20th International Conference on the Science and Application of Nanotubes and Low-Dimensional Materials

21-26 July 2019

Würzburg | Germany

Conference Organization (Local)

Tobias Hertel (Julius-Maximilians-U Würzburg, Germany)
Andreas Hirsch (FAU Erlangen-Nürnberg, Germany)
Ralph Krupke (KIT und Universität Duisburg, Germany)
Jana Zaumseil (Universität Heidelberg, Germany)

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	Jin Kong (MIT, USA)
	Yan Li (Peking University, China)
	Masako Yudasaka (AIST, Japan)
	Ming Zheng (NIST, USA)

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Symposium Organisation

Co-Chairs	**Tobias Hertel** (Julius-Maximilians-U Würzburg, Germany) **Masako Yudasaka** (AIST, Japan)

1st Symposium on Synthesis, Purification and Functionalization of Low-Dimensional Materials (SPFLD19 - ‘Synthesis’)

Chair	**Yan Li** (Peking U, China)
Local Organizer	**Ben Flavel** (KIT, Germany)
Organizers	**Sofie Cambre** (U Antwerp, Belgium) **Shigeo Maruyama** (U Tokyo, Japan) **Avetik Harutyunyan** (Honda Research Institute, USA)

2nd Symposium on Nanocarbon Materials for Energy and Sustainability (NMES19 - ‘Energy’)

Co-Chairs	**Qiang Zhang** (Peking U, China) **Feng Li** (Shenyang National Laboratory for Materials Science, China)
Local Organizer	**Maria Antonietta Loi** (U Groningen, Netherlands)
Organizer	**Suguru Noda** (WASEDA U, Japan)

7th Carbon Nanotube Thin Film Electronics and Applications Symposium (CNTFA19 - ‘Electronics’)

Co-Chairs	**Esko I. Kauppinen** (Aalto U, Finland) **Yutaka Ohno** (Nagoya U, Japan)
Local Organizer	**Christoph Strunk** (U Regensburg, Germany)

10th Symposium on Carbon Nanomaterials Biology, Medicine & Toxicology (CNBMT19 - ‘NanoBio’)

Co-Chairs	**Masako Yudasaka** (AIST, Japan) **Alberto Bianco** (CNRS, France)
Local Organizer	**Ardemis Boghossian** (EPF Lausanne, Switzerland)
Organizers	**Emmanuel Flahaut** (CNRS, France) **Dan Heller** (Sloan Kettering Center, USA) **Kostas Kostarelos** (U Manchester, UK)

10th Graphene and 2D Materials Symposium (GSS19 - ‘2D Materials’)

Chair	**Annick Loiseau** (ONERA, France)
Local Organizer	**Alexander Hoegele** (LMU Munich, Germany)

13th Symposium on Nanotube Spectroscopy, Photonics, and Applications in Metrology (NSAP19 - ‘Spectroscopy’)

Co-Chairs	**Ado Jorio** (U Minas Gerais, Brasil) **Achim Hartschuh** (LMU Munich, Germany)
Organizers	**Hiromichi Kataura** (AIST, Japan) **Yuhei Miyauchi** (U Kyoto, Japan) **Stephanie Reich** (Free U Berlin, Germany) **Jin Zhang** (Peking U, China) **Ming Zheng** (NIST, USA)

14th Symposium on Computational Challenges in Two-Dimensional Materials and Nanotubes (CCTN19 - ‘theory’)

Chair	**Yoshiyuki Miyamoto** (AIST, Japan)
Local Organizer	**Ermin Malic** (Chalmers UT, Sweden)
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Friedrich Schöppler (sponsor liaison)
Sabine Walther (conference secretary)

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Sabine Fuchs
Lucas Fuhl
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Special Thanks to

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Mandy Wagner (Conventus GmbH)
Masako Yudasaka (AIST)

Julius-Maximilians-University Würzburg

Thanks to our Sponsors

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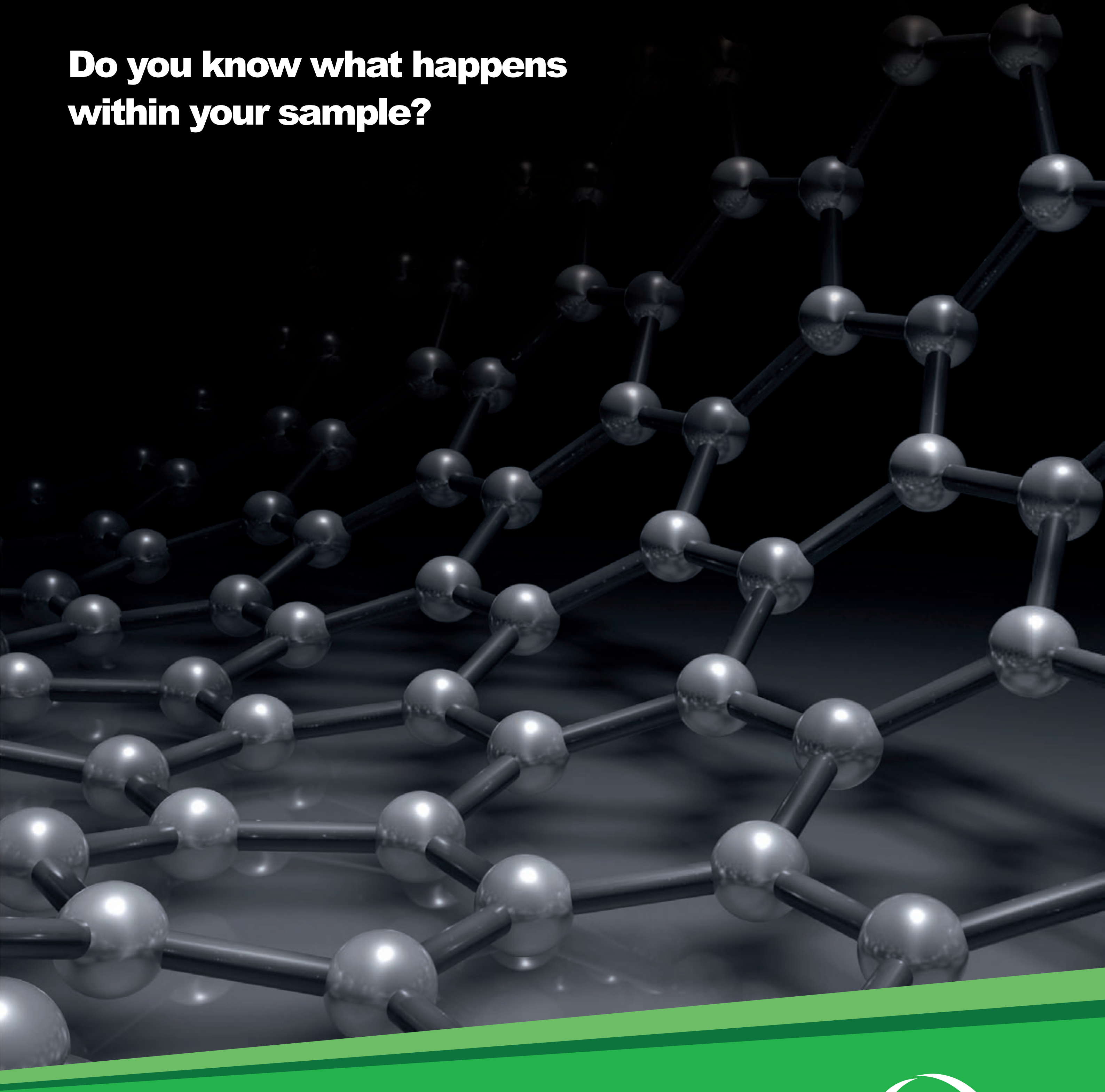

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Welcome to NT19

Dear Colleague.

We are excited about months of preparations finally coming to fruition with the opening of NT19 in Würzburg. We hope you will find the meeting enjoyable, interesting and enriching. With 142 oral and 280 poster presentations there is plenty to learn and to choose from.

Seasoned attendees of former NT conferences will notice important changes to the program layout. Most notably, we have integrated the previous Satellite Symposia into the main conference in the form of parallel afternoon sessions on Monday, Tuesday and Thursday. While this made the organization more complex we also believe that it will provide you with the opportunity to better tailor this years NT experience to your specific interests.

This conference also represents a milestone in NT history. 2019 marks the 20th anniversary of the first NT workshop, organized in 1999 by David Tománek in East Lansing, Michigan. Thanks to the efforts of David and the organizers that followed, the conference has catalyzed the formation of a strong community and has helped test ideas as well as shape future research directions.

In these 20 years, the meeting has also experienced considerable growth while trying to maintain its original spontaneity and youthfulness, a difficult balance to strike in an evolving and maturing research field. With the organization of this years meeting we aimed at providing opportunities for informal exchange in a hopefully stimulating environment. Poster sessions continue to play a central role for the NT conference as a whole, now merging presentations from the main event with those from the seven symposia.

As such, the NT conference series remains an ongoing social and organizational experiment, as exciting for organizers and attendees as the research being performed in our offices and laboratories.

With all the best for a productive and stimulating meeting.

Yours sincerely

Tobias Hertel
(*local organizer and conference chair, JMU Würzburg*)

Jana Zaumseil
(co-chair, Universität Heidelberg)

Andreas Hirsch
(*co-chair, FAU Erlangen-Nürnberg*)

Ralph Krupke

Ralph Krupke
(*co-chair, KIT & TU Darmstadt*)

STADT WÜRZBURG

Congress · Tourismus · Würzburg

1. Falkenhaus
2. Marienkapelle
3. Höfe und Bürgerhäuser
4. Rückermainhof
5. Alter Kranen
6. Alte Mainbrücke
7. Grafeneckart und Rathaus / Town Hall
8. Neumünster
9. Dom St. Kilian / Cathedral of St. Kilian
10. Domschatz / Cathedral Treasury
11. Museum am Dom
12. Riemenschneiderhaus
13. Franziskanerkirche
14. Hof zum Rebstock
15. Alte Universität
16. UNESCO-Weltkulturerbe Residenz / UNESCO-World Heritage Residence
17. Roter Bau
18. Bürgerspital zum Hl. Geist
19. Stift Haug
20. Juliusspital
21. Augustinerkirche
22. Hof Conti
23. St. Gertraud
24. Röntgen-Gedächtnisstätte / Röntgen-Memorial
25. Kunstschiff „Arte Noah"
26. Kulturspeicher
27. Don Bosco Kirche
28. Deutschhauskirche
29. Hofspitalkirche „Spitäle"
30. Festung Marienberg / Fortress Marienberg
31. St. Burkard
32. Ehemaliges Frauenzuchthaus / Former Women's Prison
33. Käppele
34. Karmelitenkirche
35. St. Peter
36. St. Stephan
37. St. Johannis
38. Sieboldmuseum Frankfurter Straße 87
39. Jüdisches Museum / Jewish Museum Shalom Europa Valentin-Becker-Str. 11
40. Botanischer Garten / Botanical Garden Julius-von-Sachs-Platz 4
41. Mineralogisches Museum / Mineralogical Museum Am Hubland

Weitere Informationen zu den Sehenswürdigkeiten/
Further information about the sights:
www.wuerzburg.de

Tourist Information

Falkenhaus am Markt
Tel. +49 (0)9 31/37 23 98
www.wuerzburg.de

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Hotel reservations, guided tours, event tickets, Würzburg guidebooks, souvenirs

Jan – März Mo – Fr 10 – 17 Uhr
Sa 10 – 14 Uhr
April, Nov, Dez Mo – Fr 10 – 18 Uhr
Mai – Okt Mo – Fr 10 – 18 Uhr
Sa 10 – 15 Uhr
So und Feiertage 10 – 14 Uhr

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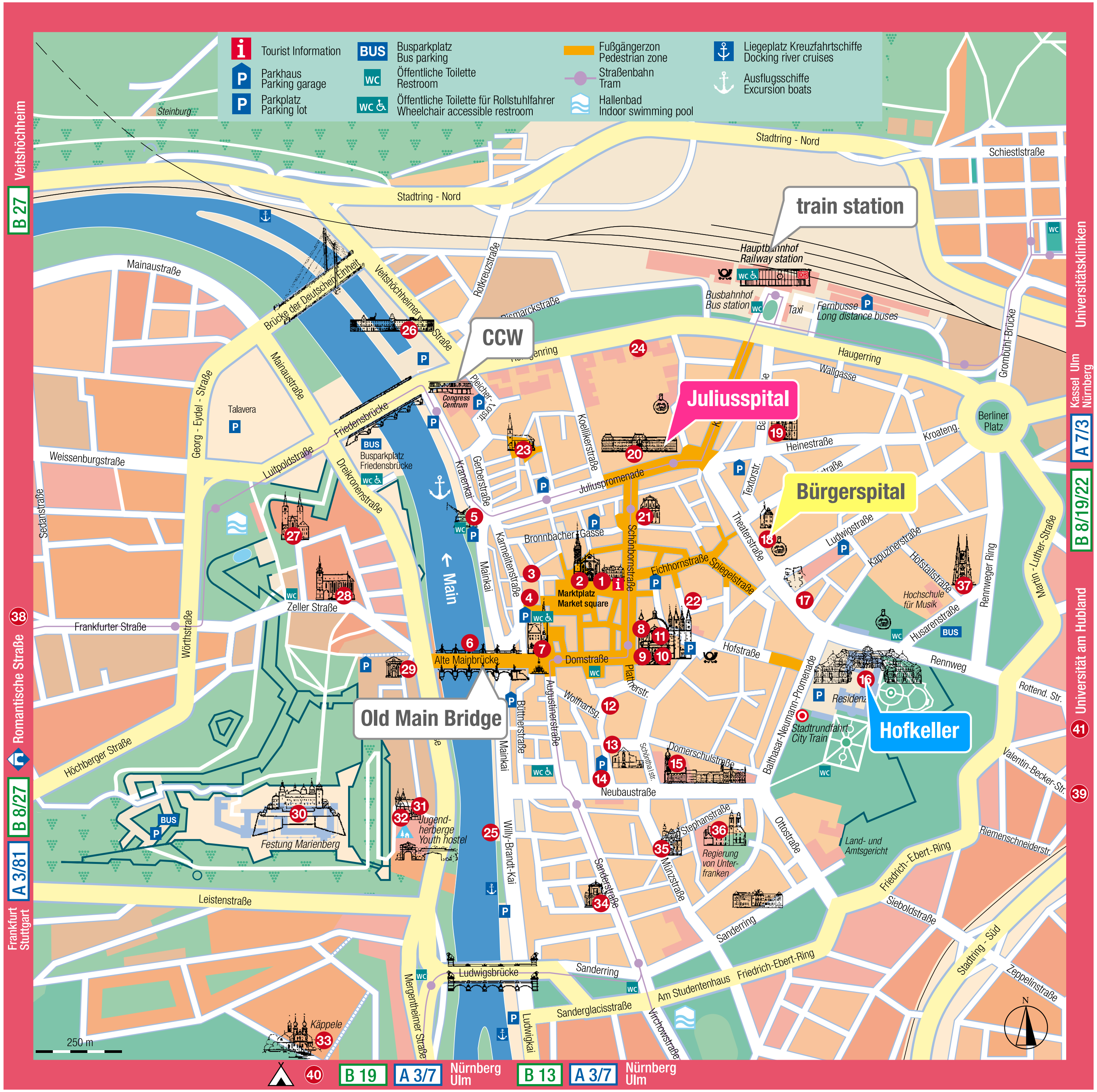


City

Traveling to Würzburg

If you arrive by plane in Frankfurt you can take one of over 20 daily direct ICE trains toward Würzburg HBF (main station). The travel time from Frankfurt airport (FRA) to Würzburg HBF is about 1:30h. The trip from Munich (MUC) to Würzburg requires at least one change and takes 3:00h or more. Seat reservations on ICE trains are not mandatory but highly recommended. For connections and online booking visit bahn.com/en/. The *DB navigator* app can be used for booking as well as for travel information and is available for android and iOS devices. Just as importantly, this app provides real-time updates on recommended travel routes and all too frequent delays.

Getting Around Town

The preferred mode of transportation is walking. Würzburg is a small town. Most points of interest east of the Main river can be reached from the centrally located Old Main Bridge in no more than 15 minutes, on foot! We have highlighted the congress center, train station, old Main bridge and three important wineries on the map to the left (map website, download pdf).

Cabs, Tram, Bus

Unfortunately, ride-sharing is currently not available in Würzburg. If you are prepared to pay with cash you can hail a white cab ‘old school’ style from the curb or from the dispatcher by phone +49 (0)931 19410. You’ll also find queues of cabs waiting for customers at some points of interest.

Connections for all modes of local public transport can be found through the versatile *DB navigator* app (android, iOS).

Bus and tram rides within the inner city are 1.40 € per trip, one-day tickets are 5.20 €. Rides to the city outskirts are 2.80 € per trip. Tickets may be purchased from vending machines at some of the major bus/tram intersections or directly from bus drivers. Bus drivers only take cash while vending machines may also accept credit cards. You need to validate a ticket at the start of each trip using one of the ticket validation boxes found as you enter buses or trams. When you enter a connecting bus on your trip, show your validated ticket to the driver (even if he appears disinterested).

Tourism and Sightseeing

A good place to start is the Würzburg webpage with plenty of useful information on events and seasonal highlights as well as major tourist attractions.

City Walk for Accompanying Persons

We offer a Monday morning city excursion for accompanying persons. Get a first look at the beautiful City of Würzburg. Discover what and where to see, eat and shop! See the city from above, experience the "Brückenschoppen" and enjoy lunch in a Biergarten! We meet on Monday morning, 9:00 o’clock, at the foot of the central market square’s obelisk next to the Marienkapelle. Check out the NT19 facebook page under ‘events’ for additional information and upcoming details.

Conference

Registration

The registration desk can be found in the lobby area of the congress center on your way from the main entrance (A) to the Franconia Lecture Hall (see blue squares on the floor plans to the right). The registration desk opens at 13:00 on Sunday and at 7:30 on all other days.

WLAN Access

Network name: CCW5 | User name: NT19guest | Password: nanomaterials .

Oral Presentations - BYOD

Please bring your own device including connectors needed to hook up to HDMI or VGA connections. All projectors are capable of wide-screen format display. Feel free to ask our students to help you try these out during coffee or lunch breaks ahead of your presentation to identify and correct possible connectivity issues.

Poster Sessions

Coffee & buffet. The 17:00-18:30 poster sessions are preceded by a coffee break. The second 19:00-21:00 poster sessions are accompanied by a complementary dinner-buffet and drinks.

Printed poster pickup. In the congress center lobby next to the main entrance Sunday 13:00-18:30, Monday 08:00-16:30 or Tuesday 08:00-16:30.

Poster setup. Following the morning session coffee break. Posters should be taken down before the end of the next days morning session coffee break. For attaching posters to poster boards, use the glue strips provided as part of your registration package.

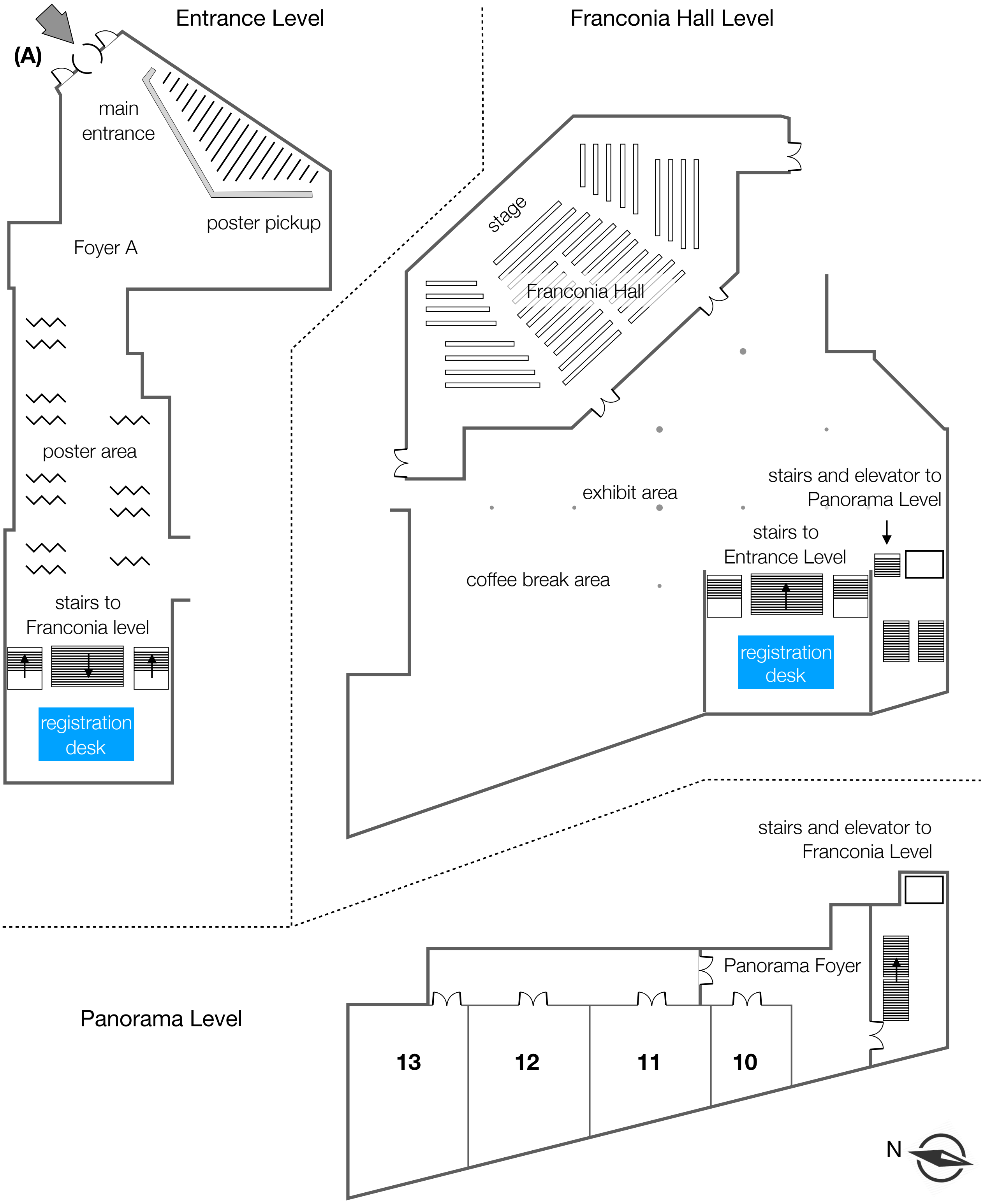
Odd-numbered posters: 17:00 - 18:30.
Even-numbered posters: 19:00 - 21:00.

Poster awards. Book vouchers are sponsored by the Royal Society of Chemistry and the Bavarian Nanoinitative. Winners will be announced during the closing ceremony.

Lunch Options

The Maritim hotel neighboring the Congress Center offers a daily lunch buffet only a few steps from the Franconia Lecture Hall. There are also less pricy alternatives within no more than 10 minute walking distance in the nearby downtown area.

Venue - Schematic Floor Plan



Wednesday City Tours at 15:45 and Wine Tasting at 18:30

Registered participants and accompanying persons meet their tour guides on Wednesday at 15:45 at the Congress Center main entrance (A). Numbers on the tour-and-wine-tasting-tickets provided with your registration package indicate the guided tour to be joined, the colors indicate your designated winery. For the wine tastings please join us at 18:30 at one of the three meeting points indicated on the map below. Alternatively you may also follow one of our students who will pick you up at the Franconia Fountain at 18:15 (see map below). Feel free to swap your ticket(s) with a colleague if you want to join another group for the wine tasting event

Meeting points

Juliusspital (magenta tickets)

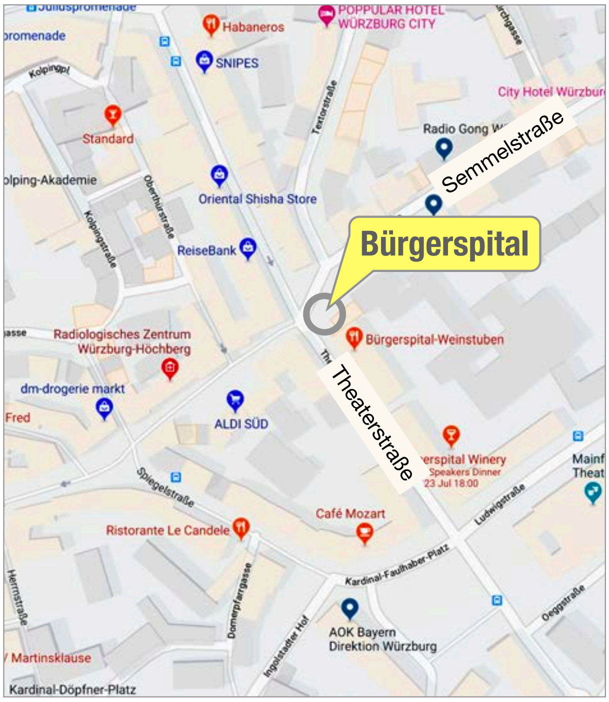
At the fountain in the center of its back-yard. The entrance to the yard is on *Juliuspromenade* about 100 m from the intersection with *Koellikerstraße*.

Bürgerspital (yellow tickets)

At the Vinothek '*Weinhaus*' at the corner of *Theaterstraße* and *Semmelstraße*.

Hofkeller (blue tickets)

At the Franconia-Fountain in front of the three-sided ceremonial court-yard of the *Würzburg Residence*.



Program at a Glance

Conference Schedule at a Glance

	Su	Mo	Tu	We	Th	Fr
Date	21. July	22. July	23. July	24. July	25. July	26. July
		Plenary	**Plenary**	**Plenary**	**Plenary**	**Plenary**
08:30-12:15		PIS 1 & 2	PIS 3 & 4	PIS 5 & 6	PIS 7 & 8	PIS 9 & 10
		lunch break	lunch break	lunch break	lunch break	closing 12:15
	Tutorials	**Symposia**	**Symposia**	**Symposia**	**Symposia**	
14:00-16:30	T1 & T2	SEI, S2D, SEn,	SEI, S2D, SEn,	SEI, …SEn, SSp, SNB	SEI, S2D, SEn,	
		SSy, STh	SSp, SNB	guided tours 15:45-18:00	SSp, SNB	
	coffee break	coffee break	coffee break		coffee break	
	Tutorial	**Poster**	**Poster**		**Poster**	
17:00-18:30	T3 to 18:15	P1 (odd #s)	P3 (odd #s)		P5 (odd #s)	
	welcome reception 18:30-20:30	break	break		break	
19:00-21:00		P2 (even #s)	P4 (even #s)	wine tasting 18:30-22:30	P6 (even #s)	

Plenary Schedule at a Glance (Franconia Hall)

	Mo	**Tu**	**We**	**Th**	**Fr**
Date	22. July	23. July	24. July	25. July	26. July
Session	**PI1**	**PI3**	**PI5**	**PI7**	**PI9**
08:30 - 09:15	Welcome - K1 - J. Zhang	- K2 - J. Maultzsch	- K3 - T.F. Heinz	- K4 - H.S.P. Wong	- K5 - C. Voisin
09:15 - 09:40	- I1 - Y. Li	- I5 - C. Cocchi	- I10 - Y.H. Lee	- I12 - M. Pasquali	- I15 - S. Noda
09:40 - 10:05	- I2 - H. Kataura	- I6 - S. Chiashi	- C4 - S. Maruyama	- I13 - Y.H. Wang	- C11 - D. Heller
	coffee break	coffee break	coffee break	coffee break	coffee break
Session	**PI2**	**PI4**	**PI6**	**PI8**	**PI10**
10:35 - 11:00	- C1 - A. Loiseau	- I7 - M. Shaffer	- I11 - R. Martel	- C8 - Y. Nonoguchi	- C12 - Y. Miyamoto
11:00 - 11:25	- I3 - M. Zheng	- I8 - M. Strano	- C5 - M. Engel	- C9 - W. Qian	- I16 - Y. Ohno
11:25 - 11:50	- C2 - H. Li	- C3 - L. Shi	- C6 - K. Mustonen	- C10 - M. Scagliotti	- C13 - C. Meyer
11:50 - 12:15	- I4 - B. Yakobson	- I9 - Q. Li	- C7 - A. Jorio	- I14 - M. Xu	poster awards & closing ceremony

Symposia Schedule at a Glance

	Electronics (CNTFA19)	**Energy (NMES19)**	**2D Materials (GSS19)**
Monday	Panorama level 11	Franconia hall	Panorama level 13
14:00 - 14:20	SEl1 - L. Peng	SEn1 - K. Hata	S2D1 - X. Marie
14:20 - 14:40			
14:40 - 15:00	SEl2 - J. Zhao	SEn2 - J. Blackburn	S2D2 - S. Borghardt
15:00 - 15:20	SEl3 - Th. Gao	SEn3 - Y. Chen	S2D3 - C. Kastl
	10 min break	10 min break	10 min break
15:30 - 15:50	SEl4 - K. Mustonen	SEn4 - C.-M. Chen	S2D4 - C. Schneider
16:10 - 16:30	SEl5 - N.F. Hartmann	SEn5 - E. Gracia-Espino	S2D5 - N.A. Peyyety
16:30 - 16:50	SEl6 - A. Sekiguchi	SEn6 - H. Ji	S2D6 - M. Kroner
Tuesday			
14:00 - 14:20	SEl7 - E Laird	SEn7 - F. Wei	S2D7 - Y.K. Yap
14:20 - 14:40			S2D8 - C. Journet
14:40 - 15:00	SEl8 - P. Hakonen	SEn8 - C. Brabec	S2D9 - J. Pang
15:00 - 15:20	SEl9 - A. Hüttel	SEn9 - E. Kaupinnen	S2D10 - Y. Wu
	10 min break	10 min break	10 min break
15:30 - 15:50	SEl10 - Y. Yaish	SEn10 - S.O. Kim	S2D11 - U. Khan
16:10 - 16:30	SEl11 - L. Cong	SEn11 - C. Liu	S2D12 - M. Heuken
16:30 - 16:50	SEl12 - A. Descombin	SEn12 - W. Lyu	S2D13 - H. Lee
Wednesday			
14:00 - 14:20	SEl13 - M. Hersam	SEn13 - R. Nicholas	S2D14 - B. Dlubak
14:20 - 14:40	SEl14 - Y. Hu	SEn14 - V. Koman	S2D15 - L. Kühl Teles
14:40 - 15:00	SEl15 - L. Liu	SEn15 - B. Wei	S2D16 - I. Kriegel
15:00 - 15:20	SEl16 - E.X. Ding	SEn16 - I. Jeon	S2D17 - P. Zeller
Thursday			
14:00 - 14:20	SEl17 - A.G. Nasibulin	SEn17 - Y. Zhu	S2D18 - Banszerus
14:20 - 14:40	SEl18 - Z. Ma	SEn18 - J. Vilatela	
14:40 - 15:00	SEl19 - T. Szkopek		S2D19 - I. Bondarev
15:00 - 15:20	SEl20 - D. Lioubtchenko		S2D20 - S. Caneva
	10 min break	10 min break	10 min break
15:30 - 15:50	SEl21 - V. Koman		S2D21 - A. Sperlich
16:10 - 16:30	SEl22 - A. Tsapenko		S2D22 - Y. Wei
16:30 - 16:50			S2D23 - B. Plaçais

Symposia Schedule at a Glance

	Synthesis (SPFLD19)	Spectroscopy (NSAP19)	Theory (CCTN19)	NanoBio (CNBMT19)
Monday	Panorama level 12		Panorama level 10	
14:00 - 14:20	SSy1 - Harutyunyan		STh1 - R. Saito	
14:20 - 14:40	SSy2 - D. Futaba			
14:40 - 15:00	SSy3 - K. Jiang		STh2 - M. Selig	
15:00 - 15:20	SSy4 - F. Yang		STh3 - H. Yu	
	10 min break		10 min break	
15:30 - 15:50	SSy5 - V. Jourdain		STh4 - H- Santos	
16:10 - 16:30	SSy6 - R. Xiang		STh5 - D. Prezzi	
16:30 - 16:50	SSy7 - L. Shi		STh6 - C. Vets	
Tuesday				
14:00 - 14:20	SSy8 - Wenseleers		STh7 - A. Page	
14:20 - 14:40	SSy9 - J. Fagan		STh8 - Z. Wang	
14:40 - 15:00	SSy10 - M. Arnold		STh9 - J. Elliot	
15:00 - 15:20	SSy11 - E. Gauffrès		STh10 - B. Flebus	
	10 min break		10 min break	
15:30 - 15:50	SEl12 - R. Nißler		STh11 - K.V. Bets	
16:10 - 16:30		SSp1 - S. Doorn		SNB1 - M.S.Strano
16:30 - 16:50				
Wednesday				
14:00 - 14:20		SSp2 - A. Loiseau		SNB2 - C. Allard
14:20 - 14:40		SSp3 - A. Riaz		SNB3 - S. Kruss
14:40 - 15:00		SSp4 - G. Gordeev		SNB4 - Y. Wang
15:00 - 15:20		SSp5 - L. Malard		SNB5 - Antonucci
Thursday				
14:00 - 14:20		SSp6 - K. Liu		SNB6 - E. Hirata
14:20 - 14:40				SNB7 - S. Florito
14:40 - 15:00		SSp7 - S. Cambré		SNB8 - M. Zhang
15:00 - 15:20		SSp8 - Y. Homma		SNB9 - D. Heller
		10 min break		10 min break
15:30 - 15:50		SSp9 - Y. K. Kato		SNB10 - M. Zheng
16:10 - 16:30		SSp10 - Joselevich		SNB11 - S. Freddi
16:30 - 16:50		SSp11 - A. Ishii		SNB12 - G. Bisker

Sunday Program

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Prof. **Alexandra Boltasseva**
Birck Nanotechnology Center, Purdue University

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Prof. **Frank Koppens**
ICFO- The Institute of Photonic Sciences

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NKT Photonics

Tutorial program

Franconia Hall

13:00 - 18:30		Registration & poster pickup	CCW Lobby
Session T1		Chair: Ralph Krupke	
14:00 - 15:15	T1	**Tutorial Lecture** **Sofie Cambré** (University of Antwerp) *Optical Spectroscopy To Characterize the Filling and Sorting of Carbon Nanotubes*	
15:15 - 16:30	T2	**Tutorial Lecture** **Shahal Ilani** (Weizmann Institute of Science) *Quantum Design in Carbon Nanotubes*	
		Coffee break	CCW Lobby
Session T2		Chair: Tobias Hertel	
17:00 - 18:15	T3	**Distinguished Tutorial Lecture** **Sumio Iijima** (Meijo University & NEC) *Aligning CNTs for Electronic Device Applications*	
18:30 - 20:30		Welcome reception	Panorama level

Tutorial Abstracts

Tutorial Session T1 (tutorial)

Franconia Hall **Su 14:00 - 15:15**

Optical Spectroscopy to Characterize the Filling and Sorting of Carbon Nanotubes

Sofie Cambré[1]

[1] *Physics Department, University of Antwerp, Belgium*

Single-walled carbon nanotubes (SWCNTs) exhibit unique, remarkably diverse electronic and optical properties that depend critically on their exact chiral structure and are extremely sensitive to the local environment of the SWCNT, thereby making optical spectroscopy one of the most valuable methods to identify the different chiral species in a particular sample and at the same time probe their interactions with the local environment. In this tutorial, I will provide an overview of how optical spectroscopy can be used to assess the filling of SWCNTs [1-5], to investigate the interaction between encapsulated molecules and SWCNTs (e.g. energy transfer) [6] and to reveal new quasi-phase transitions within a single file of encapsulated water molecules.[7] Finally, I will discuss the application of optical spectroscopy to determine the purity of chirality-sorted SWCNTs.

References:
[1] W. Wenseleers et al, Adv. Mater. 19, 2274 (2007)
[2] S. Cambré et al, Phys. Rev. Lett. 104, 207401 (2010)
[3] S. Cambré et al,, Angew. Chem. 50, 2764 (2011)
[4] S. Cambré et al, ACS Nano 6, 2649 (2012)
[5] S. Cambré et al, Nature Nanotechnol. 10, 248 (2015)
[6] S. van Bezouw et al, ACS Nano 12, 6881 (2018)
[7] X. Ma et al, Phys. Rev. Lett. 118, 027402 (2017)

Tutorial Session T2 (tutorial)

Franconia Hall **Su 15:15 - 16:30**

Quantum Design in Carbon Nanotubes

Shahal Ilani[1]

[1] *Department of Condensed Matter Physics, Weizmann Institute of Science.*

In the last decade, there have been dramatic developments in the technologies for making electronic devices based on carbon nanotubes. New growth and nano-assembly methods have allowed the creation of complex quantum devices with electronically pristine carbon nanotubes, and this has opened new frontiers of research based on carbon nanotubes. In this talk I will review the recent achievements in nanotube electronics that include their use as quantum bits, as nano-mechanical systems, as ideal substrates for studying the physics of interacting electrons in one dimension, and as the world's most sensitive scanning probe detectors of electric fields.

Tutorial Session T3 (tutorial)

Franconia Hall **Su 17:00 - 18:15**

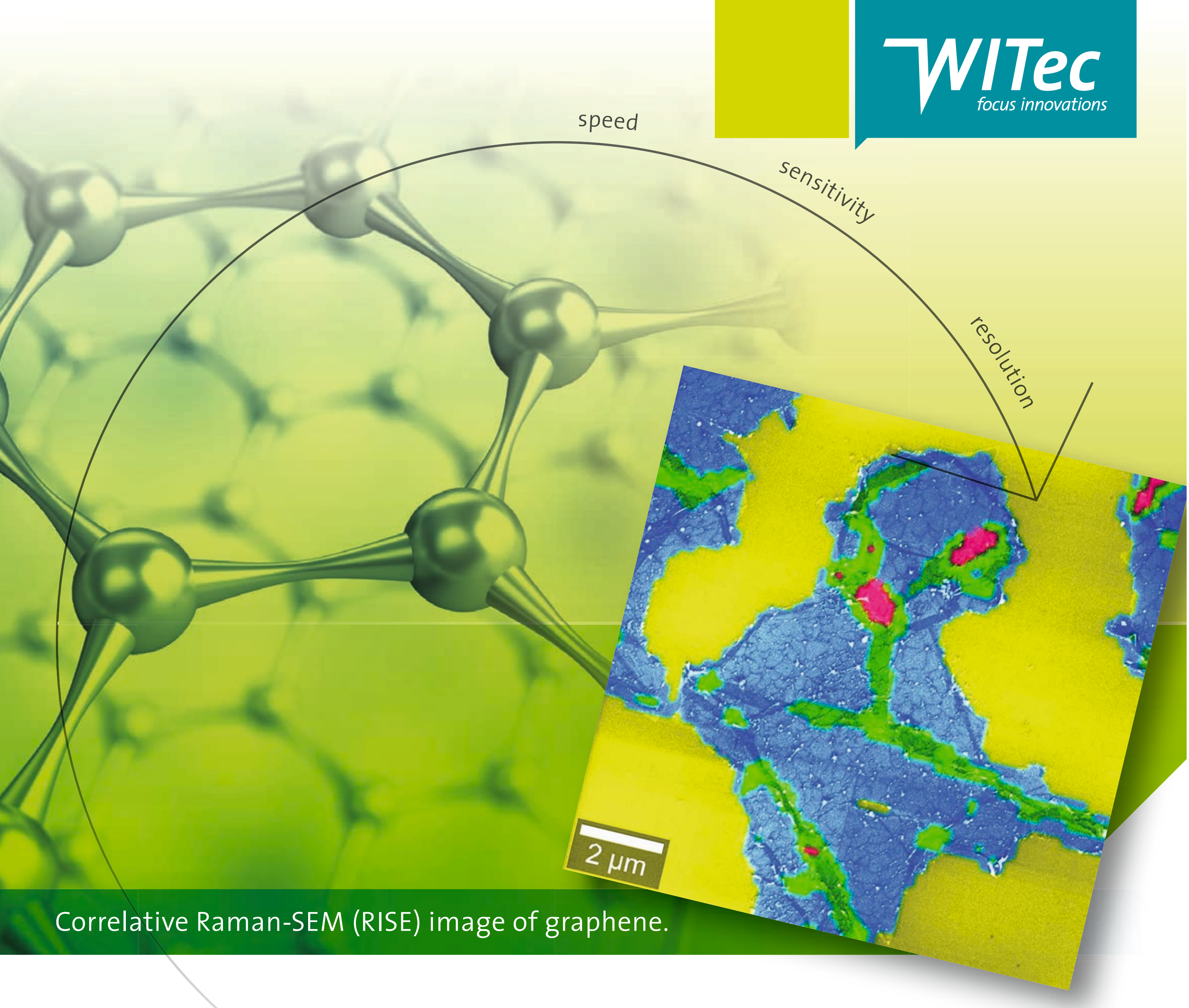
Aligning CNTs for electronic device applications

Sumio Iijima

[1]*Meijo University & NEC, Nagoya, Japan*

Space for notes.

Program Monday


WITec
focus innovations
speed
sensitivity
resolution
2 µm

Plenary program Franconia Hall

Session Pl1 Chair: Annick Loiseau

08:30 - 08:35		**Tobias Hertel** (Julius-Maximilians-U Würzburg) *Welcome Address*
08:35 - 09:15	K1	**Jin Zhang** (Peking University) *Chirality Controlled Growth of Horizontal Carbon Nanotubes Array With Designed Catalysts*
09:15 - 09:40	I1	**Yan Li** (Peking University) *In Situ Study of Single-Walled Carbon Nanotube Growth With Cobalt and Tungsten-Cobalt Intermetallic Compound Catalysts*
09:40 - 10:05	I2	**Hiromichi Kataura** (AIST) *Multiscale Hydrophobic Interaction Between Carbon Nanotubes, Surfactants, and Polysaccharide Gels*

Coffee break CCW Lobby

Session Pl2 Chair: Riichiro Saito

10:35 - 11:00	C1	**Annick Loiseau** (LEM, CNRS-ONERA) *Momentum-Resolved Dielectric Response of Free Standing Black Phosphorus Down to the Monolayer*
11:00 - 11:25	I3	**Ming Zheng** (National Institute of Standards and Technology) *Resolving Carbon Nanotube Structures by DNA*
11:25 - 11:50	C2	**Han Li** (KIT) *Separation of Single Walled Carbon Nanotubes in One to Three Steps Using pH Modulated Aqueous Two-Phase Extraction*
11:50 - 12:15	I4	**Boris Yakobson** (Rice University) *Computations To Explain or Predict, in Low-Dimensional Materials*

Lunch break

Electronics Symposium (CNTFA19) Panorama 11

Chair: Yutaka Ohno

14:00 - 14:40	SEI1	**Lian-Mao Peng** (Peking University) *Carbon Nanotube Based TFT and Optoelectronic Devices and Systems*
14:40 - 15:00	SEI2	**Jianwen Zhao** (Chinese Academy of Sciences) *High-Performance Printed Carbon Nanotube Thin Film Transistors and Their Applications for Printed Logic Gates, Circuits and Neuromorphic Devices*
15:00 - 15:20	SEI3	**Theodore Gao** (Stanford University) *Improving Inkjet-Printed Carbon Nanotube Transistors via Flocculation*

10 minute break

Chair: Lianmao Peng

15:30 - 15:50	SEI4	**Kimmo Mustonen** (University of Vienna) *Optimising Single-Walled Carbon Nanotube Network Conductivity via Tunnelling Barrier Modifications*
15:50 - 16:10	SEI5	**Nicolai F. Hartmann** (neaspec GmbH) *Nanoscale Conductivity Mapping in Graphene and Carbon Nanotubes Through Mid-IR and Terahertz Scattering-Type Scanning Near-Field Optical Microscopy*
16:10 - 16:30	SEI6	**Atsuko Sekiguchi** (AIST) *Application and Fabrication Process Development of Long Single Walled Carbon Nanotubes and its Metal Composite*

Coffee break CCW Lobby

Energy Symposium (NMES19) Franconia Hall

Chair: Qiang Zhang

14:00 - 14:40	SEn1	**Kenji Hata** (AIST) *Cu/CNT Composites: Next-Gen Lightweight High-Performance Copper Substitutes?*
14:40 - 15:00	SEn2	**Jeffrey Blackburn** (National Renewable Energy Laboratory) *Organic/Inorganic Hybrid Interfaces With SWCNTs for Energy Harvesting and Conversion*
15:00 - 15:20	SEn3	**Yuan Chen** (University of Sydney) *Carbon Materials Assisted Designs of Electrocatalysts*

10 minute break

Chair: Yuan Chen

15:30 - 15:50	SEn4	**Cheng-Meng Chen** (Chinese Academy of Sciences) *Graphene and Porous Carbon for Supercapacitor Applications*
15:50 - 16:10	SEn5	**Eduardo Gracia-Espino** (Umeå University) *Surface Activation of Carbon-Based Nanomaterials for Oxygen Reduction Reaction: in the Search of Efficient Metal-Free Electrocatalysts*
16:10 - 16:30	SEn6	**Hengxing Ji** (University of Science and Technology of China) *Carbon Based Current Collectors for Lithium-Metal Batteries*

Coffee break CCW Lobby

2D Materials Symposium (GSS19) Panorama 13

Chair: Annick Loiseau

14:00 - 14:40	S2D1	**Xavier Marie** (CNRS - INSA Toulouse) *Exciton Linewidth Approaching the Homogeneous Limit in MoS_2 Based Van Der Waals Heterostructures*
14:40 - 15:00	S2D2	**Sven Borghardt** (Forschungszentrum Jülich) *Radially Polarized Light Beams From Spin-Forbidden Dark Excitons in Monolayer WSe_2*
15:00 - 15:20	S2D3	**Christoph Kastl** (Walter-Schottky-Institut - TU München) *Effects of Defects on Band Structure and Excitons in WS2 Revealed by Nanoscale Photoemission Spectroscopy*

10 minute break

Chair: Christoph Stampfer

15:30 - 15:50	S2D4	**Christian Schneider** (Julius-Maximilians-Universität Würzburg) *Condensation and Expansion of Cavity Polaritons Based on Two-Dimensional Crystals*
15:50 - 16:10	S2D5	**Naga Anirudh Peyyety** (Technische Universität Darmstadt) *Probing Enhanced Light-Matter Interaction in Graphene on Plasmonic-Photonic Crystals by Raman Spectroscopy*
16:10 - 16:30	S2D6	**Martin Kroner** (ETH Zürich) *Pump-Probe Spectroscopy of Polaritons in a $MoSe_2$ Monolayer in the Presence of Itinerant Electrons: Signatures of Optical Amplification*

Coffee break CCW Lobby

Synthesis Symposium (SPFLD19) Panorama 12

		Chair: Yan Li
14:00 - 14:20	SSy1	**Avetik Harutyunyan** (Honda Research Institute USA Inc.) *Origin of Chirality in Carbon Nanotubes: Interplay Between Catalyst and Carbon Nuclei*
14:20 - 14:40	SSy1	**Don Futaba** (AIST) *Advances in the Synthesis of Single Wall Carbon Nanotubes by the Water-Assisted CVD Method*
14:40 - 15:00	SSy2	**Kaili Jiang** (Tsinghua University) *Growing Highly Pure Semiconducting Carbon Nanotubes for Nanoelectronics by Electrotwisting the Helicity*
15:00 - 15:20	SSy3	**Feng Yang** (Peking University) *Atomic Scale in-Situ Study on Carbon Nanotube Growth From Co-Co3C Catalysts*
		10 minute break
		Chair: Sofie Cambré
15:30 - 15:50	SSy4	**Vincent Jourdain** (University of Montpellier) *Studying the Growth of Single-Walled Carbon Nanotubes by Optical Means*
15:50 - 16:10	SSy5	**Rong Xiang** (University of Tokyo) *One-Dimensional Van Der Waals Heterostructure Nanotubes: Synthesis and Growth Mechanism*
16:10 - 16:30	SSy6	**Lei Shi** (Sun Yat-sen University) *In-Situ Synthesis of the Confined Linear Carbon Chains*
		Coffee break CCW Lobby

Theory Symposium (CCTN19) Panorama 10

		Chair: Yoshiuki Miyamoto
14:00 - 14:40	STh1	**Riichiro Saito** (Tohoku University) *Controlling Helicity of Circularly Polarized Light in Low-Dimensional Materials*
14:40 - 15:00	STh2	**Malte Selig** (Technische Universität Berlin) *Bright and Dark Exciton Dynamics in Transition Metal Dichalcogenides*
15:00 - 15:20	STh3	**Hongyi Yu** (University of Hong Kong) *Moiré Physics in Heterobilayer and Homobilayer 2D Semiconductors*
		10 minute break
		Chair: James Elliott
15:30 - 15:50	STh4	**Hernán Santos** (Autonomous University of Madrid) *Controlling Spin-Polarized Currents in Carbon Nanotubes: Rashba Spin-Orbit Effects and Defect Engineering*
15:50 - 16:10	STh5	**Deborah Prezzi** (University of Modena and Reggio Emilia) *Light Emission From Ultranarrow Graphene Nanoribbons: Insights From Ab Initio Simulations*
16:10 - 16:30	STh6	**Charlotte Vets** (University of Antwerp) *The CNT-Metal Adsorption Energy: Key for Chirality Selective Growth?*
		Coffee break CCW Lobby

Poster Sessions CCW Lobby Level

17:00 - 18:30	Poster Session 1 (odd poster numbers)
19:00 - 21:00	Poster Session 2 (even poster numbers)

Abstracts Monday
(Oral)

Plenary Venue K1 (keynote)

Franconia Hall **Mo 08:30 - 09:15**

Chirality Controlled Growth of Horizontal Carbon Nanotubes Array with Designed Catalysts

Jin Zhang[1]

[1] *Center for Nanochemistry, College of Chemistry and Molecular Engineering, Peking University, Beijing, 100871, China*

Single-walled carbon nanotubes (SWNTs) had received broad attention in the past decades due to its dramatic physical and chemical properties. As synthesis determined the future, in this talk, I will focus on the chirality controlled growth of horizontal carbon nanotubes array with designed catalysts: 1) By using open-end SWNTs as ‘seeds/catalysts’ (without metal catalysts), duplicate SWNTs could be grown and cloned from the parent segments via an open-end growth mechanism. These findings provide a new approach for growing SWNTs with controlled chirality; 2) Using symmetry matching strategy, a structure-family (2m, m) horizontally aligned SWNTs were successfully obtained on uniform carbide (WC and Mo_2C) solid catalysts. It is based on a consideration of nanotube/catalyst interfacial thermodynamics determined by symmetry, and the kinetic growth rates set by the number of kinks; 3) For the application of SWNTs in electronic device, a new family of semiconducting SWNTs, (n, n-1) carbon nanotubes, called property-family, with different diameters can be grown using near-equilibrium nucleation growth mode. This new strategy adds a new degree of freedom for selective growth of SWNTs and opens up a new route for growth of SWNTs families beyond catalysts design.

References
1. Jin Zhang et. al., Nano Lett., 9(2009), 1673-1677.
2. Jin Zhang et. al., Nature, 543(2017), 234-238.
3. Jin Zhang et. al., Chem, 5(2019), 1-12.

Plenary Venue I1 (invited)

Franconia Hall **Mo 09:15 - 09:40**

In situ study of Single-Walled Carbon Nanotube Growth with Cobalt and Tungsten-Cobalt Intermetallic Compound Catalysts

Yan Li[1], Feng Yang[1], Haofei Zhao[2], Rongming Wang[2]

[1] *College of Chemistry and Molecular Engineering, Peking University, Beijing, China*
[2] *School of Mathematics and Physics, University of Science and Technology Beijing, China*

Revealing the catalyst structure and chemistry in the reactive environment at the atomic scale is imperative for the rational design of catalysts and the investigation of mechanism for single-walled carbon nanotube (SWCNT) growth, while in situ characterization at the atomic scale in high temperature is still a great challenge. Tracking intermetallic Co_7W_6 nanoparticles with a defined structure and a high melting point by in situ environmental transmission electron microscope (ETEM) in combination with synchrotron X-ray absorption spectroscopy (XAS), we directly present the structural and chemical stability of the Co_7W_6 nanocrystals in different gases at the temperature of 700–1100 °C. Then we demonstrate the process of SWCNT growth from the catalysts. When using Co, the growth of SWNTs is realized by the cooperation of Co with Co_3C. When a carbon cap nucleates from the Co_7W_6 nanocrystal, the catalyst keeps its atomic-scale structure. No carbon penetration is observed. The observations reveal the structural template effect of Co_7W_6in SWCNT growth.

Plenary Venue I2 (invited)

Franconia Hall **Mo 09:40 - 10:05**

Multiscale hydrophobic interaction between carbon nanotubes, surfactants, and polysaccharide gels

Hiromichi Kataura[1], Guowei Wang[1], Mayumi Tsuzuki[1], Takeshi Tanaka[1]

[1]*Nanomaterials Research Institute, AIST, C5, Tsukuba, Ibaraki 305-8565, JAPAN*

Adsorption chromatography is very useful for large scale metal/semiconductor separation and structure sorting of single-wall carbon nanotubes (SWCNTs), where polysaccharide gels are used as stationary phase. However, adsorption and desorption mechanisms of SWCNTs have not been well understood to date. In this work, we have fabricated seven different allyl dextran gels by changing dextran concentrations and measured their adsorption abilities. Results show that effective adsorption site is not nanoscale but mesoscopic scale. This finding lets us know that the adsorption of SWCNT is driven by a wet-dry transition that is usually observed for macroscopic hydrophobic surfaces dipped in water. Here, the wet state means that SWCNT is covered with surfactants in water and dry state means that bare SWCNT is attached to polysaccharide polymer. Wet and dry states can be understood as metastable states where the total free energy of hydrogen bonding of surrounding water is minimized locally. Since the adsorption of surfactant is due to microscopic hydrophobic interaction, the wet and dry states can be understood as multiscale hydrophobic interaction system. This model explains all our separation data and further contributed automatic separation of 18 kinds of single chirality species.

Franconia Hall **Mo 10:35 - 11:00**

Momentum-resolved dielectric response of free standing black phosphorus down to the monolayer

Annick Loiseau[1]

[1]LEM, CNRS-ONERA, U. Paris Saclay, 92322 Chatillon, France
[2]LP2N, Institut d'optique –CNRS, 33400 Talence, France
[3]RQMP & Dpt de Chimie, U. Montréal, Montréal, Canada
[4]RQMP & Dpt de Physique U. Montréal, Montréal, Canada

Anisotropy and layer number drive the semiconducting properties of thin black phosphorus (BP), that offers promising perspectives in various fields such as electronics and photonics. However as screening effects may strongly affect these properties, it is highly desirable to investigate intrinsic properties of free-standing layers.

To that aim we have shown that investigation of spectroscopic properties can be done in a unique way using angular resolved Electron energy loss spectroscopy implemented in Transmission Electron Microscopy with the advantage to have access to their q dispersion and their symmetry properties.

By combining this technique with suitable ab initio calculations, we have studied the dielectric response of free-standing pristine BP layers. We found optical bandgap values of 1.9 eV, 1.4 eV and 1.1 eV for the 1-3 BP layers respectively. By using a simple variational model, we correlate the exciton energy with the dielectric screening. We hence demonstrate that the variations of the electronic gap are sizeably larger than the variations of the binding energy. Finally, we probe and analyze the plasmons dispersion for the 1-3 BP layers and bulk and highlight a deviation and linearization of the parabolic dispersion with strong anisotropic fingerprints.

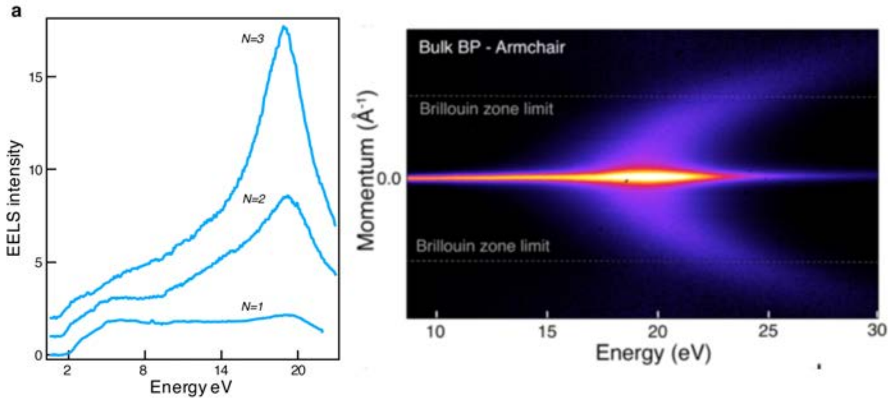


Figure caption: left: EELS spectra of suspended BP mono, bi and trilayers (N=1, 2, 3) showing the optical gap and the plasmon peak. Right: Mapping of the plasmon energy loss along the armchair direction of BP

Franconia Hall **Mo 11:00 - 11:25**

Resolving Carbon Nanotube Structures by DNA

Ming Zheng[1]

[1]*National Institute of Standards and Technology, Maryland 20899, USA*

Many fundamental studies and technology development rely on structurally well-defined CNTs as well as corresponding coating layers. DNA-CNT library has been used to select structurally well-defined hybrids using separation method. Existing selection methods have various drawbacks. In this talk, I will present our recent work in developing new spectroscopy and separation method to obtain DNA sequences that are capable of resolving different CNT structures. I will also present a multiplex sensing scheme we call “molecular perceptron”, which is based on an array of DNA-CNT hybrids to mimic human perception systems for biosensing applications.

Franconia Hall **Mo 11:25 - 11:50**

Separation of Single Walled Carbon Nanotubes in One to Three Steps using pH Modulated Aqueous Two-Phase Extraction

Han Li[1], Georgy Gordeev[2], Oisin Garrity[2], Naga Anirudh Peyyety[1,3], Pranauv Balaji Selvasundaram[1,3], Simone Dehm[1], Sofie Cambré[4], Wim Wenseleers[4], Stephanie Reich[2], Ralph Krupke[1,3], Ming Zheng[5], Jeffrey Fagan[5], Benjamin S. Flavel[1,3]

[1] *Institute of Nanotechnology, Karlsruhe Institute of Technology, Karlsruhe, Germany*
[2] *Department of Physics, Freie Universität Berlin, Berlin, Germany*
[3] *Institute of Materials Science, Technische Universität Darmstadt, Darmstadt, Germany*
[4] *Physics Department, University of Antwerp, Antwerp, Belgium*
[5] *Materials Science and Engineering Division, NIST, Gaithersburg, USA*

Separation of as-grown single-wall carbon nanotubes (SWCNTs) into single (n,m) species is important for SWCNTs to be used in advanced material applications such as electronic devices and sensors. Aqueous two-phases extraction (ATPE) has been demonstrated as an easily accessible and scalable method to separate SWCNTs through partitioning of different species across two aqueous phases. Despite the high efficiency of the approach, multiple steps (6-10 steps) and careful control of the surfactant are normally required. In our latest work we show that separation can be achieved in 1, 2 or at the most 3 steps without changing the global concentration or ratio of co-surfactants. Instead, separation is reliant upon the unique surfactant shell around each nanotube diameter at a fixed surfactant concentration. This allows for an (n,m) separation approach to be presented that is as simple as pipetting known volumes of acid into the ATPE system. This has also allowed us to demonstrate single chirality species in the diameter range 0.7—1.5 nm from a wide range of starting materials. Li, Han, et al. "Separation of Small Diameter Single Walled Carbon Nanotubes in 1-3 Steps with Aqueous Two-Phase Extraction." ACS nano (2019).

Plenary Venue I4 (invited)

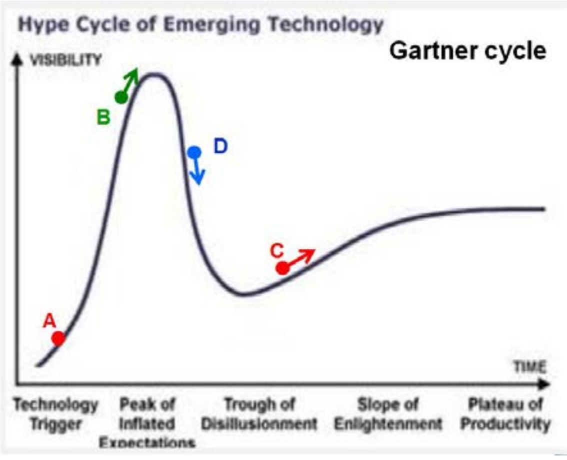
Franconia Hall **Mo 11:50 - 12:15**

Computations to explain or predict, in low-dimensional materials

Boris Yakobson[1], Ksenia Bets[1]

[1] *Rice University, Department of Materials Science and Nanoengineering*

Stare at the figure and assign the A, B, C, D to NT, graphene, 2D-materials "beyond", and perhaps your own pet-material or physical property explored in your work. Further, subdivide the affairs to experiment and theory, to put the theory-computations challenges in perspective. After this ever-useful exercise, turn to easier part of the talk, on progress in computations to explain-predict on NT or 2D-ms' synthesis and properties. For NT, the grand challenge of selective synthesis remains still that—a challenge. A few elegant theories, dislocation-growth favoring armchair, thermodynamics-kinetics tradeoff explaining (m,m-1) peaks, catalyst-symmetry matching, or entropy dominance, or transient kinetics, explaining the median (2m,m) type, all have merit. Yet the jury is still out on which will guide a truly selective growth. In 2D-ms, theory concepts do help to meet the challenge of mono-crystal growth. The evolutionary-selection or vicinal-planes approaches appear successful, while models explain and predict the ways. Beyond synthesis, the computations map the 2D-ms' optics, and the point-defects for ideal single-photon emission. The theme of borophene illustrates how theory guided experiments, from early predictions to synthesis and properties of plasmons, superconductivity, etc.



Assign A, B, C, D spots to the NT, graphene, 2D TMD, etc., as you see fit.

Panorama 11 **Mo 14:00 - 14:40**

Carbon nanotube based TFT and optoelectronic devices and systems

Lian-Mao Peng[1]

[1] *Department of Electronics, Peking University*

Carbon nanotube (CNT)-based electronics has been considered one of the most promising candidates to replace Si complementary metal-oxide-semiconductor (CMOS) technology, which will soon meet its performance limit. Prototype device studies on individual CNTs revealed that CNT based devices have the potential to outperform Si CMOS technology in both performance and power consumption, especially at sub-10 nm technology nodes, which are close to the theoretical limits; and various optoelectronic device such as light-emitting diodes, photodetectors and photovoltaic (PV) cells have been demonstrated. Very recently, both p-type devices and integrated systems were fabricated using CNT films. In this talk, I will discuss the use of randomly oriented CNT film to build CNT thin film transistors (TFTs) and optoelectronic devices, and show that the performance of CNT film devices and systems can be dramatically improved by optimizing the material purity, device structure and fabrication processes, thus yielding CNT devices with outstanding performance comparable to that of Si CMOS and ICs working in the GHz regime, and integrated electronic and optoelectronic systems for communications between nanoelectronic circuits using CNT devices.

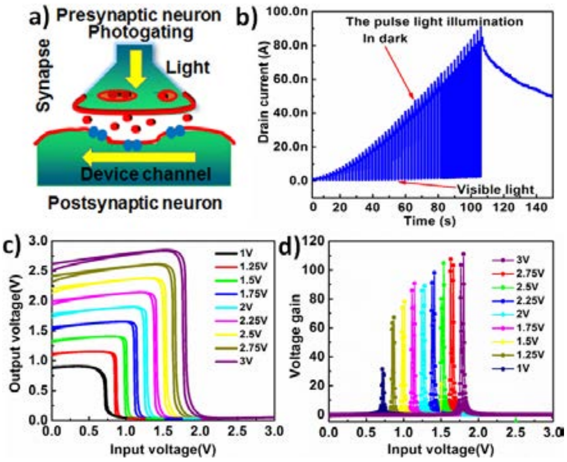
Panorama 11 **Mo 14:40 - 15:00**

High-performance printed carbon nanotube thin film transistors and their applications for printed logic gates, circuits and neuromorphic devices

Jianwen Zhao[1], Zheng Cui[1], Miaomiao Wei[1], Tianqi Gao[1]

[1] *Printable electronics research centre, Suzhou institute of nano-tech and nano-bionics, CAS*

Semiconducting SWCNTs (sc-SWCNTs) have been become a promising semiconductor for printed TFTs, especially for flexible printed TFTs, due to their excellent electrical properties, solubility, flexibility, high chemical and physical stability, and process temperatures compatible with flexible substrates. In this talk, I will show some research results about high-purity sc-SWCNT inks and high-performance printed p and n-type SWCNT TFTs, CMOS inverters, ring oscillators and neuromorphic devices. We have designed and synthesized some new conjugated organic compounds to sort sc-SWCNTs from commercial SWCNTs. More than 20 sc-SWCNT inks have been obtained, which can be used to directly construct SWCNT TFTs by printing. Flexible printed SWCNT TFTs show high effective mobility (30 $cm^2V^{-1}s^{-1}$) and on/off ratio (10^6) at operation voltage of ±2 V. The gains of printed inverters and the frequency of printed 5-stage oscillators on flexible substrates can research 40 and 3.3 kHz, respectively. Furthermore, the novel photo-neuromorphic devices based on printed photogating SWCNT TFTs are achieved. Important synaptic characteristics, such as low-pass filtering characteristics and the non-volatile memory ability, are successfully emulated in the printed light-stimulated artificial synapses.



Printed photoneuromorphic devices based on photogating SWCNT TFTs and printed SWCNT CMOS-like inverters on flexible substrates

Panorama 11 **Mo 15:00 - 15:20**

Improving Inkjet-Printed Carbon Nanotube Transistors via Flocculation

Theodore Gao[1], Francisco Molina-Lopez[2,3], Ting Lei[2,4], Zhenan Bao[2]

[1]*Stanford University/Dept. of Materials Science & Engineering, Stanford, CA 94305, USA*
[2]*Stanford University/Dept. of Chemical Engineering, Stanford, CA 94305, USA*
[3]*KU Leuven/Dept. of Materials Engineering, Leuven, 3001, Belgium*
[4]*Peking University/Dept. of Materials Science and Engineering, Beijing,100871, PRC*

Polymer sorting is a promising approach to sorting carbon nanotubes (CNTs) by electronic type, offering high selectivity and yield, in addition to low cost and scalability. However, processing conditions that maximize the sorting yield typically lead to CNT dispersions with significant amounts of excess sorting polymer, which has undesirable implications for CNT-based electronics. Here, we introduce a method for removing excess sorting polymer based on flocculation. This approach is broadly applicable to various sorting polymers and facilitates recycling of the sorting polymer. Moreover, this method utilizes materials and equipment that are commonplace in laboratories that work with CNTs.

To establish the utility of flocculated CNTs, we first tested thin-film transistors on $\mathrm{SiO_2}$. Flocculation was found to improve device performance as well as process compatibility, producing transistors with mobilities $\approx$10 $\mathrm{cm^2V^{-1}s^{-1}}$and on–off ratios $\approx 10^6$. We then leveraged the benefits of flocculation for fully inkjet-printed stretchable transistor arrays. The resulting devices have mobilities $\approx$27 $\mathrm{cm^2V^{-1}s^{-1}}$, on-off ratios > 10^4, and can be stretched to $\approx$20% strain with minimal degradation of the on-current.

Panorama 11 **Mo 15:30 - 15:50**

Optimising single-walled carbon nanotube network conductivity via tunnelling barrier modifications

Kimmo Mustonen[1], Viera Skakalova[1], Liao Yongping[2], Semir Tulic[1], Esko I. Kauppinen[2], Jani Kotakoski[1]

[1] *University of Vienna, Faculty of Physics, 1090 Vienna, Austria*
[2] *Aalto University School of Science, P.O. Box 15100, FI-00076 Aalto, Finland*

Transparent and conductive films (TCFs) are of great technological importance. The high transmittance, electrical conductivity and mechanical strength render single-walled carbon nanotubes (SWCNTs) a good candidate for their raw material. Despite the ballistic transport of individual SWCNTs, however, the electrical conductivity in their networks is limited by low charge tunnelling efficiency between the tube elements. Here, we discuss the prospects of improving the tunnelling efficiency with tuning the tube diameter and by the choice of substrate. At a constant optical density, we establish a decrease in the barrier energy with an increasing diameter and show that the (absorption normalised) conductivity of 1.9 nm SWCNTs soars by 60% by placing them on graphene. This improvement is very similar to strong chemical doping, but Raman spectroscopic measurements reveal no apparent changes in the related spectral features. Instead, temperature dependent conductivity measurements indicate that graphene substrate simply reduces the tunnelling barrier heights with only a negligible parallel conduction contribution.

Panorama 11 **Mo 15:50 - 16:10**

Nanoscale conductivity mapping in graphene and carbon nanotubes through mid-IR and terahertz scattering-type scanning near-field optical microscopy

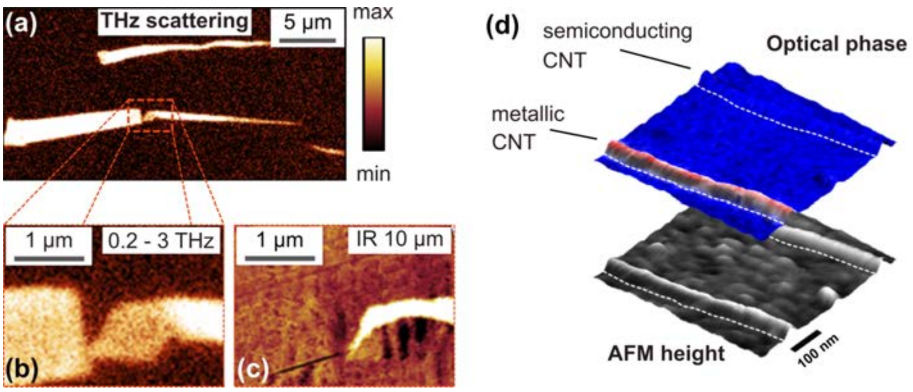
Nicolai F. Hartmann[1], Philip Schaefer[1], Adrian Cernescu[1], Andreas J. Huber[1]

[1] *neaspec GmbH, Haar, 85540, Germany*

Far-field imaging and spectroscopy in the terahertz (THz) and mid-infrared (mid-IR) spectral region is a powerful tool for contact-less conductivity measurements or the study and control of low-energy excitations in solid-state systems [1]. Scattering-type scanning near-field optical microscopy (s-SNOM) bypasses the diffraction limit, enabling these optical measurements with extreme sub-wavelength spatial resolution of below 20nm [2-4], independent of the excitation wavelength.

Graphene on h-BN is imaged with a broadband THz pulse, revealing changing amplitude contrast independently of layer number (Fig. (a), (b)). In a corresponding s-SNOM measurement at 10µm an inverted contrast (Fig. (c)) follows as a direct consequence of the frequency dependent free carrier response in graphene. In a mid-IR s-SNOM image, semiconducting and metallic CNTs can be distinguished in a device [6]. The strong contrasts in the optical phase (Fig. (d)) give access to the conductivity behavior by optical means.

[1] M. Tonouchi, Nat. Photonics 2007, 1, 97; [2] A. J. Huber et al. Nano Lett. 2008, 8, 3766; [3] P. Alonso-Gonzalez et al., Nat. Nanotechnol. 2016, 12, 31; [4] F. Keilmann, R. Hillenbrand, Phil. Trans. R. Soc. Lond. A 2004, 362, 787; [5] G. Nemeth et al. Phys. Status Solidi B 2017, 1700433.



(a) S-SNOM optical amplitude contrast of graphene on h-BN under (b) THz and (c) mid-IR illumination, corresponding to the local free carrier concentration. (d) This concept can also be used to distinguish semiconducting and metallic CNTs.

Panorama 11 **Mo 16:10 - 16:30**

Application and Fabrication Process Development of Long Single Walled Carbon Nanotubes and Its Metal Composite

Atsuko Sekiguchi[1], Atsuko Sekiguchi[1], Rajyashree Sundaram[1], Yuichi Kato[1], Guohai Chen[1], Don Futaba[1], Takeo Yamada[1], Kenji Hata[1]

[1]*National Institute of Advanced Industrial Science and Technology, Tsukuba, 305-8565, Japan*

We present the application and fabrication process of long single walled carbon nanotubes (SWCNTs) utilizing its uniqueness, which are mechanical strength, flexibility, thermal stability and lightweight. Our process is designed to be scalable, versatile and effectively utilize the merit of long SWCNTs in the various forms, such as microfabricated structures, films or wires including its metal composites. Here we demonstrate the superiority of long SWCNTs for thin films with extraordinal mechanical properties and Cu/CNT composite with prominent electrical and thermal properties by discussing the importance of quality and hierarchal structure of CNTs for each property.

We believe that these two examples have a potential to be a key application to realize sustainable CNT industry. The CNT thin films (either supported by the substrate or free-standing) are in demand for a wide-range of applications, e.g. sensing elements in flexible or stretchable electronics, ultrafiltration membranes for water purification or metal ion refinement. The Cu/CNT composite are desired as lighter and more stable substitues of Cu wiring and interconnect to reduce fuel consumption in automobile and aircraft, or to improve reliability in microelectronics.

Franconia Hall **Mo 14:00 - 14:40**

Cu/CNT composites: next-gen lightweight high-performance copper substitutes?

Kenji Hata[1]

[1] *AIST/CNT-Application Research Center, Tsukuba, Ibaraki, Japan*

In this talk, we present the progress made and next challenges in developing Cu/CNT as a realistic competitor to copper. Neat CNT materials have not fulfilled intensifying demands for lightweight copper substitutes for sustainable future technologies. Despite advances, the best CNT assembly conductivities are 10 times lower than that of copper. We believe this deficiency can be overcome by marrying CNTs with copper.

First, we will review the considerable progress made in Cu/CNT fabrication despite inherently weak Cu-CNT affinity. Current literature confirms Cu/CNT electrical and mechanical properties rival that of copper, demonstrating the material's potential as future Cu replacements. In this context, we summarize our group's results. We have reported homogeneously mixed composites 2/3rd as light as copper with high CNT vol% as well as excellent electrical conductivities and heat/current stabilities. Our group's results suggest that Cu/CNT performances not just compete with copper, but also has potential to surpass copper. In the final portion of the talk, we lay out challenges that lay ahead for Cu/CNT to beat copper-performances with possible directions for future research.

Franconia Hall **Mo 14:40 - 15:00**

Organic/Inorganic Hybrid Interfaces with SWCNTs for Energy Harvesting and Conversion

Jeffrey Blackburn[1], Dana Sulas[1], Hyun Suk Kang[1], Severin Habisreutinger[1], Justin Johnson[1], Andrew Ferguson[1], Elisa Miller-Link[1]

[1] *National Renewable Energy Laboratory*

Low-dimensional semiconductors provide a rich tapestry of tunable optical and electrical properties for a wide variety of applications. Semiconducting single-walled carbon nanotubes (s-SWCNTs) have shown tremendous potential in applications ranging from digital logic, biological imaging, quantum information processing, photovoltaics, and thermoelectric energy harvesting. Energy harvesting applications rely critically upon the creation of tailored interfaces that enable the movement of energetic species (excitons, electrons, holes) in specified directions. While organic energy harvesting devices often employ interfaces between distinct organic species such as polymers, fullerenes, and carbon nanotubes, hybrid interfaces between organic and inorganic semiconductors have unique properties that are relatively unexplored. In this talk, I will discuss our recent efforts at constructing novel hybrid interfaces between s-SWCNTs and low-dimensional inorganic semiconductors. I will highlight time-resolved spectroscopy results that illustrate exceptionally long-lived photoinduced charge separation across such interfaces. These studies provide insight into some of the remarkable properties of these interfaces that can enable efficient solar energy harvesting and conversion to fuels.

Energy Symposium SEn3 (invited)

Franconia Hall **Mo 15:00 - 15:20**

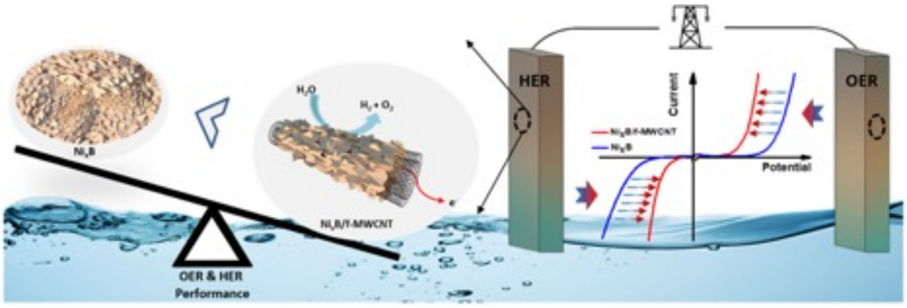
Carbon Materials Assisted Designs of Electrocatalysts

Yuan Chen[1]

[1] *The University of Sydney, Sydney, NSW, 2006, Australia*

Electrocatalysts are critical for realizing efficient energy conversion. Carbon materials can serve as catalyst substrates or act as metal-free catalysts themselves. Here we introduce our efforts in designing novel electrocatalysts for water splitting and zinc-air batteries with the assistance of carbon materials. First, N-containing polymers and metal-organic frameworks were carbonized to yield N doped porous carbon.[1-3] Second, biomaterials containing proteins, such as microbes or milk powders, are cost-effective precursors to produce N and P dually doped carbon.[4-7] Last, we demonstrate that carbon nanomaterials, such as graphene oxide, carbon nanotubes, and their hybrids, can be tailored to assist the synthesis of structurally controlled metal oxide, metal boride, and metal nanoparticles.[8-12]

[1] J. Mater. Chem. A, 2013, 1, 11061; [2] Mater. Chem. Front., 2018, 2, 102; [3] Batteries & Supercaps, 2019, 10.1002/batt.201800143; [4] Catal. Today, 2015, 249 228; [5] J. Mater. Chem. A, 2015, 3, 7210; [6] J. Energy Chem., 2016, 25, 189; [7] Energy Storage Mater., 2018, 11, 134; [8] Nanoscale, 2013, 5, 3457; [9] Adv. Mater., 2017, 29, 1701410; [10] J. Mater. Chem. A, 2019, 7, 764; [11] Sens. Actuators, B, 2019, 283, 304; [12] Small, 2019,1900358



Ultrathin nickel boride nanosheets anchored on functionalized carbon nanotubes as bifunctional electrocatalysts for overall water splitting

Franconia Hall **Mo 15:30 - 15:50**

Graphene and Porous Carbon for Supercapacitor Applications

Cheng-Meng Chen[1]

[1] *Institute of Coal Chemistry, Chinese Academy of Sciences*

Supercapacitor is a rising energy storage device of high power density and long cycle life. For commercial EDLC, carbon is the primary electrode materials, with graphene and porous carbon to be highly concerned. On one hand, the ton scale pilot production of graphene materials was achived by oxidation-reduction strategy from graphite. On the other hand, various porous carbon materials of tunable structure were prepared from biomass, polymer and coal precursor, and a 10 ton/y pilot line was constructed. Graphene and porous carbon was hybrided into composite electrode, and further assembled into cylindrical and pouch devices, with application demonstration in EVs and road stud light. At the same time, the structural evolution, surface chemistry and nano-assembly of carbon materials was systematically studied, so as to pave the way for industrial production and application of these carbon materials.

Franconia Hall **Mo 15:50 - 16:10**

Surface Activation of Carbon-based Nanomaterials for Oxygen Reduction Reaction: In the search of efficient metal-free electrocatalysts

Eduardo Gracia-Espino[1]

[1] *Department of Physics, Umea University, 90187 Umea, Sweden*

The enhanced chemical reactivity seen on defective nanocarbons has been already put to the test, particularly for oxygen reduction electrocatalysis. The promising performance has motivated the further development of doped and defective carbon-based nanomaterials, and nowadays, this approach is seen as alternative pathways to achieve inexpensive but efficient metal-free electrocatalysts. Unfortunately, the intricate atomic configuration of such defective materials significantly complicates their design and optimization. In recent years, the use of computational tools have facilitated the electrocatalysts design by providing detailed information about possible reaction mechanisms, limiting steps, and nature and distribution of active sites, among others. Therefore, in this talk I will describe some of the computational strategies used to identify trends in catalytic activity caused by the presence of edges, defects, and dopants in nanocarbons.

Franconia Hall **Mo 16:10 - 16:30**

Carbon based current collectors for lithium-metal batteries

Hengxing Ji[1], Song Jin[1], Zhaowei Sun[1]

[1]*Department of Applied Chemistry, University of Science and Technology of China*

As an important component of the battery, current collectors in both cathode and anode are used to support the active materials, deliver electrons between active materials and the external circuit, and expand internal thermal heat generate in the electrode film. In order to achieve this function, the current collectors have to be (1) free-standing or self-supporting with macro-scale size, (2) mechanically robust, (3) electronically and thermally conductive, (4) electrochemically inert, (5) light in weight, and (6) low cost.

sp^2-hybridized carbon materials exhibit excellent electric/thermal conductivity, structural stability, and chemical inertness due to the highly delocalized pi electrons. In addition, carbon allotropes have a lower mass density than metal used for current collectors. Combination of these carbon materials used in complementary ways makes it the promising building constituents for current collectors.

We introduce our recent progress in constructing of 3D scaffolds made of sp^2-hybridized carbon constituents as current collectors for lithium based batteries. The requirements and the challenges of the 3D carbon based current collector's design are discussed, which provide inspiration for further exploitation of the current collectors for Li-ion batteries.

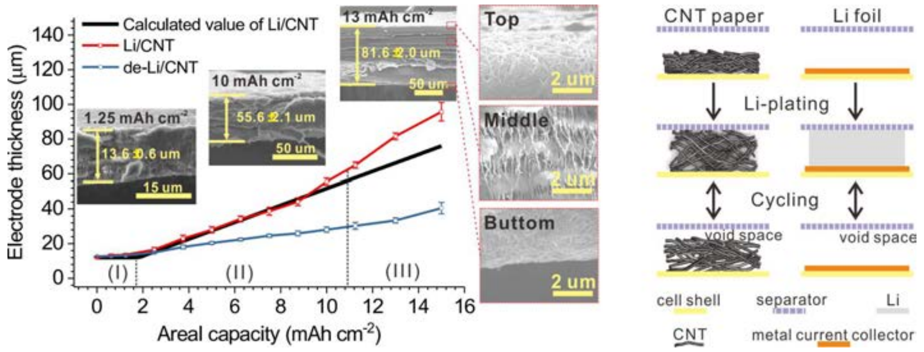


Fig.1 Thicknesses of Li/CNT and de-Li/CNT at different Li loadings. Insets show SEM images obtained from cross sections of Li/CNT with Li loadings of 1.25, 10, and 13 mA h cm^{-2}. Schematic of volume expansion Li/CNT and Li-metal foil.

Panorama 13 **Mo 14:00 - 14:40**

Exciton Linewidth Approaching the Homogeneous Limit in MoS_2 based Van der Waals Heterostructures

Xavier Marie[1], C. Robert[1], B. Han[1], H. Fang[1], E. Courtade[1], B. Urbaszek[1], T. Amand[1], M. Glazov[2], M. Semina[2], L. Golub[2], T. Taniguchi[3], K. Watanabe[3]

[1] *Université de Toulouse, INSA-CNRS-UPS, LPCNO, 135 Av. Rangueil, 31077 Toulouse, France*
[2] *Ioffe Institute, 194021 St.Petersburg, Russia*
[3] *National Institute for Materials Science, Tsukuba, Ibaraki 305-0044, Japan*

In this talk we will review the key characteristics of excitons in transition metal dichalcogenide monolayers [1]. We show that encapsulation of MoS_2ML in hBN can efficiently reduce the inhomogeneous contribution to the exciton linewidth, as we measure in photoluminescence and reflectivity a FWHM down to 2 meV [2]. Similar results are obtained with encapsulated $MoSe_2$, $MoTe_2$, WSe_2 and WS_2MLs [3].
Among the new possibilities offered by the well-defined optical transitions we evidence the optical selection rules for in-plane propagation of light. These studies yield a direct determination of the bright-dark exciton splitting [4]. We also uncover new information on exciton-exciton interactions [5] and exciton-photon weak coupling regime in these Van der Waals heterostructures. The exciton spontaneous emission time can be tuned by one order of magnitude depending on the thickness of the surrounding hBN layers as a result of the Purcell effect [6]

[1] Wang et al, Rev. Mod. Phys. 90, 21001 (2018)
[2] Cadiz et al, PRX 7, 21026 (2017)
[3] Manca et al, Nature Com. 8, 14927 (2017)
[4] Wang et al, PRL 119, 47401 (2017)
[5] Han et al, PRX 8, 31073 (2018)
[5] Fang et al, ArXiv 1902.00670 (2019)

Panorama 13 **Mo 14:40 - 15:00**

Radially polarized light beams from spin-forbidden dark excitons in monolayer WSe_2

Sven Borghardt[1], Jhih-Sian Tu[1], Takashi Taniguchi[2], Kenji Watanabe[2], Beata Kardynal[1]

[1] *Peter Grünberg Institute 9 (PGI-9), Forschungszentrum Jülich, DE-52425 Jülich, Germany*
[2] *National Institute for Materials Science, Tsukuba, Ibaraki 305-0044, Japan*

Transition-metal dichalcogenide monolayers have been shown to act as an ideal playground to study excitonic physics in low-dimensional semiconductors. Especially tungsten-based compounds, where the uppermost valence band and the lowermost conduction band are spin-inverted at the K- and K'-points, host a large diversity of excitonic complexes. So called spin-forbidden dark excitons and trions in WSe_2emit light through an out-of-plane dipole transition and can, therefore, be probed only when collecting light in the plane of the monolayer or using a high numerical aperture objective.

In our work, we show that dark excitons and trions in WSe_2monolayers hold great promise for the facile generation of radially polarized light beams. Photoluminescence emitted from these states is collected using a high numerical aperture objective and its spatial disctribution of state of polarization is resolved.

Although the light emitted through the photoluminescence process is incoherent, we propose strategies to generate radially polarized light beams from dark excitonic states in tungsten-dichalcogenide monolayers. We consider our approach a compact alternative to state of the art systems for the generation of cylindrical vortex beams, as these systems are based on very complex optical system.

Panorama 13 **Mo 15:00 - 15:20**

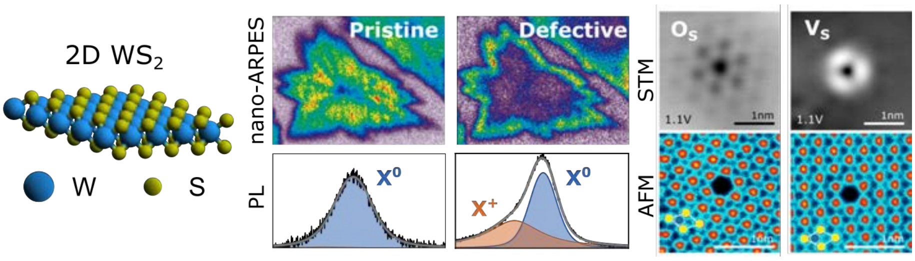
Effects of Defects on Band Structure and Excitons in WS_2 Revealed by Nanoscale Photoemission Spectroscopy

Christoph Kastl[1,2]

[1] *Walter-Schottky-Institut, Technische Universität München, 85748 Garching, Germany*
[2] *Molecular Foundry, Lawrence Berkeley National Laboratory, CA 94720, United States*

Here, we correlate band structure, chemical state, and optical properties of 2D transition metal dichalcogenides at the nanoscale. We employ spatially resolved angle resolved photoemission spectroscopy (nano-ARPES) to map variations in band alignment and chemical composition of monolayer $WS_2$with an unprecedented spatial resolution down to 150 nm. [1] Correlating nano-ARPES with hyperspectral photoluminescence data, we reveal the interplay between local material properties, such as defect density or chemical composition, and the formation of charged trions, defect-bound excitons and neutral excitons. Finally, we compare this to combined atomic force and scanning tunneling microscopy, where we can unambiguously identify the occurring point defects and their electronic structure at the atomic level. [2] Surprisingly, in as-grown WS_2 sulfur vacancies are initially completely absent, and oxygen atoms at sulfur sites are the dominant defect instead. While the sulfur vacancies exhibit electronic states in the gap, the oxygen substitutions recover the band structure of pristine WS_2.

[1] C. Kastl et al. ACS Nano, 13, 1284 (2019).
[2] S. Barja et al. arXiv:1810.03364.



Nano-ARPES reveals nanoscale variations in the band structure of WS_2, which are correlated to the local excitonic properties. High resolution scanning probe microscopy identifies the underlying structure and electronic properties of point defects.

2D Materials Symposium S2D4 (invited)

Panorama 13 **Mo 15:30 - 15:50**

Condensation and expansion of cavity polaritons based on two-dimensional crystals

Christian Schneider[1]

[1] *Lehrstuhl für Technische Physik, Universität Würzburg, Germany*

Semiconducting monolayer crystals, and in particular, transition metal dichalcogenides (TMD) have emerged as a new platform for studies of manyparticle excitations, strongly bound excitons, and most recently, exciton-polaritons in ultimately thin materials. I will discuss the formation of a bosonic condensate driven by excitons hosted in an atomically thin layer of $MoSe_2$, strongly coupled to light in a hybrid GaAs solid-state Resonator, which manifests by a superlinear increase of emission intensity from the hybrid polaritons.

While we capture indications of valley-selective polariton condensation, in turn, high fidelity spin-selective, as well as valley-coherent injection of exciton-polaritons is facilitated via quasi-resonant, non-linear spectroscopy. Valley polarization and coherence can be retained to a very high degree (90%) in the $MoSe_2$ polariton-system. This strongly suppressed valley relaxation and dephasing allows us to study valley selective polariton currents in our structure. Pseudo-magnetic fields, induced by the microcavity's polarization-anisotropic resonance, yield a manifestation of the optical valley Hall effect in the hybrid light-matter system.

2D Materials Symposium S2D5 (contributed)

Panorama 13 **Mo 15:50 - 16:10**

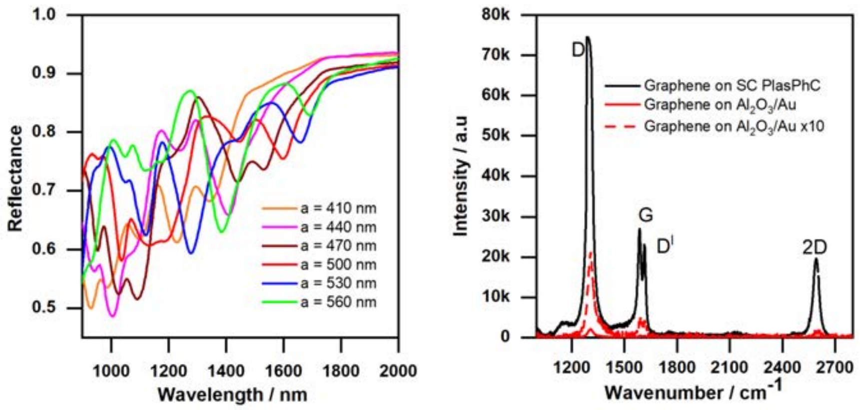
Probing enhanced light-matter interaction in graphene on plasmonic-photonic crystals by Raman spectroscopy

Naga Anirudh Peyyety[1,2], Aimi Abass[1], Adnan Riaz[1,2], Simone Dehm[1], Carsten Rockstuhl[1], Aravind Vijayaraghavan[3], Martin Kalbac[4], Ralph Krupke[1,2]

[1] *Institute of Nanotechnology, Karlsruhe Institute of Technology, Germany*
[2] *Institute of Materials Science, Technische Universität Darmstadt, Germany*
[3] *School of Materials, The University of Manchester, UK*
[4] *J. Heyrovsky Institute of Physical Chemistry, Prague, Czech Republic*

Graphene and carbon nanotubes have unique optical and electrical properties and are of great interest for applications in nanoscale light emitting and light detection devices. Unfortunately, the intrinsic light-matter interaction of these graphene based nanomaterials is rather weak due to their low-dimensionality and measures to enhance it such as, e.g., the integration into optical microcavities and photonic crystals have been considered [1,2]. In our present work, emphasis is laid on enhancements via so-called stacked complementary plasmonic-photonic crystal (SC PlasPhCs), which combine localized plasmonic and high-Q photonic guided resonances to give rise to hybrid plasmonic-photonic resonances at visible and near infrared frequencies. SC PlasPhCs were previously employed as platforms to enhance fluorescence from molecules [3]. Here, we study the enhancement of the light-matter interaction in graphene transferred onto SC PlasPhC substrates by Raman spectroscopy, reflection measurements, and simulations. By tuning the SC PlasPhC structural parameters enhancement contributions of Raman excitation and emission can be tailored.

[1] M. Engel et al., Nat. Comm. 3, 906 (2012)
[2] R-J. Shiue et al., Nat. Comm. 10, 109 (2019)
[3] M. Iwanaga et al., Nano Lett. 3, 1904 (2015)



Left: Reflectance spectra of plasmonic-photonic crystals (SC PlasPhCs) for different air-hole lattice distances. Right: Raman scattering enhancement of graphene on SC PlasPhC is about two orders of magnitude as compared to graphene on 5nm-Al_2O_3/Au.

2D Materials Symposium S2D6 (invited)

Panorama 13 **Mo 16:10 - 16:30**

Pump-Probe Spectroscopy of Polaritons in a $MoSe_2$ Monolayer in the Presence of Itinerant Electrons: Signatures of Optical Amplification

Martin Kroner[1]

Owing to their large exciton binding and strong light-matter coupling, two dimensional semiconductors provide an ideal platform for the exploration of linear exciton and polariton physics. The observation of non-linear optical effects however is hindered by reduced exciton-exciton interactions. In my presentation, I will show that electrical injection of itinerant electrons into monolayer molybdenum diselenide allows us to overcome this limitation. In order to demonstrate optical gain by stimulated cooling of polaritons by electrons, we carry out pump-probe measurements and observe transmission gain of the probe field. Our findings demonstrate that itinerant electron exciton interactions provide an invaluable tool for electronic manipulation of optical properties and pave the way for realization of active optical devices.

Panorama 12 **Mo 14:00 - 14:20**

Origin of Chirality in Carbon Nanotubes: Interplay Between Catalyst and Carbon Nuclei

Avetik Harutyunyan[1]

[1] *Honda Research Institute USA*

The tremendous potential of unique applications of carbon nanotubes is hindered by one key factor: nanotube properties are delicately reliant on their chirality, and yet there is no established technology for monochiral production. The root of the challenge is deeply fundamental - the origin of chirality. More than two decades of studies have revealed the essential contributions of a catalyst features in chirality abundance of grown nanotubes. However, it is hard to rule out the bottom-up approach where carbon nuclei structure dictates the chirality. In this presentation, we target this dilemma by decoupling the influence of catalyst properties on the grown tubes chirality. The revealed fine interplay between these two chirality formation paths suggests the strategy for achieving selective growth.

Practical opportunities toward unique industrial scale applications of carbon nanotubes, particularly for high energy density batteries, will be addressed shortly as well.

Panorama 12 **Mo 14:20 - 14:40**

Advances in the Synthesis of Single Wall Carbon Nanotubes by the Water-Assisted CVD Method

Don Futaba[1]

[1] *CNT-Application Research Center, AIST JAPAN*

In the nearly 30 years since the elucidation of the carbon nanotube structure, the reality of mainstream commercial applications, such as nonplanar touch panels, sealing materials, high performance power sources, etc. are now in the foreseeable future. However, for these dreams to become reality, a practical, developmental obstacles need to be resolved. This is precisely the work which is undertaken by the CNT-Application Research Center, AIST. Our center has been working with companies to support the establishment of a carbon nanotube-based industry in Japan. We have teams working on various topics which are fundamental to the development of applications, such as synthesis, processing, and evaluation at each step. In one section of my presentation, I will describe our efforts toward the economical mass-production of single-walled carbon nanotubes (SWCNT) based on the water-assisted chemical vapor deposition technique, from which highly efficient synthesis of vertically aligned SWCNTs grow from substrates (SWCNT forests). In addition, I will present some recent achievements in the development of commercial CNT products. Finally, I will discuss some of our ongoing work to resolved existing obstacles in the area of synthesis.

Panorama 12 **Mo 14:40 - 15:00**

Growing Highly Pure Semiconducting Carbon Nanotubes for Nanoelectronics by Electrotwisting the Helicity

Kaili Jiang[1], Jiangtao Wang[1], Xiang Jin[1], Zebin Liu[1], Bingyu Xia[1]

[1]*Department of Physics & Tsinghua-Foxconn Nanotechnology Research Centre, Tsinghua University, Beijing, 100084, China*

Carbon nanotubes (CNTs) are anticipated to be the successor to silicon in next generation integrated circuits. However, great challenges to the practical application of this concept include the need to grow horizontal semiconducting CNT (s-CNT) arrays with very high purity. Recently, we found that charge is generated during the CVD growth of CNTs[1], which inspired us to use electric field to twists the helicity of the CNTs during synthesis. As a result, nearly-defect-free s-CNTs horizontally-aligned on the substrate have been synthesized with less than 0.1% residual metallic CNT (m-CNT), thus offers a potential pathway to practical applications of CNT nanoelectronics[2].

[1] J. Wang, P. Liu, B. Xia, et al. Nano Letters 16, 4102-4109 (2016).
[2] J. Wang, X. Jin, Z. Liu, et al. Nature Catalysis 1, 326-331 (2018).

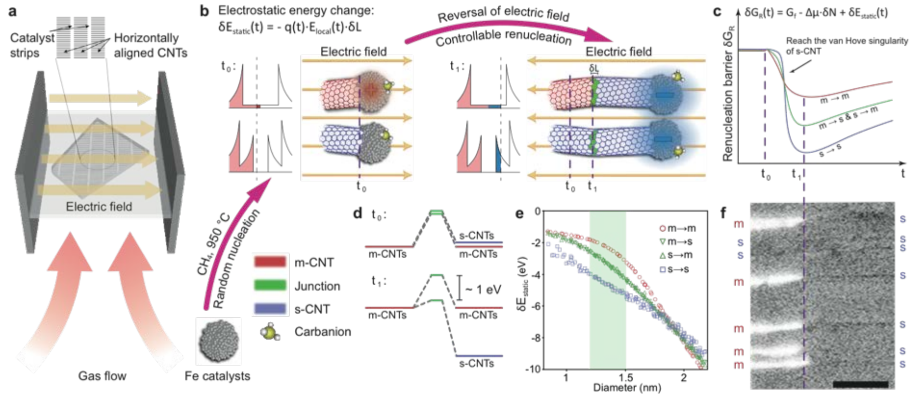


Figure 1 Controllably twisting the chirality of CNTs from metallic to semiconducting. (a) Schematic diagram of the Electro-ReNucleation system. (f) SEM image of the CNTs with chirality changing from m-CNTs(bright) to s-CNTs(dark).

Panorama 12 **Mo 15:00 - 15:20**

Atomic Scale In-Situ Study on Carbon Nanotube Growth from Co-Co3C Catalysts

Feng Yang[1], Yan Li[1]

[1]*College of Chemistry and Molecular Engineering, Peking University, Beijing 100871, China*

Atomic Scale In-Situ Study on Carbon Nanotube Growth from Co-Co3C Catalysts
Feng Yang, Yan Li*
College of Chemistry and Molecular Engineering, Peking University, China
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The metal catalysts play important roles in chemical vapor deposition (CVD) of single-walled carbon nanotubes (SWNTs). It was reported that solubility of carbon in transitional metal nanoparticles such as Fe, Co, and Ni is associated with the SWNT growth, which is generally believed to via a vapor–liquid–solid mechanism [1, 2]. Revealing the catalyst structure with atomic resolution under reactive environment is crucial for understanding the controlled growth mechanism.

Here, using Co as a model catalyst, we investigated the role of active species Co-Co3C in catalyzing SWNT nucleation and growth by using aberration-corrected environmental transmission electron microscope (ETEM). We recorded the carbon atoms dissolving into Co nanoparticles and formation of inhomogeneous Co-Co3C structure during CVD. The growth of SWNTs was realized only by the cooperation of Co and Co3C in proper carbon feeding conditions. The evidences are in situ and real time with atomic scaled resolution. These findings are crucial for the rational design of catalysts for high efficiently catalyzing SWNTs.

Panorama 12 **Mo 15:30 - 15:50**

Studying the Growth of Single-Walled Carbon Nanotubes by Optical Means

Vincent Jourdain[1], Huy-Nam Tran[1], Vladimir Pimonov[1], Léonard Monniello[1], Hugo Navas[1], Matthieu Picher[1], Thierry Michel[1], Rémy Vialla[1], Guillaume Prévot[1], Saïd Tahir[1], Eric Anglaret[1], Amandine Andrieux-Ledier[2], Frédéric Fossard[2], Annick Loiseau[2], Akinari Kozawa[3], Takahiro Maruyama[3]

[1] *Laboratoire Charles Coulomb (University of Montpellier / CNRS)*
[2] *Laboratoire d'étude des microstructures, CNRS-ONERA, Châtillon, France*
[3] *Department of Applied Chemistry, Meijo University, Nagoya, Japan*

We will report on the use of optical methods to address the relation between nanotube structure and growth conditions. First, we will present in situ and ex situ Raman studies of the evolution of the SWCNT population during their growth by CCVD [1]. Importantly, this study reveals that the nanotube diameter distribution strongly evolves during growth but in dissimilar ways depending on the growth conditions which is explained by the kinetic competition between catalyst ripening and nanotube growth. Second, we will show how recently developed polarization-based methods [2] can be used to image the growth of individual SWCNTs on substrate with time resolution of a few tens of ms. Third, we will describe a comprehensive model of the spectra of individual SWCNTs on substrate obtained with the same polarization-based setup [3]. Importantly, this model includes the influence of the commonly used anti-reflection substrates (e.g. SiO_2/Si), and of coherent and non-coherent depolarization by the optics. This model allows extracting both the real and imaginary parts of the nanotube susceptibility and improving the methodology of chirality assignment.

[1] Navas et al, ACS Nano (2017), 11, 3081
[2] Liu et al, Nature Nanotech. (2013), 8, 917
[3] Monniello al., PRB (2019), in press.

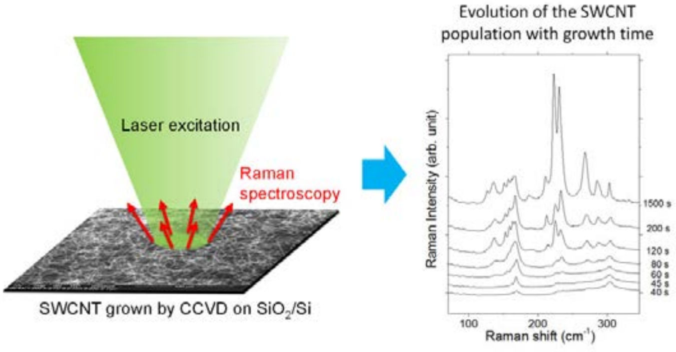

Illustration of the optical-based approach and of the strong evolution of nanotube diameter distribution during the growth observed in numerous growth conditions (Navas et al, ACS NAno (2017), 11, 3081)

Panorama 12 **Mo 15:50 - 16:10**

One-dimensional van der Waals heterostructure nanotubes: synthesis and growth mechanism

Rong Xiang[1]

[1]*Department of Mechanical Engineering, The University of Tokyo, Tokyo 113-8656, Japan*

Recently, we proposed a conceptually new structure, in which single- or few-walled hexagonal boron nitride nanotube (BNNT) and/or MoS_2nanotube seamlessly wrap around a single-walled carbon nanotube (SWCNT), and result in an atomically smooth coaxial nanotube consisting different materials. As different shells are stacked by van der Waals (vdW) force and in one-dimensional (1D) geometry, we name it “1D vdW heterostructure” nanotubes (1D heteroNTs).[1] TEM/STEM characterizations confirm each layer is single-crystal nanotube.

In this presentation, we will further extend the exploration of this new structure, with the focus on controlled synthesis and growth mechanism. Overall, 1D heteroNTs follow an open-end chiral growth mechanism. In this scenario, three different nucleation modes (one-end nucleation, two-end nucleation and center nucleation) can be distinguished. In a two-end mode, we confirm that two outer nanotubes with different chiralities can form on the same SWCNT and merge into a junction. Similarly, a chirality analysis in SWCNT-MoS_2heteroNTs reveals no noticeable structure recognition between two different shells. Finally, we show two strategies to control the nucleation and growth site of 1D heteroNTs.

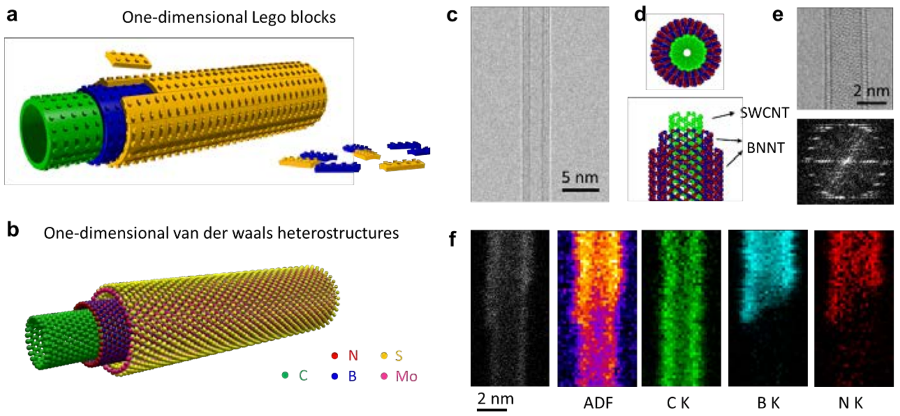

Figure Overview of 1D vdW heterostructures. (a) concept and (b) atomic model 1D vdW heterostructures; (c-f) TEM image and EELS mapping of a SWCNT-BNNT 1D vdW heterostructure.

Panorama 12 **Mo 16:10 - 16:30**

In-situ synthesis of the confined linear carbon chains

Lei Shi[1,2], Ryosuke Senga[3], Kazu Suenaga[3], Paola Ayala[2], Thomas Pichler[2]

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[2]University of Vienna, Faculty of Physics, 1090 Wien, Austria
[3]AIST, Nanomaterials Research Institute, 305-8565 Tsukuba, Japan

Recently we demonstrated synthesis of confined one-dimensional linear carbon chains (LCCs) inside double-walled carbon nanotubes (DWCNTs) using high-temperature annealing method in high vacuum. The shortest chains consist of around 30 carbon atoms (polyyne) and the longest ones are with a record length of more than 6000 carbon atoms (carbyne) [1]. However, synthesis of specific length of LCCs is still challenging. In this presentation, I will show our recent efforts on tailoring the length of the confined LCCs using different carbon nanotubes as hosts [2]. Also, a new method will be introduced to grow different length of LCCs monitored by in-situ Raman spectroscopy [3].

[1] L. Shi, et al. Nature Mater. 15, 634-639 (2016)
[2] L. Shi, et al. Submitted (2019)
[3] L. Shi, et al. In preparation (2019)

Panorama 10 **Mo 14:00 - 14:40**

Controlling helicity of circularly polarized light in low-dimensional materials

Riichiro Saito[1]

[1] *Tohoku University, Department of Physics*

We overview our recent works on optical properties by using circularly polarized light in carbon nanotubes and two-dimensional materials. Electric field of circularly polarized light rotates as a function time, clockwise (left-handed, LH) or anti-clockwise (right-handed, RH) when we observe the rotation from the propagating axis. The freedom of LH and RH is a "spin" of a photon which can be applied for doubling the information in optical signal transmission. A photon of circularly polarized light has an angular momentum of $\pm\hbar$ which we call helicity of the phonon. Circular dichroism (CD) is defined by the difference of optical absorption for LH and RH circularly polarized light, which can be seen in chiral carbon nanotubes. We will discuss how the CD is calculated [1] and observed [2] as a function of chirality of carbon nanotubes. CD generally appears in two-dimensional materials, too, which we discuss in connection with valley polarization or pseudo-spin polarization by using so-called Haldane model [3] or modified Haldane model [4] that covers the Hamiltonian of many two-dimensional materials such as graphene, h-BN etc. In the Raman spectroscopy, we will discuss the origin of helicity-changing Raman spectra [5] and the relevant conservation law of angular momentum [6]. Finally, we will discuss surface plasmon of two-dimensional materials which is coupled with circularly polarized light [7].

References: *This work is supported JSPS KAKENHI No. JPB18H01810.
[1] N. Sato, Y. Tatsumi, R. Saito, Phys. Rev. B. 95, 155436 (2017).
[2] X. Wei, T. Tanaka, Y. Yomogida, N. Sato, R. Saito, H. Kataura, Nat. Comm. 7, 12899 (2016).
[3] K. Ghalamkari, Y. Tatsumi, R. Saito, J. Phys. Soc. Jpn., 87, 063708 (2018).
[4] M. Villa, N. T. Hung, S. Roche, R. Saito, Phys. Rev. B, 99, 161404 (2019).
[5] Y. Tatsumi, R. Saito, Phys. Rev. B 97, 115407 (2018).
[6] Y. Tatsumi, T. Kaneko, R. Saito, Phys. Rev. B, 97, 195444 (2018).
[7] M. S. Ukhtary, M. Maruoka, R. Saito, unpublished.

Theory Symposium

STh2 (invited)

Panorama 10

Mo 14:40 - 15:00

Bright and Dark Exciton Dynamics in Transition Metal Dichalcogenides

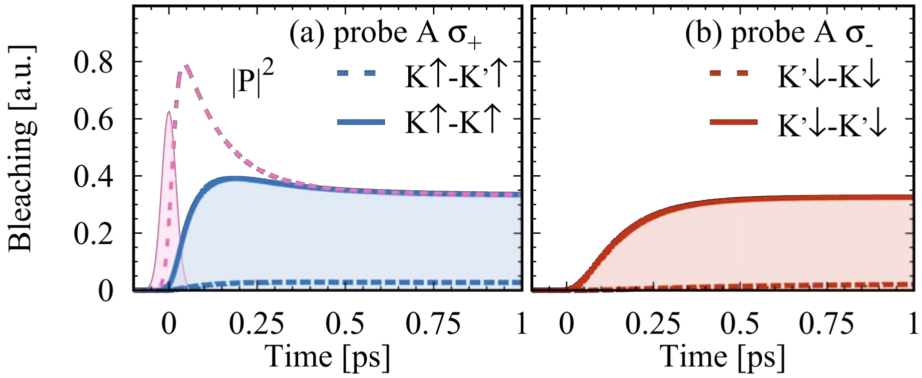
Malte Selig[1], Dominik Christiansen[1], Florian Katsch[1], Ermin Malic[2], Andreas Knorr[1]

[1] *Institut für Theoretische Physik, Technische Universität Berlin, Berlin, Germany*
[2] *Chalmers University of Technology, Gothenburg, Sweden*

Atomically thin transition metal dichalcogenides exhibit strongly bound excitons dominating the optical spectra. Besides bright excitons, a variety of dark exciton states exist being formed by electrons and holes with opposite spin, or by excitons with non-vanishing center of mass momentum well above the lightcone, including intervalley excitons. Here, we present an excitonic theory within the Heisenberg equation of motion framework [1]. We investigate the impact of exciton phonon interaction on the excitonic lineshape [2,3,4] as well as the phonon mediated formation and thermalization of exciton densities [5]. It turns out, that dark states

as a ground state in tungsten based TMDs strongly influence the temporal dynamics of the exciton relaxation, as well as their luminescence yield and their resulting decay. Additionally we will discuss the impact of such dark exciton states on the Pauli blocking contributions in pump probe experiments, cf. figure 1, where it turns out that they give rise to an unintuitive signal at the energetically higher B transition. Our theoretical results explain several recent experimental results.

[1] pssb 255 1800185 (2018).
[2] Nat Commun. 7 13279 (2016).
[3] PRL 18 1751 (2018).
[4] Nano Lett. 18 187402 (2017).
[5] 2D Mater. 5 035017 (2018).



Bleaching contributions of different valley excitons to the polarization resolved pump probe signal after resonant excitation to the A exciton.

Panorama 10 **Mo 15:00 - 15:20**

Moiré physics in heterobilayer and homobilayer 2D semiconductors

Hongyi Yu[1]

[1] *Department of Physics, University of Hong Kong, Hong Kong, China*

In bilayer structures of transition metal dichalcogenides, a small twist angle between the two layers leads to the appearance of a large scale moiré pattern, i.e., the real space texture of atomic configurations. In a heterobilayer, we find these moiré effects realize superstructures of nanodot confinements for long-lived interlayer excitons. At given atomic registry, the spin-triplet and spin-singlet excitons have distinct valley polarization selection rules, allowing the selective optical addressing of both the exciton valley and the spin-singlet/triplet configurations. In a homobilayer moiré superlattice, we introduce a three-orbital tight-binding model to describe the three lowest hole bands. These bands are found to exhibit nontrivial topological structures depending on the moiré periodicity.

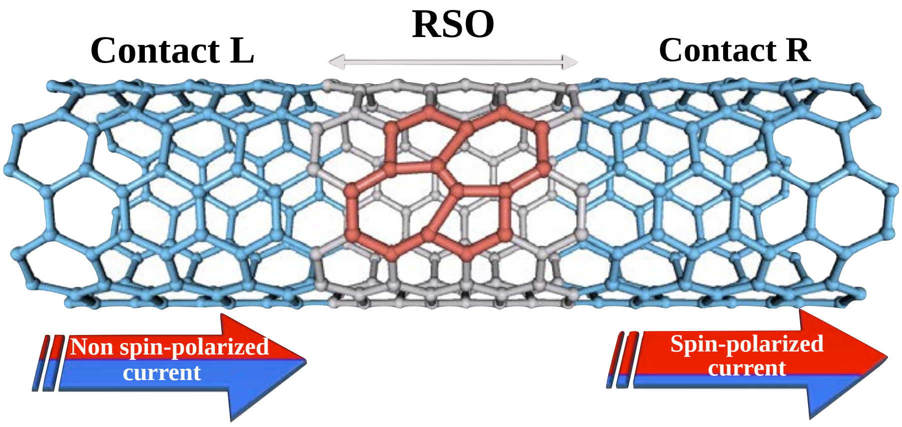
Panorama 10 **Mo 15:30 - 15:50**

Controlling spin-polarized currents in Carbon Nanotubes: Rashba spin-orbit effects and defect engineering

Hernán Santos[1], Leonor Chico[2], José Enrique Alvarellos[3], Andrea Latgé[4]

[1]*Dep. de Física de la Materia Condensada, U. Autónoma de Madrid, 28049 Madrid, Spain*
[2]*Inst. de Ciencia de Materiales de Madrid, ICMM-CSIC, 28049 Madrid, Spain*
[3]*Dep. de Física Fundamental, U. Nacional de Educación a Distancia (UNED), Madrid, Spain*
[4]*Inst. de Física, Universidade Federal Fluminense, Niterói, 24210-340, RJ-Brazil*

The production of spin-polarized currents at the nanoscale continues to be a challenge for the development of real spintronic devices. Carbon nanotubes (CNTs) are good candidates for spintronic applications due to their unbeatable transport properties. The production of spin-polarized currents in pristine carbon nanotubes with Rashba spin-orbit (RSO) interactions has been shown to be very sensitive to the symmetry of the tubes and the geometry of the setup in concordance with its planar counterpart [1,2]. Here we study the role of defects as hydrogen adatoms and Stone-Wales defects on the spin-polarized currents in CNTs [3] (see Fig. 1). Actually a single-defect scenario is insufficient to generate significant spin-dependent currents. However, an equispaced array of a few defects enhances considerably spin-polarized currents. We explain this as a result of resonant tunnelling produced by multiple defects. We also show that certain arrangements of defects can yield a reversal of the spin polarization, which can be exploited for spin switches. Our results can open a way for the design of spintronic CNT devices.



Schematic drawing of the proposed device. Pristine CNT forms the left (L) and right (R) contacts. The central region is composed by the same CNT in the presence of RSO, but with topological defects (a Stone-Wale topological defect is plotted in red).

Panorama 10 **Mo 15:50 - 16:10**

Light Emission from Ultranarrow Graphene Nanoribbons: Insights from Ab Initio Simulations

Deborah Prezzi[1]

[1] *Nanoscience Institute of the National Research Council (CNR-NANO), Modena, Italy*

Owing to their width-dependent sizable band gaps, graphene nanoribbons (GNRs) have attracted increasing attention in the last decade as a viable route for graphene-based nano- and opto-electronic applications. More recently, the successful production of ultranarrow and structurally well-defined GNRs by means of bottom-up techniques has further boosted this research line. While absorption properties have been addressed in depth [1,2], emission properties are still largely unexplored.

We here report on the optical response of finite-length GNRs as resulting from state-of-the-art ab initio calculations beyond mean field [3,4]. Our results indicates that bulk-like excitations coexist with below-bandgap states localized at the GNR extremities, which are almost independent on the length. By investigating both the presence of defects and the effect of the substrate, our simulations allow us to identify unpredicted optical transitions in GNRs and to elucidate the origin of below-bandgap STM-induced light emission recently observed in suspended GNRs [3], providing a promising route for the realization of bright, robust, and controllable graphene-based light-emitting devices.

[1] R. Denk et al., Nat. Commun. 5, 4253 (2014)
[2] G. Soavi et al., Nat. Commun. 7, 11010 (2016)
[3] M. Chong et al., Nano Lett. 18, 175 (2018)
[4] C. Cardoso, A. Ferretti, D. Prezzi, EPJB, 91, 286 (2018)

Theory Symposium STh6 (contributed)

Panorama 10 **Mo 16:10 - 16:30**

The CNT-metal adsorption energy: key for chirality selective growth?

Charlotte Vets[1], Daniel Hedman[2], J. Andreas Larsson[2], Erik C. Neyts[1,3]

[1]*University of Antwerp, Antwerp, BE-2610, Belgium*
[2]*Luleå University of Technology, Luleå, SE-971 87, Sweden*
[3]*NANO Centre of Excellence, Antwerp, Belgium*

While chirality selective growth of CNTs is a topic of paramount importance, the mechanisms governing chirality formation have not yet been unraveled. [1] Bimetallic catalysts have received much attention in experiments, [2] and the computation of adsorption energies on monometallic nanoparticles has been well documented. [3] However, a combination of both is a topic that has remained largely unexplored. This work seeks to elucidate whether the adsorption energy is the key for chirality selective growth. Drawing on a density functional theory approach, we analyzed adsorption energies of armchair, zigzag, and chiral CNTs on Ni, Fe and NiFe alloyed nanoparticles. Finding the most stable atom distributions within NiFe alloys was achieved in our previous work. [4] Our current findings were validated with experimental results. [2] Taking into account the limitations of the chosen systems, the results demonstrate that the adsorption energy alone is not sufficient for chirality selective growth.

References

1. Neyts, E. C. et al. J. Am. Chem. Soc. 133, 17225-17231 (2011).
2. Chiang, W.-H. et al. ACSNano 3, 12, 4023-4032 (2009).
3. Silvearv, F. et al. J. Mater. Chem. C 3, 3422-3427 (2015).
4. Vets, C. and Neyts, E. C. J. Phys. Chem. C 121, 15430-15436 (2017).

Abstracts Monday (Poster)

P001 **Mo 17:00 - 18:30**

Optical spectroscopy of doped single wall carbon nanotubes

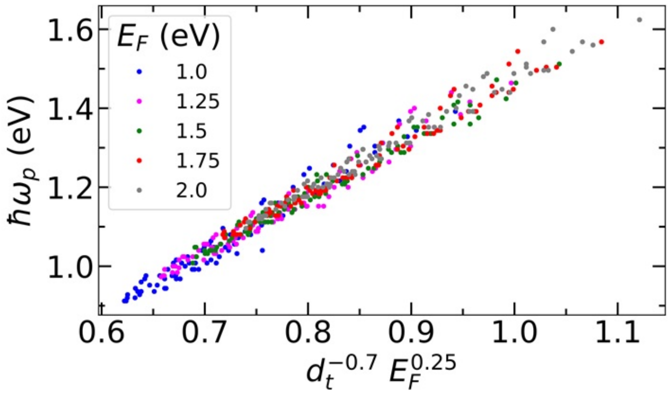
Riichiro Saito[1], Daria Sacco[2], Ahmad R. Nugraha[1], Shoufie Ukhtary[1], Daria Kopylova[2], Albert G. Nasibulin[2]

When single wall carbon nanotube is heavily doped, the E_{ii} optical absorption is suppressed and the new peak appears at a different energy. When the Fermi energy is located in the conduction (or valence) band of a semiconducting or a metallic nanotube, we expect intraband, optical conductivity which makes a strong optical absorption that is known as surface-plasmon absorption peak. Yanagi has observed the plasmon peak using the aligned nanotube sample by changing the polarization of light. [1] Thus it is important to investigate the chirality dependence of the plasmon frequency and the intensity of the plasmon peaks as a function of (n,m) of nanotube and the Fermi energy.

In this presentation, we will show “Plasmon Kataura Plot as a function of the Fermi energy” theoretically for characterizing nanotubes by plasmon peaks. [2] In particular, we discuss (1) the most contributed cutting lines (one-dimensional Brillouin zone) for observing the each plasmon peak and (2) scaling the plasmon peak as a function of the diameter. This information will be useful for designing nano-antenna.

References:

[1] K. Yanagi et al., Nature Commn., 9,. 1121 (2018)
[2] D. Sacco et al., Phys. Rev. B99, 075403, (2019).



Plasmon Kataura plot for doped carbon nanotubes. Energy positions of the optical absorption by surface plasmon can be scaled by $d_t^{-0.7}E_F^{0.25}$. This plot is useful for spectroscopy of doped nanotubes.

P003 **Mo 17:00 - 18:30**

Drawable single- and double-walled carbon nanotube forest grown from dip-coated Iron nanoparticle

Yuya Abe[1], Motoyuki Karita[1], Takayuki Nakano[1], Yoku Inoue[1]

[1] *Department of Electronics and Materials Science, Shizuoka University*

For high drawability (dry-spinnability) of a carbon nanotube (CNT) forest, it is important to grow CNTs with high density. When a catalyst layer is formed by sputtering, it is difficult to independently control the nanoparticle size and density by thermal condition. In this study, we synthesized CNT forests with a mixture of single- and double-walled CNTs showing drawability from size-controlled iron nanoparticles.

Iron catalyst nanoparticles were synthesized by a polyol method using iron acetylacetonate. The prepared nanoparticles were densely supported on an Al_2O_3layer formed on a thermally oxidized Si substrate by dip coating. Then CNT forests were grown by thermal chemical vapor deposition CVD with acetylene as a carbon source. Height of the synthesized CNT forest was 200 μm and average CNT diameter was 3.9 nm. Diameter of the CNTs and the iron nanoparticles had the same size distribution. 60% of grown CNTs were DWCNT and the rest was SWCNT. The CNT forest had drawability. A CNT web was easily drawn out from the CNT forest.

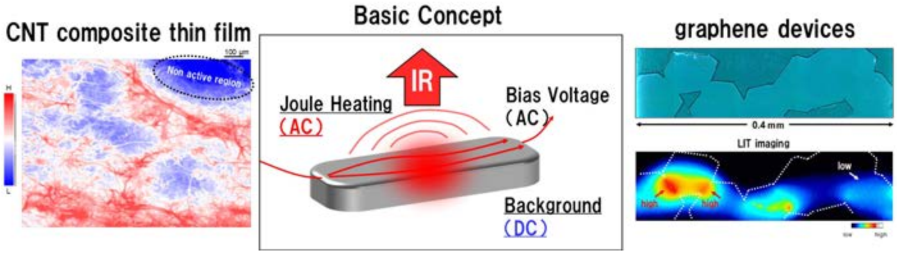


Fig.1 (a) SEM image of a drawable CNT forest, and (b) diameter distribution of the CNT forest

P005 **Mo 17:00 - 18:30**

Role of sulfur in floating-catalyst CVD growth of single-walled carbon nanotubes for transparent conductive film applications

Saeed Ahmad[1], Er-Xiong Ding[1], Qiang Zhang[1], Hua Jiang[1], Esko I. Kauppinen[1]

[1]*Aalto University School of Science, P.O. Box 15100, FI-00076 Aalto, Finland.*

Sulfur-containing molecules have been widely utilized as a promoter for the growth of single-walled carbon nanotubes (SWCNTs) in floating-catalyst chemical vapor deposition (FC-CVD) process to fabricate SWCNT-based transparent conductive films (TCFs). However, in-situ catalyst particle formation and SWCNT growth conditions hinders to correlate the substantial role of sulfur in tuning yield, morphology and structure of SWCNTs. Herein, we have systematically studied the roles of sulfur on yield, morphology and structure of FC-CVD grown SWCNTs, using ex-situ Fe and Co catalyst particles. Firstly, we synthesized SWCNTs without sulfur and then sulfur-assisted SWCNTs were obtained using H_2S. We found that the yield of SWCNTs has considerably changed by adding sulfur into the reaction depending on sulfur concentration and catalyst composition. More importantly, the addition of an optimized amount of sulfur has enhanced approximately three times, performance of SWCNT-TCFs, by increasing diameter and bundle length along with improving quality of SWCNTs. Surprisingly, detailed atomic structure determination revealed that SWCNTs from both Fe and Co have a wide chirality distribution spanning from zig-zag to armchair edges and sulfur promotor has no role in controlling chirality of SWCNTs.

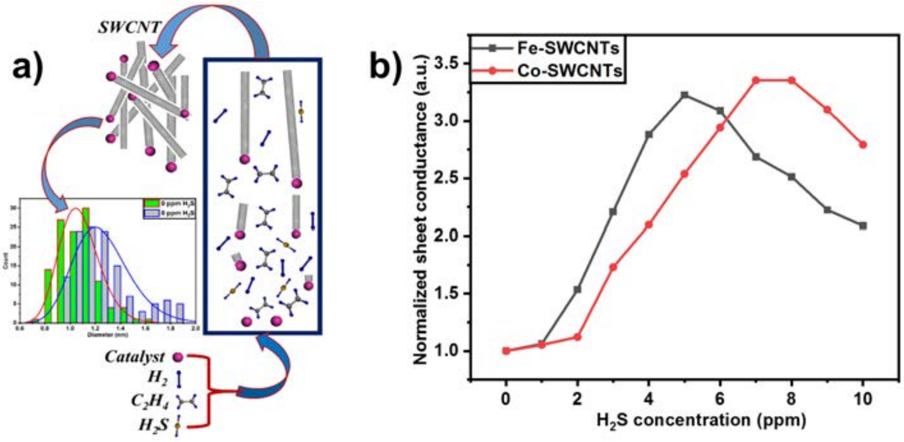


Fig. 1. a) A schematic for FC-CVD growth of sulfur-assisted SWCNTs using ex-situ catalyst particles. b) Variation in sheet conductance of SWCNTs film as a function of sulfur concentration.

Plenary Venue Poster

P009 **Mo 17:00 - 18:30**

Modulating single-walled carbon nanotube opto-electronic properties by dye confinement

Laurent Alvarez[1], Romain Chambard[1], Geraud Delport[2], Lucie Orcin-Chaix[2], Nicolas Izard[1], Bruno Jousselme[3], Stéphane Campidelli[3], Yuta Sato[4], Kazu Suenaga[4], Pascal Puech[5], Jean-Sébastien Lauret[2], Guillaume Cassabois[1], Jean-Louis Bantignies[1]

[1] *Laboratoire charles Coulomb, Montpellier, France*
[2] *Laboratoire Aimé Cotton, Orsay, France*
[3] *LICSEN CEA Saclay, France*
[4] *AIST, Tsukuba, Japan*
[5] *CEMES, Toulouse, France*

Dye encapsulation into host single-walled carbon nanotubes is an elegant way to create hybrid nano-systems with tunable opto-electronic properties. To this aim, different kinds of molecules (either electron donor or acceptor, absorbing either in the blue or the red visible range) are encapsulated into metallic or semiconducting nanotubes displaying different diameters. Up to now, we have mainly studied encapsulated quaterthiophene derivatives (4T), tetracyanoquinodimethane (TCNQ) and phthalocyanine (MPc) molecules. In this work, we discuss the supramolecular organization of dyes inside the nanotube, the optical properties and the charge transfer for some of our hybrid systems. For instance, using Raman spectroscopy, a significant electron transfer is reported with 4T, whose magnitude strongly depends on the nanotube diameter, and on the metallic or semiconducting character. Experiments also suggest a photo-activated electron transfer for small diameter (~9 Å) semiconducting and metallic tubes. Confinement of electron donor (4T) (respectively electron acceptor (TCNQ)) into small diameter tubes leads to a red shift (blue shift) of the optical absorption energy and an increase (decrease) of the photoluminescence intensities, evidenced by the photoluminescence excitation maps.

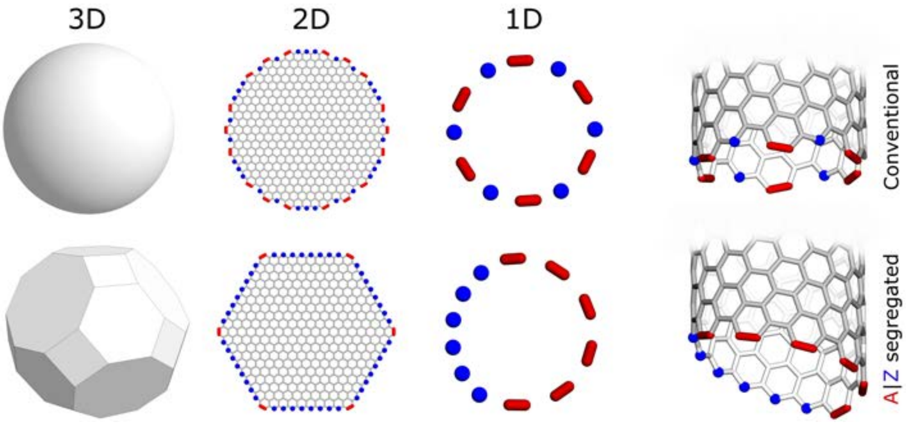
P011 **Mo 17:00 - 18:30**

Carbon nanotube-catalyst interface segregation and the quest for chirality control

Ksenia V. Bets[1], Evgeni S. Penev[1], Boris I. Yakobson[1]

[1] *Rice University, Materials Science and NanoEngineering Department, Houston, 77005, USA*

The structure of the carbon nanotube-catalyst interface during catalytic synthesis controls both thermodynamics and kinetics of the growth process that in turn prescribe chirality distribution of the growing nanotube (CNT). Despite its importance, the structure of such interface was never investigated but rather assumed to be a minimal-length circle, which is analogous to postulating spherical shape of 3D particles or circular shape of 2D flakes, clearly contradicting faceted Wulff construction in both cases (Fig.1). We present a systematic analysis of the CNT-catalyst interface energetics revealing a drastic change in the interface structure with the solidification of the catalyst. A circular edge is weakly preferred in contact with a liquid catalyst, but interface with rigid catalyst shows a strong preference towards the segregation of the CNT edge into two segments (Fig.1). This trend is further confirmed with the first-principles calculations for a set of representative catalysts (Co7W6, WC, Ni, Co). A|Z-segregation lowers the energy of the chiral tubes, largely enhancing their nucleation probability. Kinetics is also greatly influenced, as we demonstrate on the example of selective (2m,m) growth on solid Co7W6 catalyst exemplifying the importance of the interface structure.



Minimal-surface versus faceted shapes in 3D (generic nanoparticle), 2D (graphene flake), and 1D (carbon nanotube edge, also shown in side view, demonstrating conventional circular and A|Z-segregated edges).

Plenary Venue Poster

P013 **Mo 17:00 - 18:30**

Chemistry of carbon nanotubes as π-conjugated macromolecules – realizing the promise of properties-by-design approach

Slawomir Boncel[1], Rafal Jedrysiak[1], Bertrand Jozwiak[1], Anna Kolanowska[1], Anna Kuziel[1], Patrycja Wasik[1], Marzena Dzida[2], Artur Herman[3]

[1] *Silesian University of Technology, Faculty of Chemistry, NanoCarbon Group*
[2] *University of Silesia, Institute of Chemistry*
[3] *Wroclaw University of Science and Technology, Faculty of Fundamental Problems of Technol.*

Individualization of carbon nanotubes (CNTs) plays a vital role in manufacturing CNT-based composites of enhanced thermal, mechanical and/or electrical properties at low percolation thresholds. Similarly, debundling of CNT agglomerates is crucial in numerous biomedical and catalytic applications. On the other hand, macroscopic assembling of CNTs into desired forms and geometries of superior properties requires ultra-long CNTs and hence problematic processing.

Being inspired by organic chemistry methods, we have employed several reactions to functionalize CNTs and enhance their compatibility with aqueous media or polymer matrices. Inter alia, we have functionalized CNTs via: electrothermal halogenation, 'doping' with iodine monochloride, (2+3)-cycloaddition of nitrile N-oxides, (1+2)-cycloaddition of nitrenes, Ullmann-type reactions, Rieche formylation, Friedel-Crafts alkylation and many subsequent reactions (including cross-linking). The elaborated protocols combining covalent and noncovalent CNT functionalization methods allowed us to manufacture heat transfer IoNanoFluids, screen-printable electroconductive on-textile coatings, efficient/selective nanobiocatalysts and targeted drug delivery systems.

P015 **Mo 17:00 - 18:30**

Carbon-coated silver nanowires as interconnects and their electrical breakdown mechanism

Pedro Costa[1], Nitin Batra[1]

[1] *King Abdullah University of Science and Technology, Thuwal 23955-6900, Saudi Arabia*

For the most part, the solution chemistry synthesis of Ag nanowires (NW) induces the formation of a thin carbon shell that stabilizes the metallic silver. Amongst other uses, these one-dimensional (1D) nanostructures have been proposed as interconnectors for the next-generation of electrical devices. Strangely, there has not been much consideration on how the carbon-shell or the overall shape of the NWs affect their response to electrical currents. In this communication, we report a study on the correlation of electrical and structural responses of suspended Ag NWs exposed to increasing electrical current densities, as analyzed using in situ TEM [1]. These discrete-level experiments revealed that the behaviour of carbon-coated Ag NW is dependent on their initial shape (Figure 1). Accordingly, at low rates of bias application, initially straight nanowires showed trivial behaviour up to their breakdown, with electromigration and gradual necking taking place. By contrast, those nanowires with an initially bent configuration exhibit a mixed set of responses which included string-like resonance and structural rearrangements.

[1] Batra, N. M.; Syed, A.; Costa, P. M. F. J., Current-induced restructuring in bent silver nanowires. Nanoscale (2019), 11, 3606.

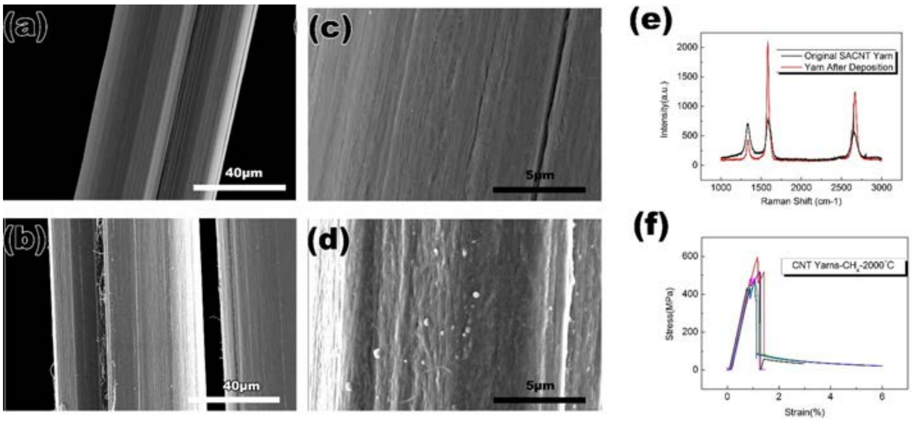


Figure 1: The application of bias at slow rates induces responses from carbon-coated Ag nanowires that are dependent on their initial shape (straight or bent).

P017 **Mo 17:00 - 18:30**

Versatile Manipulation of Nanostructured Noble Metal Aerogels

Ran Du[1]

[1] *Physical Chemistry, Technische Universität Dresden, Bergstr. 66b, Dresden 01062 , Germany.*

Combining the chemical nature of noble metals and monolithic porous architecture of aerogels, noble metal aerogels (NMAs) have emerged as a rising star in material science. Sol-gel process is the most frequently used strategy to fabricate NMAs. To date, quite a few systems (Au, Ag, Pd, Pt, Pd-Pt, etc.) have been demonstrated and diverse applications have been investigated. However, a superficial understanding of underlying gelation mechanism retard the flexible manipulation of NMAs, thus hindering investigating composition/structure-property/performance relationship for material design and optimization.
In this regard, we introduced specific-ion effects to address above issues,1 where a delicate modulation of ion-nanoparticle interactions afford versatile manipulation of NMAs. As a result, NMAs with highly tunable compositions (Au, Ag, Pd, Pt, and their alloys), ligament size (3.1~142.0 nm), special morphologies (e.g. core-shell structure) are directly produced from dilute nanoparticle precursor solutions in 4~12 hours. More importantly, an overall physical picture regarding the gelation process has been proposed by combined experimental and theoretical approaches, which may pave the way for on-target designing manifold NMFs for various applications.

1. R. Du, Y. Hu, R. Hübner, J.-O. Joswig, X. Fan, A. Eychmüller, Sci. Adv. 2019, accepted.

P019 **Mo 17:00 - 18:30**

Analytical Ultracentrifugation based Quantification of the Packing Density of Linear Alkanes Inside Electric Arc SWCNTs

Jeffrey Fagan[1]

[1] *NIST, Gaithersburg, Maryland, USA*

The effects of confinement on the transition from bulk-like to atomic scale molecular packing is of great current interest. For studying the effects of packing at the nanoscale in a 1-D geometry, confinement inside single-wall carbon nanotubes (SWCNTs), well-defined cylindrical structures of sp^2-bonded carbon, has been of particular interest. As such, a variety of physical experimental methods and computational experiments have reported on the quantity or structure of adsorbed molecules inside SWCNTs, but by methods probing heterogeneous nanotube powders or without valid experimental references.
In this contribution we report the precise determination via analytical ultracentrifugation (AUC) of the packing density of linear alkane molecules inside SWCNTs of ~1.45 nm in diameter, fixing a reference point for future computational and experimental efforts. Comparison of density differences from isotopic alkane-filled variants, along with empty and water-filled SWCNTs, suggests near bulk like densities for both eicosane and water filler molecules despite the strong confinement, $\approx$ 1.1 nm diameter, of the SWCNT interior. These results provide specific constraints to analytical and computational models of SWCNT filling and the diameter of transition to pseudo-bulk behavior.

P021 **Mo 17:00 - 18:30**

Separation of Large Diameter Single Walled Carbon Nanotubes using Aqueous Two-Phase Extraction

Benjamin Flavel[1], Han Li[1], Georgy Gordeev[2], Oisin Garrity[2], Selvasundaram Pranauv[1], Anirudh Peyyety[1], Sofie Cambré[3], Wim Wenseleers[3], Ralph Krupke[1,4], Stephanie Reich[2], Ming Zheng[5], Jeffrey Fagan[5]

[1]*Karlsruhe Institute of Technology, Karlsruhe, Germany*
[2]*Department of Physics, Freie Universität Berlin, Berlin, Germany*
[3]*Physics Department, University of Antwerp, Antwerp Belgium*
[4]*Institute of Materials Science, Technische Universität Darmstadt, Darmstadt, Germany*
[5]*National Institute of Standards and Technology, Gaithersburg, USA*

Recently we have shown that the aqueous two phase method to separate single-wall carbon nanotubes (SWCNTs) can conveniently be modulated by pH and that (n,m) pure fractions can be obtained in 1, 2 or at the most 3 steps. Using alkane- filled ($\epsilon \approx 3$) SWCNTs to improve the observability of their optical properties and simplify spectroscopic analysis, we now build upon our approach using the titration of acid into the two-phase system to extract several large diameter, single chirality SWCNTs from the arc-discharge raw soot with a diameter spanning $\approx$ 1.4 nm – 1.7 nm. We show that the unique surfactant shell around certain species allows for their discrimination from the raw material and their separation in 2 steps. Metallic, semiconducting and also enantiomer separation is demonstrated as well as an insensitivity to the raw material used. All fractions have been characterised with Raman and photoluminescence-excitation contour maps and the enantiomers with circular dichroism spectroscopy.

P023 **Mo 17:00 - 18:30**

Characterization of the purity of sorted SWCNT samples by comparing absorption, resonant Raman scattering and PLE spectroscopy with HR-TEM.

Salome Forel[1], Alice Castan[2], Joeri Defillet[1], Dmitry Levshov[1], Frederic Fossard[2], Wim Wenseleers[1], Sofie Cambré[1], Annick Loiseau[2]

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[2] *Laboratoire d'Etude des Microstructures, ONERA-CNRS, Chatillon 92322, France*

Single-wall carbon nanotubes (SWCNTs) possess unique electronic and optical properties, strongly dependent on their exact chiral structure. Recent progress in the structure sorting or the selective synthesis of specific SWCNT chiralities, with increasing chiral purity, demands an effective characterization methodology to be developed. Very often, fluorescence-excitation (PLE) spectroscopy is used to assess the chirality distribution in a sample, but PL quantum efficiencies are structure-dependent and depend strongly on other factors such as the specific internal and external environment of the SWCNTs. In this work, we systematically compare the intensity chirality distribution obtained from three different optical spectroscopic techniques, i.e. absorption, PLE and wavelength-dependent Raman scattering spectroscopy, with the chirality distribution obtained from high-resolution transmission electron microscopy for both sorted and unsorted HiPco SWCNTs. This combined approach allows for identifying the advantages and disadvantages of each technique, and demonstrates that information from all is important for a reliable characterization of SWCNT chirality distributions.

P025 **Mo 17:00 - 18:30**

Comprehensive study on the device performance of ultra-scaled CNTFETs

Florian Fuchs[1,2,3,4], Anibal Pacheco-Sanchez[4,5], Andreas Zienert[1,2], Sven Mothes[4,5], Martin Claus[4,5], Sibylle Gemming[1,3,4], Jörg Schuster[1,2,4]

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We study ultra-scaled carbon nanotube based field-effect transistors (CNTFETs) with channel lengths down to 5.1 nm. Computationally expensive atomistic quantum transport simulation (AQS) as well as numerical device simulations (NDS) are employed (Pacheco-Sanchez et al., IEEE TNANO 17, 100, 2018).

The NDS approach is critically tested and verified by comparing the results with the more expensive AQS approach. A simplified device with ohmic-like contacts is studied for this purpose, consisting of an (16,0)-CNT. We demonstrate that tunneling processes in the transistor are adequately described by the NDS approach and discuss deviations, which we attribute to a different description of the contact physics.

Having verified the NDS, we apply it to compare different device architectures with Schottky contacts, including gate-all-around, buried gate, and top-gate designs. Different figures of merits such as the switching speed, the subthreshold slope, and the Ion/Ioff ratio are compared. It is shown that the buried gate CNTFET is the most suitable structure for high performance logic applications. Also the benefits of having doped spacer regions are demonstrated. Structural changes such as displaced gates and feedback gates are also studied towards improving the device performance.

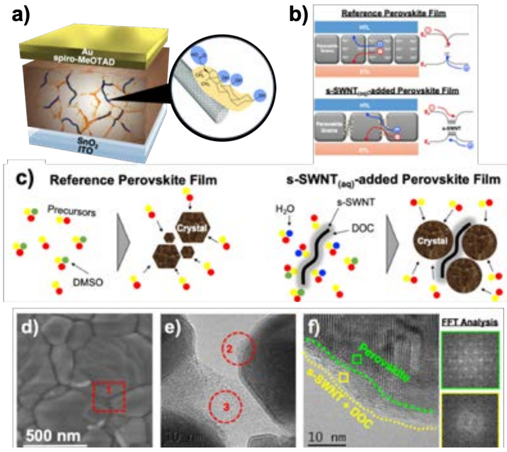

Fig. 1: (a) Exemplary device structure used in AQS. The contacts are n-doped, yielding Ohmic-like contacts. (b) Device characteristics for CNTFETs with Schottky contacts and with different gate architectures.

P027 **Mo 17:00 - 18:30**

Covalent honeycomb networks comprising triptycene and polyphenyl

Yasumaru Fujii[1], Mina Maruyama[1], Susumu Okada[1]

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Hybrid networks of sp^2 and sp^3C atoms show interesting variations in their geometric and electronic structures that do not appear in sp^2C materials. Lacking π electrons, sp^3C atoms act as spacers for π electron networks while giving structural flexibility, allowing the materials to form two- and three-dimensional structures. Triptycene is an example of such sp^2/sp^3 hybrid carbon molecule, which possesses a Y-shaped ridged structure consisting of three benzene panels connected via bridgehead sp^3C atoms with fourfold coordination situated at the molecular axis. Following the synthesis of the triptycene polymers containing phenyl groups, in this work, we aim to investigate the energetics and electronic structure of the triptycene polymers in terms of phenyl conformations and length, using the density functional theory. Our calculation showed that the triptycene polymers are energetically stable with a total energy similar to that of an isolated benzene. The polymers are semiconductors with a direct band gap of about 2eV, which is inversely proportional to phenyl length. The polymers possess peculiar electronic band structures in both the valence and conduction states originating from the kagome topology of sp^2 hydrocarbon networks.

P029 **Mo 17:00 - 18:30**

Efficient CVD Growth of Single-Wall Carbon Nanotube Carpets Using Industrial Gaseous Waste as a Feedstock

Placidus Amama[1], Haider Almkhelfe[1], Xu Li[1], Rahul Rao[2]

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[2]*Air Force Research Laboratory, Materials and Manufacturing Directorate, Wright-Patterson AFB, OH 45433, United States*

A gaseous product mixture from Fischer-Tropsch synthesis (FTS-GP) has been utilized as an efficient feedstock for growth of high-quality, well-aligned, single-wall carbon nanotube (SWCNT) carpets of millimeter-scale heights on Fe and (sub) millimeter-scale heights on Co catalysts via chemical vapor deposition (CVD). Growth conducted at optimal temperatures for Co and Fe catalysts yielded predominantly SWCNTs that are largely free of carbon impurities. Growth on Fe is characterized by a growth rate of ~50 μm/min and catalyst lifetime that is longer than 90 min, with the catalyst showing no decay of activity. In contrast, growth on a Co catalyst shows a lifetime of ~60 min, with a slower growth rate of ~7μm/min. Resulting area densities of SWCNT carpets grown on Fe and Co catalysts, determined by the weight-gain method, were 1.0 × 10^{12} and 6.0 × 10^{12} cm^{-2}, respectively. The catalyst lifetime and area densities of SWCNTs are among the highest achieved on standard catalysts. Unlike SWCNT carpet growth involving conventional feedstocks (such as $C_2\,H_2$, C_2H_4, and CO), growth rate and density of SWCNTs on Fe are less sensitive to the FTS-GP fraction and thus allow for relatively easy optimization and scale-up.

P033 **Mo 17:00 - 18:30**

Brightening of Long, Polymer-Wrapped Carbon Nanotubes by Large Scale sp^3 Functionalization

Felix Berger[1,2], Tobias Kutsch[3], Tim Nowack[1], Jan Lüttgens[1,2], Sebastian Lindenthal[1], Lucas Kistner[1], Lukas Bongartz[1], Jana Zaumseil[1,2]

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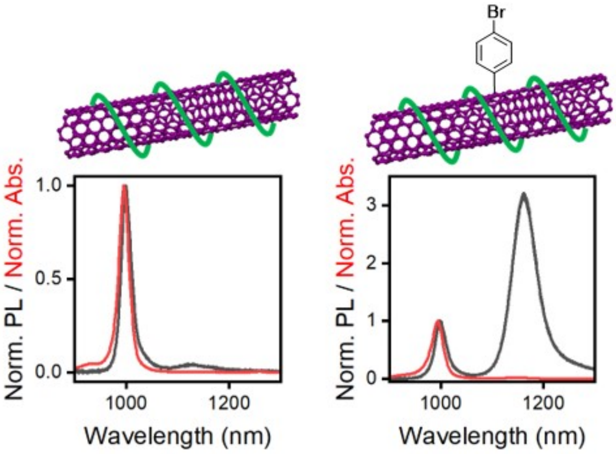
Narrowband emission in the near-infrared and electrical generation of excitons make semiconducting single-walled carbon nanotubes (SWNTs) desirable materials for light-emitting devices (Adv. Mater. 2018, 30, 1706711). Up to now, the efficiency of these devices has been limited by the low photoluminescence quantum yield (PLQY) of SWNTs. To tackle these shortcomings, the controlled introduction of sp^3 defects as exciton trapping sites emerged; leading to red-shifted emission, longer exciton lifetimes and higher PLQYs. However, the synthetic methods to achieve the required low-level functionalization are limited to aqueous dispersions of SWNTs with often very short tube lengths. Here, we report a method for simple and large scale sp^3 functionalization of polymer-wrapped SWNTs in organic, non-halogenated solvents, thereby making it compatible with nanotubes dispersed by shear-force mixing. The low density of exciton quenching sites on shear-mixed SWNTs (Carbon 2016, 105, 593) enables efficient channeling of excitons to emissive defect sites and absolute PLQYs of 4 % for dispersions of long and polymer-wrapped (6,5) SWNTs in toluene. The resulting access to large quantities of high-quality sp^3-functionalized SWNTs facilitates their application in thin film optoelectronic devices.



P035 **Mo 17:00 - 18:30**

Growth of vertically aligned carbon nanotubes on aluminium substrate at low temperature through a one-step thermal CVD process

Antoine Combrisson[1], Fabien Nassoy[2], Mathieu Pinault[1], Cécile Reynaud[1], Emeline Charon[1], Martine Mayne-L'Hermite[1]

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This study addresses the vertically aligned carbon nanotubes (VACNT) growth on specific substrates by thermal aerosol assisted CCVD at low temperature (LT). This one-step continuous process is based on the simultaneous injection of catalytic and carbon precursors into a reactor to form in-situ catalytic particles leading to the VACNT growth. It has initially been developed at high temperature (800-850 °C) [Pinault et al 2005, Castro et al 2013] and is easily scalable. Recently it has been adapted to grow VACNT on Al foils to fabricate ultracapacitor electrodes, requesting a lower process temperature [Nassoy thesis 2018].
According to our previous work, hydrogen adjunction in the gas phase promotes the catalyst precursor decomposition at LT. Using acetylene as a carbon precursor is more favorable for decomposition at LT. Recent results enabled to obtain clean, long and dense VACNT at LT with growth rates at the best level of state of the art for multi-step assisted CVD. However, a decrease in growth rate and a catalytic particle poisoning are observed for long time synthesis, inducing a carpet height caping. The main goal is to strengthen our understanding of VACNT growth at LT and to identify mechanisms involved, in order to have a better control of the growth process.

P037 **Mo 17:00 - 18:30**

In situ PANI/MWNTs nanocomposites hydrothermal synthesis

Fahima Djefaflia[1,2], Ouanassa GUellati[1,2], Assia Nait-Merzoug[1,2], Aicha Harat[1], Simon Detriche[3], Zineb Mekhalif[3], Mohamed Guerioune[1]

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The preparation of conductive polymer nanocomposites consisting of nanofiller, such as carbon black, carbon nanotubes (CNTs) or graphene, with enhanced properties compared to pure polymers has recently become a popular topic in nanomaterials science [1-3].

In this investigation, nanocomposites based of Polyaniline (PANI) and MWNTs were synthesized via in situ hydrothermal method, in the presence of the ammonium persulfate (APS) and hydrochloric acid (HCl) as oxidant and dopant, respectively. The success of the PANI/MWNT nanocomposites synthesis was proved using x-ray diffraction (XRD), Fourier-Transform Infrared (FTIR), Raman spectroscopy, Field Emission Scanning Electron Microscopy (FE-SEM) and Transmission Electron Microscopy (TEM) techniques, Brunauer–Emmett–Teller (BET) method, Thermal-Gravity analysis (TGA) and (XPS) analysis.

P039 **Mo 17:00 - 18:30**

Self-assembly of polymer-grafted carbon nanotubes: controlling interactions from the nano to the macroscale

Martha V. Escarcega-Bobadilla[1], Gustavo A. Zelada-Guillen[1]

[1] *School of Chemistry, National Autonomous University of Mexico (UNAM)*

Chemical modification of carbon nanotubes to selectively introduce functional groups either at the sidewalls or at the termini has been recently explored as a tool to achieve nanomaterials with enhanced properties at the nanoscale. However, the possibility to translate these nanoscale physicochemical characteristics into macroscale tunable attributes with potential applications at industrially viable conditions has remained a challenge.

With this in mind, we employed a selective chemical oxidation synthesis to introduce useful reactive sites either at the termini or at the sidewalls of pristine multiwalled carbon nanotubes. This strategy was carried out in order to differentially introduce polymer chains to different regions in the nanostructures, thus making it possible to confer anisotropic supramolecular interactions at the nanoscale.

Herein, we present a family of grafted and non-grafted 1D nanostructures, which autonomously yielded spatially oriented self-assemblies at the microscale and, depending on the process conditions and nanotube history, spontaneously organized mesoscale networks. Moreover, these structures were easily melt-processed to yield polymer nanocomposites with appealing macroscopic mechanical properties.

P041 **Mo 17:00 - 18:30**

Tuning bimetallic catalysts for a selective growth of SWCNTs

Salome Forel[1], Alice Castan[2], Hakim Amara[2], Ileana Florea[1], Frederic Fossard[2], Laure Catala[3], Christophe Bichara[4], Talal Mallah[3], Vincent Huc[3], Annick Loiseau[2], Costel-Sorin Cojocaru[1]

[1]LPICM, CNRS, Ecole Polytechnique, Palaiseau, 91128 , France
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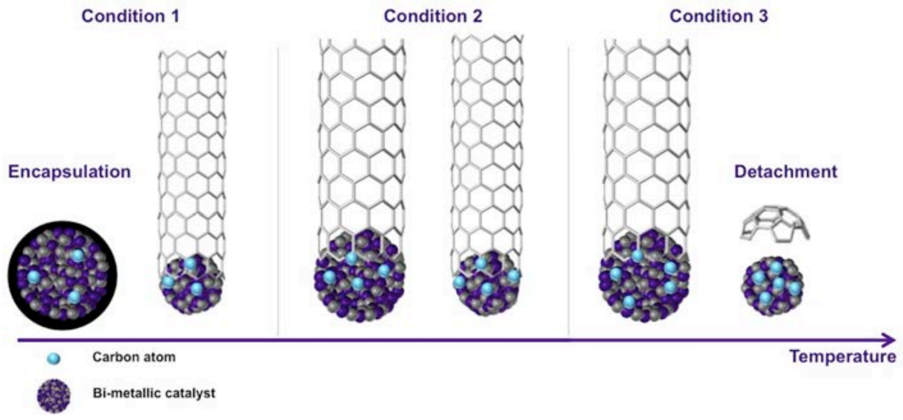
Recent advances in structural control during the SWCNT synthesis rely on the use of bimetallic nanoparticles as catalysts, despite the fact that their exact role is not fully understood. We therefore analyze the effect of the catalyst's chemical composition on the structure of the resulting SWCNTs by comparing three bimetallic catalysts with different thermodynamic properties with respect to carbon (FeRu, CoRu and NiRu). Setting all the CVD parameters except the temperature we demonstrate a global shift of distributions towards larger diameters with increasing temperature. Assuming a tangential growth mode, based on TEM images after growth, we were able to establish a link between the evolution of diameter distributions, not with an increase in the size of the catalyst NPs, but rather with a phenomenon of selective activation of different catalyst size populations in the same initial pool of available catalysts by tuning the growth temperature. We assume that this effect can be correlated with the difference in carbon solubility in NPs according to their size and chemical composition and propose a phenomenological model. This work provides a rational understanding of the key factors that determine SWCNT diameters, providing new elements to grow SWCNTs with defined chiralities.



Schematic view of the proposed mechanism of selective activation of catalyst NPs based on the growth temperature and NP size.

P043 **Mo 17:00 - 18:30**

Growth Mechanism and Controllable Preparation of High-purity Semiconducting Carbon Nanotubes

Jun Gao[1], Zhenxing Zhu[1], Fei Wei[1]

[1]*Department of Chemical Engineering, Tsinghua University, Beijing, 100084,China*

In recent years, the performance of silicon-based integrated circuit(IC) is approaching the physical limit. Carbon nanotube (CNT) is a promising alternative for semiconductor materials. To achieve its large-scale application in IC, there is a big challenge to achieve extremely high semiconducting selectivity.

Based on our previous work, we propose an idea of solving the problem by increasing the length of CNTs. However, it is not completely clear about the growth of decimeter-long CNTs. To illustrated the mechanism, we analyzed the analogy of the electrons of CNTs and laser photons based on non-mass and uncertainty principle, then we proposed a conjecture that the former have a similar restrained volume. Furthermore, we deduced electron restrained volume of CNTs and estimated the growth length limit theoretically.

Then the conjecture was explored experimentally. The statistical results we have collected exhibit similar trend with the model. Our work can provide guide for the growth of ultra-long CNTs with high semiconducting selectivity. Based on the model, the ultra-long growth requires a good linearity, which means the stability of growth environment is essential. Therefore, a large-scale preparation of CNTs by optimizing and stabilizing the growth conditions is undertaking.

P045 **Mo 17:00 - 18:30**

Engineering Polymer Conformation for Efficient Carbon Nanotube Sorting

Theodore Gao[1], Zehao Sun[2,3], Xuzhou Yan[2,4], Zhenan Bao[2]

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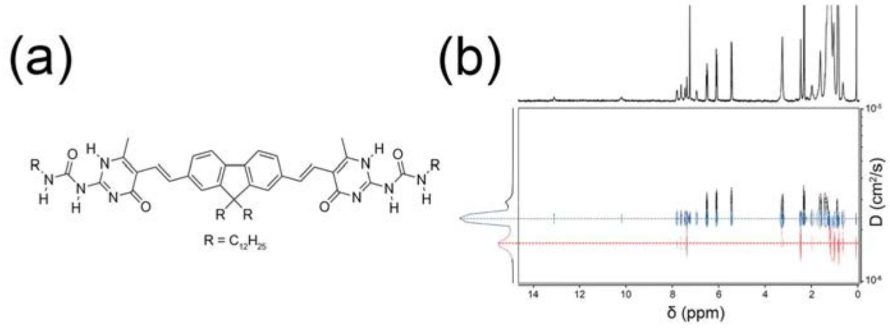
[3] *Peking University/College of Chemistry & Molecular Engineering, Beijing 100871, PRC*
[4] *Shanghai Jiao Tong University/Dept. of Polymer Science & Engineering, Shanghai 200240, PRC*

Polymer sorting is a promising approach to selecting carbon nanotubes (CNTs) by electronic type, offering rapid processing (1-2 hours), high purity (>99%), and excellent sorting yields (>20%). Recent demonstrations have shown that supramolecular polymers are effective and versatile for CNT sorting. They can be easily removed from CNTs by the addition of a bond-disrupting agent, enabling the fabrication of electronically pristine CNT electronics. The removed polymer can also be recycled without any kind of chemical resynthesis, which has significant advantages for large-scale CNT sorting.
Optimization of polymer structure for CNT sorting has been explored extensively in the past decade, though primarily for conjugated polymers. A similar optimization is desired for supramolecular polymers but requires improved understanding of polymer-CNT dynamics. Towards this end, we have applied a suite of characterization techniques to CNT solutions sorted by a fluorene-based H-bonding polymer. We discovered that this polymer exhibits ring-chain tautomerism – the polymer can exist either as linear chains or as cyclic rings, which have differing degrees of CNT sorting efficacy. Altering the conformation of the polymer was found to double the sorting yield without compromising purity.



(a) Chemical structure of the fluorene-based H-bonding polymer. (b) Diffusion-ordered NMR spectra showing the coexistence of distinct species in the polymer solution. Blue indicates linear chains while red indicates cyclic rings.

P047 **Mo 17:00 - 18:30**

A cross-linked graphene/diketopyrrolopyrrole hybrid with intriguing far-red to near infrared absorption features

Teresa Gatti[1,2,3]

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[2]Center for Materials Research (LaMa), 35392 Giessen, Germany
[3]Institute of Physical Chemistry, Justus Liebig University, 35392 Giessen, Germany

The combination of organic dyes with graphene-based materials can bring to novel hybrid species with peculiar optoelectronic properties.

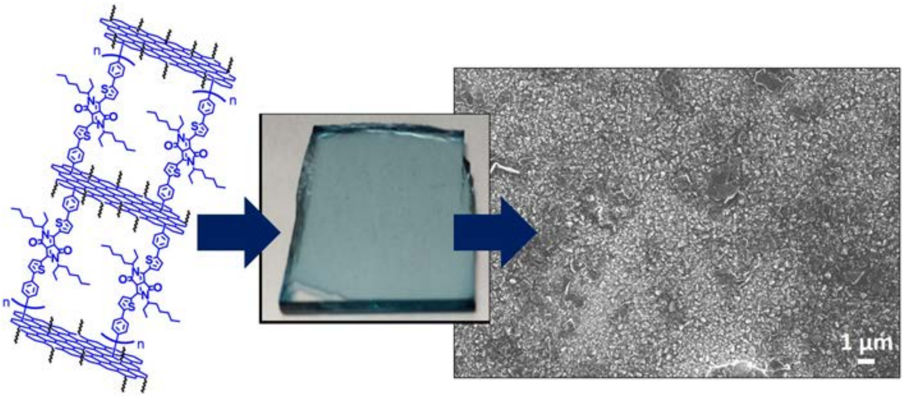
In the past, we investigated the covalent anchoring of a donor-π-acceptor (D-π-A) dye to reduced graphene oxide and applied the resulting hybrid as a photosensitizer in standard dye sensitized solar cells.(1,2)

We present here the complete physico-chemical characterization of a recently prepared covalent functional nanocarbon hybrid obtained by combining a bi-functional diketopyrrolopyrrole dye (DPP, again a D-A system) with few layers graphene coming from the mechanical exfoliation of graphite.

This species is a 3D material and can be intended as a sort of DPP polymer containing graphene, therefore a covalent composite. It has outstanding filming properties and features a continuous absorption from UV to NIR (due to the graphene moiety), coupled to a further peculiar feature in the far-red to NIR region.

The hybrid holds great promise for future use in technological applications requiring photoactive and conductive constituents.

1) T. Gatti, N. Manfredi et al.; Carbon, 2017, 115, 746-753.
2) P. Guarracino, T. Gatti et al.; Phys. Chem. Chem. Phys., 2017, 19, 27716-27724.



P049 **Mo 17:00 - 18:30**

Synthesis and characterization of gold-decorated nanosheets from liquid-exfoliated WS_2

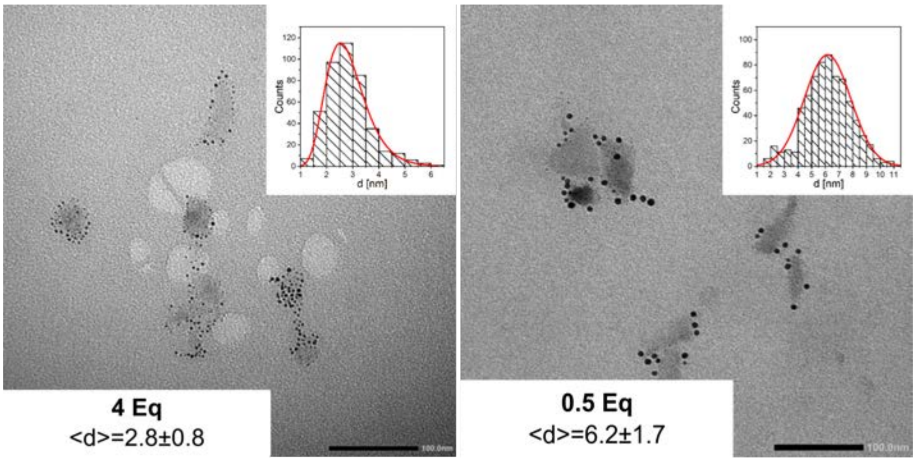
Sebastian Grieger[1], Claudia Backes[1]

[1] *Applied Physical Chemistry, Univsertiy of Heidelberg, Heidelberg, Germany*

Liquid-phase exfoliation has become a popular method for exfoliation of layered crystals owing to its high throughput and universal applicability to numerous compound classes, like graphene and transition metal dichalcogenides (TMDs). The produced colloidal dispersions are polydisperse, so a size-selecting process such as liquid cascade centrifugation is required to yield dispersions with defined nanosheet dimensions. They can be used to investigate size-dependent properties of the materials[1] or to explore further functionalization.[2] For example, WS_2 is capable of spontaneously reducing chloroauric acid (CA) to form gold nanoparticles (AuNPs).[3]

In our work, we present a method for the controlled growth of AuNPs on WS_2 using CA. The acid is added dropwisely to a liquid exfoliated, size-selected dispersion. Work up of the resulting material is done via centrifugation. This technique does not only allow for the production of preferentially edge-decorated nanosheets, it also enables the extraction of predominantly monolayers (up to ~90% after workup). Utilizing transmission electron microscopy, we could show, that the AuNPs size and density can be tuned via the used CA concentration.

[1] ACS Nano 2016, 10, 1589.
[2] Chem. Soc. Rev. 2018, 47, 6845.
[3] NPJ 2D Mat. App. 2018, 1, 43.



TEM images of the gold-decorated WS_2 nanosheets with high (left) and low (right) chloroauric acid concentrations. Inset: Statistical evaluation of nanoparticle sizes of the corresponding decorated nanosheets.

P051 **Mo 17:00 - 18:30**

Synthesis condition of CNT arrays for fabricating the double-walled carbon nanotube yarns by dry-spinning

Hirotaka Inoue[1], Tomohiro Nakagawa[1], Paneer Selvam Karthik[1], Masaki Hada[1,2], Takeshi Nishikawa[1], Yoshifumi Yamashita[1], Yasuhiko Hayashi[1]

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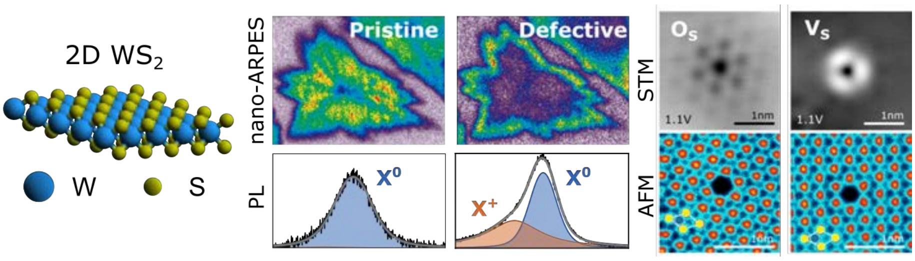
[2]*University of Tsukuba, Ibaraki 305-8573, Japan*

The carbon nanotube (CNT) yarn consisting of mainly double-walled CNTs (DWCNTs) has several superior properties, such as high physical properties, chemical stability, environmental tolerance and realistic-cost for realistic bulk-scale devices. Very few reports have been published regarding the DWCNT yarns because the synthesis window for the dry spinnable tall and dense DWCNT arrays is narrow. Here, a parametric approach was carried out on both synthesis temperature and time of synthesis to identify the spinnability of the CNT arrays. Based on the relationship between the bulk-density, height and the spinnability of CNT arrays, the results revealed that there are optimum values for spinnable CNT arrays in both their height (150–300 μm) and bulk-density (80–150 mg/cm^3). Briefly explaining that the spinnable DWCNT arrays are synthesized by the precise temperature controlling at the initial stage of CNT synthesis. We also characterized the CNT tube diameter and the surface roughness of the iron catalyst layer as a function of particularization temperature. The precise temperature control helps to facilitate the suitable surface where the catalyst particles are sufficiently dispersed and lead to successful synthesize of the spinnable CNT arrays containing a majority of DWCNTs.



The schematics of dry-spinning method of DWCNTs.

P053 **Mo 17:00 - 18:30**

Isolation of carbon nanotubes with narrow-band light emission characteristics in a single step

Dawid Janas[1], Edyta Turek[1], Tomohiro Shiraki[2], Tomonari Shiraishi[2], Tamehito Shiga[2], Tsuyohiko Fujigaya[2]

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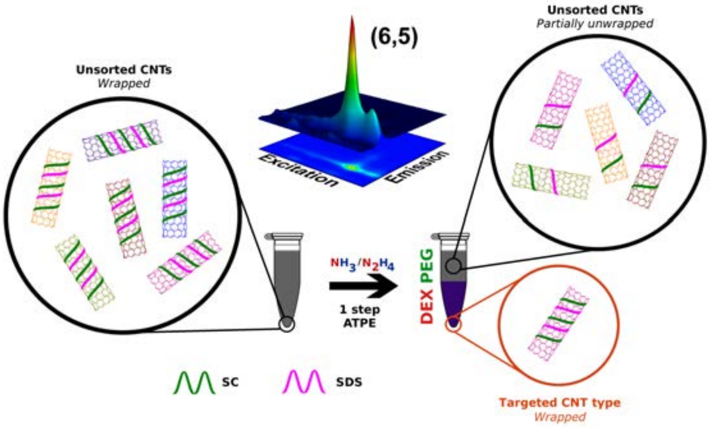
Carbon nanotubes have shown a wide range of promising properties on many fronts [1], but the inability to fully control their chirality still remains a major impediment factor for their implementation. Recently, the community has come to the conclusion that post-synthesis sorting of carbon nanotubes could be the solution, and so an arsenal of techniques has been developed to reach this goal [2]. Unfortunately, despite their obvious merits, to obtain carbon nanotubes of certain chirality tedious multistep processing must be executed. In this presenation, we would like to show how we have adopted and modified the method of aqueous two-phase extraction [3] to aim for separation of selected carbon nanotube type in a single step [4]. We were able to separate minor chiral species from the unsorted CNT mixture with very high efficiency without any unnecessary iterations. What is interesting, we observed emergence of new optical features under certain circumstances.

References:
[1] M.-F. Yu et al., Science 287, 2000, 637.
[2] D. Janas, Mater. Chem. Front. 2, 2018, 36.
[3] J. Fagan et al., Adv. Mater. 26, 2014, 2800.
[4] E. Turek et al., Sci. Rep. 9, 2019, 535.



Single-step separation of carbon nanotubes

P055 **Mo 17:00 - 18:30**

Rheological and thermal properties of IoNanoFluids prepared from various morphology CNTs synthesized using selected organometallic catalysts

Rafał G. Jedrysiak[1], Bertrand Józwiak[1], Anna Kolanowska[1], Anna Kuziel[1], Marzena Dzida[2], Sławomir Boncel[1]

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[2]University of Silesia in Katowice, Bankowa 14, 40-007 Katowice

Recently dispersions of carbon nanotubes (CNTs) in ionic liquids (ILs) have attained a raised scientific interest mainly due to their very interesting rheological, thermal and electrical properties. This unusual combination of properties of IoNanoFluids could be very useful in many technical and industrial applications, e.g. as heat exchangers and cooling systems, lubricants and polymer additives. Nevertheless, to date IoNanoFluids still remain not fully investigated and analysed.

We decided to examine a wide range of dispersions of CNTs of different morphology and concentrations in commercially available and in-house synthesized ILs. Multi-walled CNTs used in our experiments were synthesized via catalytic chemical vapour deposition (c-CVD) method in a horizontal furnace using different metalloorganic compounds as catalysts.

P057 **Mo 17:00 - 18:30**

Sulfur-source independent production of predominantly single-wall carbon nanotube fibres

Adarsh Kaniyoor[1], John Bulmer[2], Thurid Gspann[1], Jenifer Mizen[1], James Ryley[2], Jeronimo Terrones[1], Alan Windle[1], James Elliott[1]

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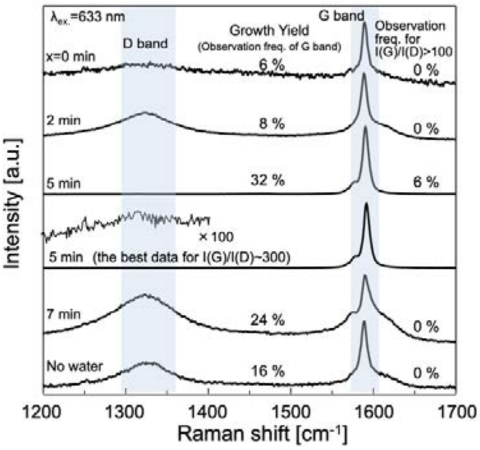
Continuous production of carbon nanotube (CNT) fibres in a single step is now routinely achieved by methods based on floating catalyst chemical vapour deposition (FC-CVD), with mass yields of around 1 g/day. However, most processes produce fibres composed mainly of multi-wall CNTs (MWCNTs), or single-wall CNTs (SWCNTs) with low-yields. In this work, we present a new strategy to obtain larger yields of high-quality fibres predominantly composed of SWCNTs, independent of the choice of sulfur precursor. At a sufficiently low sulphur-to-iron atomic ratio and high flow rates, the fibres exhibit highly intense RBMs (radial breathing modes) and large asymmetry in the G band, both consistent with the presence of small-diameter metallic CNTs. By correlating these measurements with thermogravimetric and Raman data, we show that the increase in RBM intensity is associated with a change in the quantity of the dominant nanotube species. We explain the phenomenon via fluid flow modelling – an increased jetting of the carrier gas changes where individual precursors breakdown and thereby affects the type of nanotubes produced. Further, we also show the choice of carbon source does not affect the type of CNTs produced but the impurity content, and therefore, overall fibre quality.

P059 **Mo 17:00 - 18:30**

Efficient synthesis of defect-free single-walled carbon nanotube from solid nanoparticles by chemical vapor deposition at high-temperature

Yoshihiro Kobayashi[1]

We successfully grew highly crystalline single-walled carbon nanotube (CNT) from solid seeds of carbon nanoparticle (CNP) using chemical vapor deposition (CVD) process at high temperature around 1000ºC. The CNP seeds composed of sp^2-carbon shells are obtained by thermal transformation of purified nanodiamond without metal contamination, and are completely stable without aggregation, contrary to conventional metal nanoparticles catalyst, even at high temperature, resulting in preserving the catalytic activities as the growth seed of CNT. The water addition in the growth gas and two-stage growth with varying the growth temperature were significantly effective in preventing deposition of contaminations such as amorphous carbon, and improving the growth efficiency of CNT. Delay time to introduce the water from the beginning of the growth and the temperature of the first growth stage were particularly influential in improving growth efficiency. The analysis of Raman spectra in the RBM region indicates that no additional cap structure was nucleated after the water addition. After the optimizing the growth condition including the water concentration, we achieved the growth of almost defect-free CNTs where I(G)/I(D) ratio up to 300 was observed in the Raman spectra.



Typical Raman spectra of CNTs grown from CNP with various delay time for water addition x min. The spectra were normalized by G band intensities. All spectra were averaged from a lot of spectra more than 50.

P061 **Mo 17:00 - 18:30**

Friedel-Crafts alkylation of carbon nanotubes toward synthesis of thermally active components of IoNanoFluids

Anna Kolanowska[1], Rafał Jedrysiak[1], Bertrand Józwiak[1], Anna Kuziel[1], Marzena Dzida[2], Sławomir Boncel[1]

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Carbon nanotubes (CNTs) tend to self-assemble into bundles which are held together by van der Waals forces. In order to fully take advantage of CNTs, separation of the individual nanotubes is the essential step. It is therefore important to functionalize CNTs with moieties enabling transfer of CNTs' unique properties to the macroscopic scale materials.

Friedel-Crafts alkylation is Lewis acid catalyzed electrophilic aromatic substitution allowing the synthesis of alkylarenes via alkyl halides. In the case of CNTs, this method provides new C-C bond formation on CNT surface. The introduced hydrophobic chain may be used as the linker for further functionalization and for reduction of thermal contact resistance between CNTs. For this reason, this reaction could be used to improve CNTs dispersibility while maintain wall integrity.

In our studies, we investigated the effect of alkyl chain length on CNT dispersion stability in ionic liquids (ILs) and thermal properties. Functionalization caused the disruption of intermolecular interactions while the electrostatic attractions between the CNT surface and IL led to stable dispersions. The modified CNTs were comprehensively analyzed using TGA, TEM and Raman spectroscopy.

P063 **Mo 17:00 - 18:30**

Synthesis and thermal properties of helical CNTs ionic liquid nanofluids

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Nanofluids have attained a large scientific interest being adopted as heat transfer media or energy storage systems. Ionic liquids (ILs) are eco-friendly solvents and their thermophysical properties fulfill the requirements of heat transfer fluids. Combining those with carbon nanotubes (CNTs) one could obtain IL nanofluids (IoNanoFluids) with enhanced thermal properties. Herein, we propose the synthetic routes of helical carbon nanotubes (h-CNTs) via catalytical chemical vapour deposition (c-CVD) method using ethanol or toluene as a carbon source and catalyst nanoparticles (Co, Ni, Zn, Cu, Fe, In) deposited on the tetraethoxysilane (TEOS) or silica gel (SiO_2-gel). Manipulating the diameter of growing nanoparticles one may influence on the curvature and diameter of the obtained h-CNTs. The structure and physicochemistry of nanomaterial was confirmed using SEM, TEM, TGA and Raman spectroscopy. Subsequently, the prepared IoNanoFluids based on alkylated imidazole ILs containing h-CNTs and other types of CNTs different in geometry and aspect ratio were characterized using optical microscope and cryo-TEM. Finally, the dependence between IL types, concentration and geometry of CNTs versus stability, thermal conductivity, heat storage and rheological properties were determined.

P065 **Mo 17:00 - 18:30**

Synthesis of thin multi-walled carbon nanotubes with narrow diameter distribution induced from molybdenum-cobalt alloy catalyst

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Research on the synthesis of carbon nanotubes (CNTs) with uniform physical properties has been receiving many interests in various scientific fields. To dramatically enhance the properties, in particular, CNTs with uniform diameter are strongly required because each diameter of CNTs has intrinsic properties. In other words, various diameters of the CNTs cause non-uniform properties. However, the control of nanoscale materials with specific properties demands a great deal of effort, and substantive progress is slow because the results are unpredictable. In this study, we fabricated molybdenum (Mo)-Cobalt (Co) alloy catalyst with constant diameter of ~5 nm for synthesizing thin multi-walled carbon nanotubes (MWNTs) with narrow diameter distribution. In addition, our experimental approach is simple without complex molecular designing of catalyst. This reasonable study is expected to open a new perspective of synthesizing specific controlled CNTs.

P067 **Mo 17:00 - 18:30**

Facile Catalyst Deposition Using Mist for Fluidized-Bed Production of Sub-Millimeter-Long Carbon Nanotubes

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Fluidized-bed chemical vapor deposition (FBCVD) has enabled mass-production of carbon nanotubes (CNTs) [1]. By using spherical ceramic beads as catalyst supports and depositing Fe/AlOx catalyst on them, we have realized semi-continuous production of sub-millimeter-long CNTs [2,3]. To improve the controllability over catalysts, a new method of catalyst deposition on ZrO_2beads in fluidized bed by feeding catalyst solution mist is reported. Low-cost $Fe(NO_3)_3$and $Al(NO_3)_3$aqueous solutions mist is supplied and deposited on the beads by using fluidized-bed technology. CNTs of ca. 7 nm in diameter, triple-wall on average, 0.6 mm in length are synthesized with a yield of 16.6 mgCNTs/gBeads. These results benefit from the uniform catalysts realized by mist-deposition and proper amount of Al, which is considered to play an important role in controlling the diffusion and aggregation of Fe atoms (Fig. 1). These results indicate that mist deposition to be a facile and effective method toward high-yield production of CNTs.

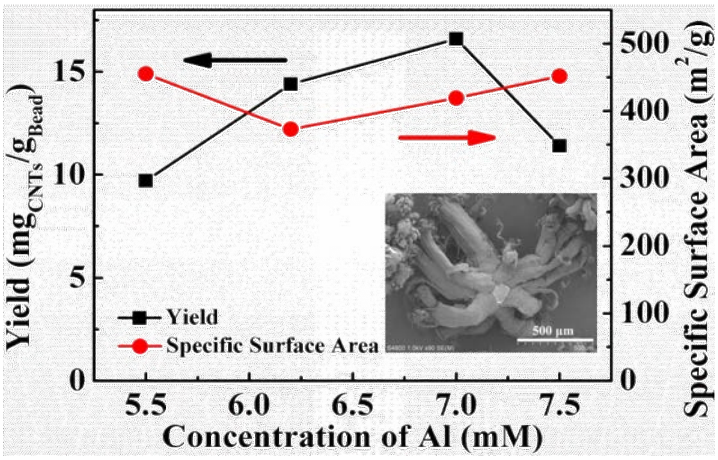

Fig.1 Effect of Al source concentration on the yield and specific surface area of CNTs. Insert figure: SEM image of CNTs on the beads.

P069 **Mo 17:00 - 18:30**

Carburization of Fe/Ni Bimetal Catalyst for Efficient Growth of Single-walled Carbon Nanotubes

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Scale-up production of single-walled carbon nanotubes with high quality and purity are in pursuit, since the subsequent post purification treatment of residual metal or amorphous carbon were complicated and would restrict the further application. Here, we reported that the slight pre-carburization of the Fe/Ni bimetal catalysts, as a compatible method , could be utilized to efficiently synthesize pure SWNTs on various supports. The carburization reaction at lower temperature for Fe/Ni bimetal with good catalytic graphitization performance and moderate carbon solubility would enhance the activity greatly. By using micro-quartz sands as recyclable supports, high-quality SWNTs with yield of 50 mg/h were prepared with 60% metal precursors utilization, 81% carbon source utilization and only 0.12% (m/m) metal residues. Taking advantage of carburized Fe/Ni bimetal catalysts and appropriate supports would make it accessible to balance the quantity, purity and quality among SWNTs growth. Furthermore, this method would provide a straightforward pathway to strongly combine SWNTs and diverse composite materials for further potential applications.

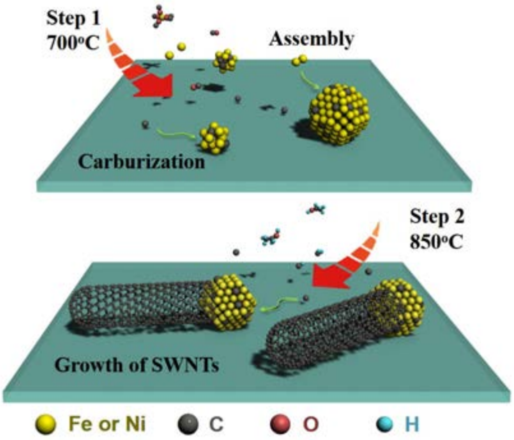

Figure1. Schematic showing the procedure designed for deposition of Fe/Ni bimetal catalysts and directly growth of SWNTs.

P071 **Mo 17:00 - 18:30**

Multiple-cycle Deposition of Pure Metal Catalyst to Grow High-density SWNT Arrays

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Single-walled carbon nanotube (SWNT) has been considered as one of the most promising candidate to replace silicon in integrated circuits. The density of SWNT arrays is essential which can limit the performance of devices. Recent years, many efforts have been achieved to grow high-density SWNT arrays by controlling the morphology and dispersion of catalysts. However, it is still a challenge to obtain SWNT arrays with a density more than 80 SWNTs µm-1 on quartz. Herein, we develop a new method of multiple-cycle deposition of pure metal catalyst and obtain horizontally aligned SWNT arrays with density more than 80 SWNTs µm-1 on quartz. The catalysts obtained by vapor deposition have very high reactivity and can be removed by a short time annealing, which is essential to multiple-cycle growth. Besides, by controlling the cycle times, we can synthesis SWNT arrays with different density varying from 10-80. Using these arrays, we can get a relation between current density and density of SWNTs, which indicates the potential of SWNTs in nanoelectronics.

P105 **Mo 17:00 - 18:30**

Mechanism of Global Alignment of Carbon Nanotubes during Vacuum Filtration

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For real-world applications of carbon nanotubes in electronics, photonics, and thermoelectrics, it is crucial to find a way to prepare macroscopically ordered nanotube assemblies, preserving the extraordinary one-dimensional properties of individual nanotubes. Recently, we have developed a simple and well-controlled method for fabricating wafer-scale monodomain films of highly aligned carbon nanotubes based on spontaneous alignment that occurs during vacuum filtration. However, the mechanism of such global alignment has not been fully understood. Here, we report new findings regarding the nanotube alignment direction with respect to the surface morphology of the filter membrane used in the vacuum filtration process. Through atomic force microscopy, we observed that a large number of parallel grooves exist on the surface of all membranes we used. Furthermore, using polarization-dependent optical transmission measurements, we found that the groove direction dictates the direction of the resulting global alignment of nanotubes.

P073 **Mo 17:00 - 18:30**

Ring GQDs in Fluorinated Graphene Matrices

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We report about new types of QDs in graphene films functionalized by atoms or molecules. Rapid heating of the local area formed pore during ion beam influence leads to defluorination around pore -Ring graphene QD surrounded CFx area 1. We studied the fluorine graphene CFx RGQDs with the diameter 1-3 nm in the dielectric CF graphene or C_2F diamane with gap 3.5 or 4.3 eV. The atomic and electronic band structures were investigated by DFT method. Dots in CF are similar to GQD rings. RGQD in C_2F is half-torus formed from two folded graphene rings. Electronic structures change view after creation of a nanopore surrounded by defluorinated area. We computed structures with RGQDs of different forms and estimated electron tunnelling through dielectric bridge between pores. The properties are different from the electronic properties of another known GQDs]. The meshes of RGQDs with period 1.5 nm are presented. The nm width between pores surrounded by CFx areas is enough for detection of their quantum properties. Formation of electronic levels near Fermi energy are associated with the electrons localized in RGQDs. The properties will be useful for applications in electronic and energy-related fields. The work was supported by RFBR 16-29-06201.

1 N Nebogatikova., et al., Nanoscale 10 (2018)

P075 **Mo 17:00 - 18:30**

The Effects of Sulfurization on the MoS_2 Growth

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In order to get a facile 2D molybdenum disulfide (MoS_2), we varied Mo thickness and post-sulfurization flow rate under hydrogen sulfide (H_2S, 5%) and nitrogen (N_2) mixture ambient. Depending on Mo thickness (1 ~ 5 nm) and $H_2S + N_2$ mixture flow rate (250 ~ 500 sccm), resulting MoS_2 thin films are turned out to be isolated or continuous grains, which are triangular and polyhedral. The continuous MoS_2 thin films show energy band gap range from 1.81 eV to 1.86 eV depending on the process condition. In addition, its structure corresponds to a hexagonal structure. From XPS analysis, Mo to S ratio is 1:1.7. This method is relatively easy and facile approach to attain the uniform MoS_2 and can be applicable to other TMD materials.

P077 **Mo 17:00 - 18:30**

Scalable production of graphene using electrochemical exfoliation in compressed reactors

Micah Green[1]

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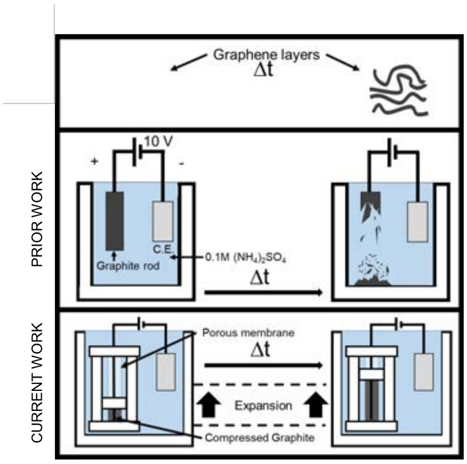
Electrochemical exfoliation is a promising bulk method for producing graphene from graphite; in this method, an applied voltage drives ionic species to intercalate into graphite where they form gaseous species that expand and exfoliate individual graphene sheets. However, a number of obstacles have prevented this approach from becoming a feasible production route; the disintegration of the graphite electrode as the method progresses is the chief difficulty. Here we show that if graphite powders are contained and compressed within a permeable and expandable containment system, the graphite powders can be continuously intercalated, expanded, and exfoliated to produce graphene. Our data indicate both high yield (65%) and extraordinarily large lateral size in the as-produced graphene. We also show that this process is scalable and that graphene yield efficiency depends solely on reactor geometry, graphite compression, and electrolyte transport. The resulting material is significantly less oxidized than typical Hummers' Method graphene oxide and avoids many of the safety and scalability issues associated with graphene oxide production.



(top) Prior electrochemical exfoliation efforts resulted in the graphite working electrode disintegrating during intercalation. (bottom) Schematic of our process for electrochemical exfoliation of graphite in a permeable expandable container.

P079 **Mo 17:00 - 18:30**

Facile Preparation of Thin Film Transistors Based on van der Waals Heterostructures with MoS_2 and Single-walled Carbon Nanotube films

Chao Jiang[1]

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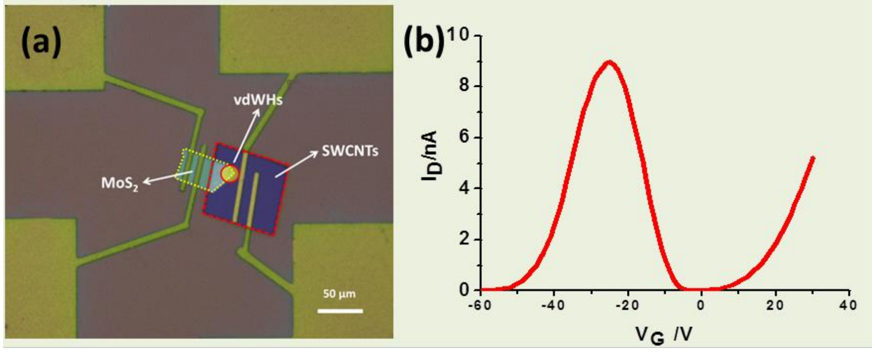
A p-n junction via van der waals (vdW) interaction can be easily realized with stacked p-type and n-type materials without the constraints of epitaxy with lattice match, which hopefully replaces a traditional p-n junction and becomes the important component in future electronics and optoelectronics. Furthermore, single-walled carbon nanotubes (SWCNTs) is an ideal p-type channel material due to its high carrier mobility, high physical and chemical stability, and compatible with low-temperature solution process for large-area flexible electronics.
Herein, we proposed an electron-beam lithography-assisted solution process to fabricate a high performance transistor based on SWCNTs/few-layered MoS_2 van der waals heterostructures with high-quality interface. The as-prepared heterojunction device shows an effective gate tunable property with typical p-n junction anti-ambipolar electrical characteristics. By optimizing dielectric material, an ultra-low voltage drived p-n vdWHs transistor has been realized. The constructed frequency doubler exhibits a good frequency doubling response. The preparation technique developed in this work might realize high performance p-n vdWHs transistors and be expected to obtain applications in large-area flexible integrated circuits.



P081 **Mo 17:00 - 18:30**

Fabrication of Mo6S6 nanowire terminated edges in monolayer molybdenum disulfide

Chuanhong Jin[1], Xiaowei Wei Huang[1], Xujing Ji Wang[1]

[1]*Zhejiang University*

Edge structures provides an additional freedom to tune the materials structure and properties, particularly in two-dimensional materials with reduced dimensionality, and needs precisely tailoring for the desirable applications. In this work, we report the formation of novel Mo6S6 nanowire (NW) terminated edges in a monolayer molybdenum disulfide (MoS_2) via an e–beam irradiation process combined with high temperature heating inside a TEM. Atomic structures of NW terminated edges and the dynamic formation process were observed experimentally. Further analysis shows that NW terminated edge could form on both Mo-zigzag (ZZ) edge and S-ZZ edge which can exhibit even higher stability superior to the pristine zigzag and armchair edge. In addition, the analogous edge structures can be also formed in MoS_2 nanoribbon and other TMDs material such as MoxW1-xSe_2. We believe that the presence of these novel edge structures in 2D and 1D TMD materials may provide novel properties and new opportunities for their versatile applications including catalytic, spintronic and electronic devices.

P083 **Mo 17:00 - 18:30**

Photophysical properties and applications of exfoliated near infrared fluorescent calcium copper silicate nanosheets

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Imaging in the near infrared range of the spectrum is beneficial due to reduced light scattering, absorption, toxicity and autofluorescence. However, there are only few near infrared fluorescent materials known and suitable for biomedical applications. Here, we exfoliate the near infrared fluorescent layered pigment CaCuSi4O10 (known as Egyptian Blue, EB) into nanosheets (EB-NS) via tip sonication. Dimensions of the nanosheets decreased with sonication time < 20 nm in diameter and heights of single EB layers (around 1 nm). The near infrared fluorescence of EB at 910 nm and the fluorescence life-times are retained in EB-NS and the total fluorescence intensity scales with size. Furthermore, we demonstrate that EB-NS display ultra-high photostability (no bleaching) and are extremely bright compared to other nIR fluorophores. The versatility of EB-NS as nIR fluorophores for biological imaging is demonstrated by in vivo single-particle tracking and microrheology measurements in developing Drosophila embryos. Furthermore, EB-NS can be uptaken by plants and used for remote detection. In summary, we introduce 2D CaCuSi$_4$O$_1$0 nanosheets as versatile material for nIR imaging.

P085 **Mo 17:00 - 18:30**

Thermoelectric properties of chemically modified carbon nanotubes: first principles simulations

Nayu Araki[1]

Carbon nanotubes (CNTs) are expected to be potential candidates for flexible thermoelectric materials with high Power Factor (PF). In contrast to high PF, the thermoelectric efficiency of a CNT is not so high because of its high thermal conductivity. Recently, several techniques to reduce the thermal conductivity of CNTs have been proposed. The diazonium salt modification of CNTs is known as one of such techniques. However, the details of influence the diazonium salt modification on thermoelectric properties of CNTs have not clarified yet.
In this work, we theoretically investigate thermoelectric properties of CNTs modified by diazonium salts using the NEGF+DFT method. We clarify the dependence of the coverage of diazonium salts on the electrical conductivity, the Seebeck coefficient and the PF.
As the modification density increases, the sp^3hybridizations acts as scatterers of electrons, so the electrical conductivity decreases greatly. On the other hand, the Seebeck coefficient increases due to a charge transfer from the diazonium salts to the CNT. The PF decreases due to the rapid reduction of electrical conductivity, but ZT is known to be increased by the diazonium-salt modification because of the rapid reduction of thermal conductivity.

P087 **Mo 17:00 - 18:30**

Calculating Lattice Thermal Conductivity of Carbon Nanotubes: A Comparison of Results from Molecular Dynamics Simulation and Boltzmann Tranport Theory

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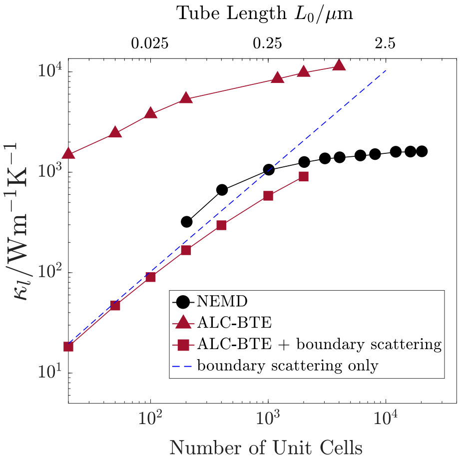
Pristine Carbon Nanotubes (CNTs) exhibit high structural order, rigid sp^2-bonds and a low atomic mass which result in an exceptionally high lattice thermal conductivity (TC). Pinpointing exact TC values of individual defect-free CNTs, however, remains a challenge both experimentally and computationally. The thermal transport properties of ideal CNTs are dominated by phonon-phonon scattering, and a theoretical prediction of TC has to include anharmonic terms in the interatomic potential energy which give rise to phonon-phonon interaction. Here we compare two commonly applied computational approaches that take into account lattice anharmonicity to predict TC: classical molecular dynamics simulation vs. a perturbative treatment of lattice anharmonicity in the framework of Boltzmann transport theory. Taking the same empirical interaction potential as input to both approaches, we contrast phonon-phonon scattering rates and TC results as a function of temperature and tube length. This comparison allows us to critically evaluate several assumptions in the different methods, namely the description of anharmonicity by a truncated Taylor expansion of the interaction potential, the use of classical vs. quantum phonon statistics, and the importance of Umklapp processes for the TC.



Length dependence of CNT thermal conductivity at T=300K as obtained from nonequilibrium molecular dynamics simulation (NEMD) and from a perturbative anharmonic lattice calculation by solving the Boltzmann transport equation for phonons (ALC-BTE).

P089 **Mo 17:00 - 18:30**

Actuation of aligned Carbon Nanotube Arrays

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The active behaviour of carbon nanotubes (CNTs) can be observed when CNTs are positioned within an electric field and immersed into an electrolyte. Several explanations are given, ranging from nanoscopic effects such as carbon bonds weakening by electron doping or atomistic double layer-induced interaction of electron orbitals. Also macroscopic effects such as volume changes as result of ion intercalation, gas generation or electrostatic effects have been proposed. In this paper experiments aligned, continuous CNT-arrays of macroscopic dimensions (3mm) are tested electromechanically in contrast to former tested CNT-papers. Their behaviour is tested at different conditions and by using different electrolytes within a modified tensile testing machine. The tests reveal almost no condition dependency, which can be explained by the presence of the neat carbon bonds. The specimen orientation and the test approach exclude macroscopic effects such as volume effects by ion diffusion. The measured free strain and the behavior of the force can be assigned to an elongation of the neat carbon structure. Furthermore, asymmetric progressions of the results at negative and positive potentials seem to be related to ion-interaction. It must be assumed that superimposing effects are measured.

P091 **Mo 17:00 - 18:30**

Novel plasmonics and transports of topological Dirac materials

Eddwi Haseo[1]

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Twisting of electronic wave function can dramatically alter transport properties. The chief among them is the anomalous Hall effect, namely, a transverse motion even in the absence of magnetic field. Gapped Dirac systems serve as ideal platforms to observe this anomalous Hall effect. Importantly, when the sign of the gap is flipped in real space, topological states arise at the boundary. The gap inversion naturally arise in gapped bilayer graphene with stacking faults (AB- and BA-) or in a split dual-gate geometry wherein perpendicular applied electric field in adjacent regions have opposite signs. In this talk, we present the properties of plasmonic collective excitation of this topological boundary modes. The domain wall plasmons (DWP) exhibit long lifetimes because of topological protection at the boundary [1]. Next, we will discuss a cyclotron motion without magnetic field appearing in gapped Dirac systems with broken time reversal symmetry [2]. Berry curvature, that is analogous with magnetic field in reciprocal space, drives electron in a circular fashion under non-adiabatic (ac) electric field.

[1] E. H. Hasdeo and J. C. W. Song, Nano Lett. 17, 7252-7257 (2017)
[2] E.H. Hasdeo, Alex Frenzel, and J. C. W. Song, arXiv:1807.00014

P093 **Mo 17:00 - 18:30**

Reactive molecular dynamics simulations of van der Waals epitaxy: can we grow phosphorene?

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[1] *Furukawa Electric Institute of Technology*
[2] *Budapest University of Technology and Economics*

Van der Waals heterostructures of two dimensional materials attracted considerable interest because of their unique properties and potential applications. Due to its favorable band gap, high carrier mobility and unique chemical properties, phosporene is one of the most interesting member of 2D materials. Its growth on graphene is not only a promising future synthesis method, but can lead to novel materials with new catalytic properties.

Successful growth of phosphorene by van der Waals epitaxy needs careful precursor and substrate selection and also the proper choice of the conditions, therefore we analyzed the growth process by reactive molecular dynamics simulations.

Our simulations showed that the dissociation of white phosphorus and phosphine proceeds at different temperatures, but yield the same P_2 active compound. P_2 oligomerizes easily at typical reaction conditions. However the reaction starting from white phosphorus and phosphine precursors yield different products and phosphorene forms only from the latter. The mechanism clearly shows that the presence of hydrogen is indispensable to achieve the desired structure.

We hope, our results will contribute to the understanding of growth mechanism and will help the synthesis of phosphorene van der Waals heterostructures.

P095 **Mo 17:00 - 18:30**

Computational study on electronic transport in doped carbon nanotubes focusing on disappearance of localization phenomena due to phonon scattering

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Impurity-doped carbon nanotubes (CNTs) are expected to be used as materials of field effect transistors or thermoelectric devices. Electronic transport properties of doped CNTs are characterized mainly by impurity and phonon scatterings. Previous studies have shown that resistance of CNTs with a lot of defects, in which impurity scattering dominates, increases exponentially with tube length, while the dependence of CNTs with few defects, in which phonon scattering dominates, shows linear behavior. Therefore, although it is expected that electronic transport properties of doped CNTs also varies depending on the dopant concentration or temperature, the details have not been clarified.
In the present study, we investigated electronic transport properties in doped CNTs at finite temperatures using our developed simulation method. We revealed that tube length dependence of resistance shows exponential behavior at 0 K, which is originated from localization phenomena. On the other hand, resistance at 300 K decreases compared to one at 0 K and the length dependence becomes linear behavior. This means that phonon scattering reduces localization phenomena. This work is the first report to investigate disappearance of localization phenomena in doped CNTs originated from phonon scattering.

P097 **Mo 17:00 - 18:30**

Formation process of 2D materials on substrates using evolutionary algorithm

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[2]National University of Science and Technology MISiS, Moscow, 119049, Russian Federation
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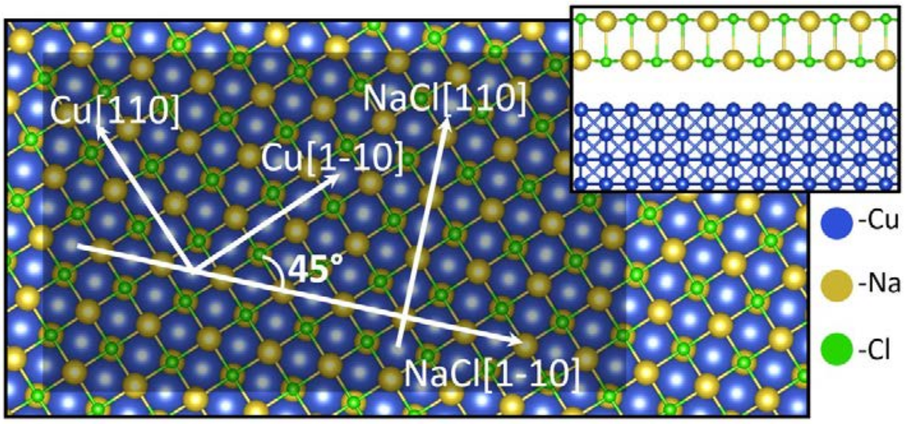
Nowadays it is already possible to obtain fundamentally new atomically thick films with unique physical properties with various composition. At first stages it is possible to form 2D films from the crystals having layered structure (graphene, h-BN, MoS_2, etc.) by mechanical exfoliation technique. Then great interest attracts formation of novel two-dimensional materials with structure and properties having no analogues in 3D, such as silicene, borophene, CuO, Fe, FeO, CoC etc.

Currently, there is a very limited set of methods for simulation the formation process of nanostructures. Presented methods can only partially describe formation process and have significant limitations in simulation and obtaining result.

Here we presented an effective method for simulation of formation process of two-dimensional materials with one and several layers thickness on substrates of different composition based on Evolutionary algorithm USPEX. Formation of 2D nanostructures with several layers thickness films of NaCl and LiCl on various substrates (including Cu, Ni, Ag, graphene, diamond) were carried out. Obtained results has an excellent agreement with available experimental data.

Authors acknowledge the financial support of the RSF according to the research project No 18-73-10135.



Supercell of theoretically predicted NaCl film on the Cu substrate. Atomic species presented in the inset.

P099 **Mo 17:00 - 18:30**

Multiphase Coexistence of MBE-growth Stanene on Cu (111)

Jia Li[1]

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Stanene, a two-dimensional material with hexagonal lattice, has extraordinary physical properties. After theoretical prediction as promising topological insulator for many years, synthesis of high-quality stanene is vital for the future practical application. Bi_2Te_3(111), PdTe(111) and Ag(111) have been explored as the substrate for the epitaxial growth of stanene[1-3]. Recently, the Cu(111) has been reported as the substrate to grow the stanene island, shape of which is hexagonal[4]. In this talk, the growth mechanism of hexagonal stanene on Cu(111) has been explored in the view of thermodynamics and kinetics. In addition, other phases of stanene on Cu(111) have also been revealed by first-principles molecular dynamics calculations combined with versatile experimental methods. In addition, other substrates have been theoretically explored the effect of substrate on the growth of different phases of stanene.

[1] Nat. Mater., 2015, 14, 1020-1025.
[2] Nat. Phys., 2018, 14, 344-348.
[3] 2D Mater., 2018, 5, 025002.
[4] Nat. Mater., 2018, 17, 1081-1086.

P101 **Mo 17:00 - 18:30**

Ab initio Simulation on Thermoelectric Properties of Nitrogen-doped Carbon Nanotubes

Manaho Matsubara[1], Takahiro Yamamoto[1]

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Significant enhancements could be realized by employing one dimensional (1D) thermoelectric materials. Carbon nanotubes (CNTs) are of particularly interest as high-performance thermoelectric 1D materials. Although both n- and p-type semiconducting CNTs are needed to develop CNT-based thermoelectric devices, the thermoelectric properties of n-type CNTs are not yet fully characterized in contrast to p-type CNTs. Recently, we theoretically found that nitrogen-doped (N-substituted) CNTs (a potential n-type CNT) exhibit extremely high thermoelectric power factor at band edges originating from van Hove singularity of 1D materials. This result demonstrates that “band-edge engineering” will be crucial for solid development of high-performance thermoelectric materials. In addition to N-substituted doping, there are various types of N-doping structure, e.g. pyridine-like N doping. However, thermoelectric properties of the pyridine-like N-doped CNTs remain to be resolved yet. In this work, we theoretically investigate the electrical conductance, Seebeck coefficient, and power factor of pyridine-like N-doped CNTs by NEGF+DFT simulation. We found that the extremely high power factor of N-substituted CNTs decreases due to existence of the pyridine-like N doping.

P103 **Mo 17:00 - 18:30**

Effects of Local Distortion on Thermoelectric Properties of Carbon Nanotubes

Keiichiro Matsumoto[1], Takahiro Yamamoto[1,2]

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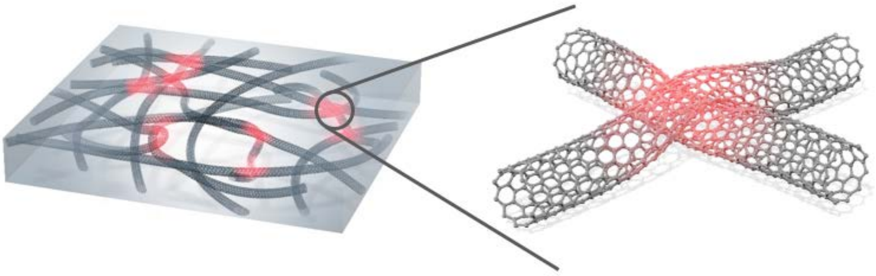
[2] *RIST, Tokyo University of Science, Tokyo 125-8585, Japan*

Thermoelectric generation is expected to use for the self-sustaining sources, which are required to realize IoT society. As a material used for the thermoelectric generation devices, a carbon nanotube (CNT) is a potential candidate for flexible devices. In the CNT film, some of the CNTs are considered to be locally distorted and/or bent. In fact, the previous experimental studies confirmed the existence of bent CNTs and showed that the thermoelectric properties vary when the CNT film is deformed by external forces. However, the detailed influence of such mechanical deformation on thermoelectric properties of CNTs has not been clarified thus far.

In the present study, we have theoretically investigated thermoelectric properties of a locally distorted semi-conducting CNT using the non-equilibrium Green's function method combined with the tight-binding method. We show that the Seebeck coefficient, the electrical conductivity and the power factor of semiconducting CNTs are almost independent with the local distortion when it is less than ~30%. On the other hand, when the local distortion is larger than ~30%, the Seebeck coefficient increases with increasing the local distortion, whereas the both electrical conductivity and the power factor decrease.



Schematic illustration of CNTs which are locally distorted by contact between CNTs in the CNT film

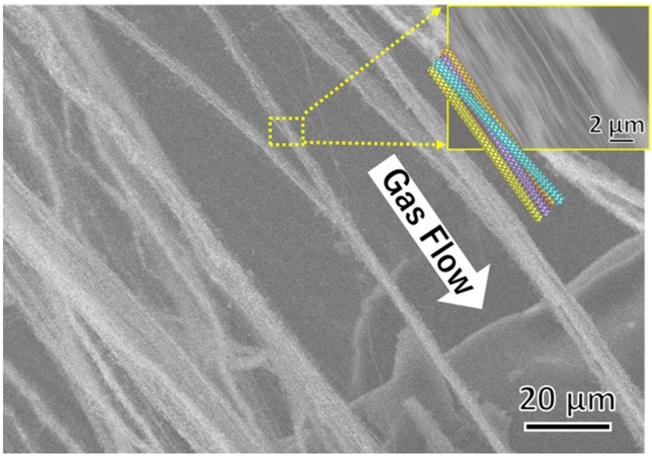
P002 **Mo 19:00 - 21:00**

One-Step Fabrication of Carbon Nanotube Fibers using Chemical Vapor Deposition Method

Toshihiko Fujimori[1], Koichiro Nakamura[2], Kanade Matsuo[2], Hideki Masuda[2], Jun Otsuka[1], Daisuke Tanioka[1], Takeshi Hikata[1], Soichiro Okubo[1], Yoshikazu Ito[2], Jun-ichi Fujita[2]

[1]*Sumitomo Electric Industries, Ltd., Osaka 554-0024, Japan*
[2]*University of Tsukuba, Tsukuba 305-8573, Japan*

The global demand in light-weight and high-strength wires has increased due to the ongoing development of next-generation electric vehicles. We report herein the one-step fabrication of carbon nanotube (CNTs) fibers using a laboratory-designed thermal chemical vapor deposition (CVD) system. Based on the conventional floating-catalyst CVD method, we further modified our horizontal reactor using a “gas-rectifier” inside the furnace. We found that the gas-rectifiers induces the formation of CNT fibers (Fig. 1). This observation indicates that the controlled gas flow is essential for assembling floating CNTs into a fiber. Furthermore, our fluid analysis shows that the gas-rectifier accelerates the velocity of reaction gases, resulting in a possible elongation of CNT fibers by shearing stress. In this presentation, we will demonstrate structural characterizations, orientation analysis, and mechanical properties of the resulting CNT fibers.



SEM images of CNT fibers fabricated directly by the chemical vapor deposition process. Due to the gas rectification, CNTs are aligned along the direction of gas flow, forming an aligned fiber.

P004 **Mo 19:00 - 21:00**

Long CNT growth with plastic deformation of spindle-shaped bottom graphitic shells in laminar-flow CVD

Jun-ichi Fujita[1], Kanade Matsuo[1], Kentaro Wayanabe[1], Yu Kikuchi[1], Hideki Masuda[1], Toshihiko Fujimori[2], Soichiro Okubo[2], Takeshi Hikata[2]

[1]*University of Tsukuba, Tsukuba 305-8573, Japan*
[2]*Sumitomo Electric Industries, Ltd., Osaka 554-0024, Japan*

We demonstrated long carbon nanotube (CNT) growth over 3cm having the highest breaking stress exceeds 80 GPa, using the kite growth mode with Fe_2O_3 powder catalyst and pure CH_4 laminar flow (Fig. (a)). The furnace temperature was 940 to 980 °C, and the CH_4 flow rate was 5 cm/sec. The characteristic feature of our CNTs was the remarkable appearance of hairpin-shaped CNT which can be visualized using additional pyrolytic decoration (Fig. (b)), and the spindle-shaped bottom of the CNT(Fig. (c)). To understand the long CNT growth mechanism under strong laminar flow, we traced the time evolving growth images by developing the CNT growth technique on a TEM membrane.
We triggered the initial seeds growth with methane flashing for spreading of the Fe_2O_3 particles(Fig. (d)). Then the carburized iron became to split into some fragments connected with stringy graphitic tubes(Fig. (e)). The tube seemed to grow accompanying the plastic deformation at the interface with the carburized liquid-like iron(Fig. (f)). We think the splitting of the carburized iron at the initial gas flow resulted in the hairpin-shaped seeds. The carburized irons encapsulated in the large graphitic spindle plays an important role in high efficiency supplying of carbon source for long CNT growth.

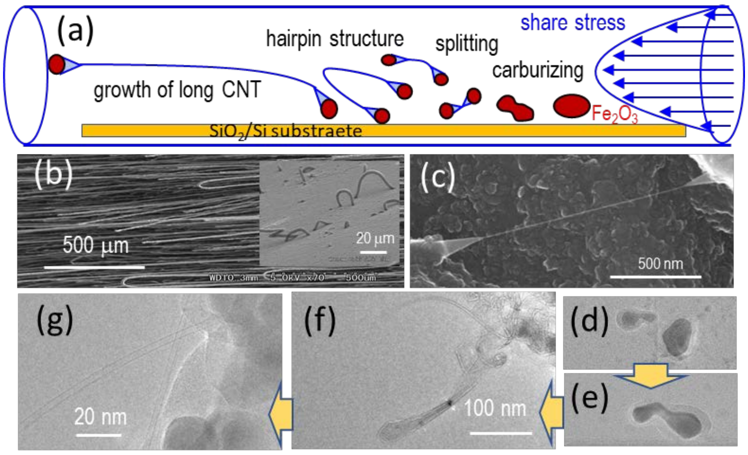


Figure shows (a)the CNT growth sequence. (b)the hairpin-shaped CNT and (c)the spindle-shaped bottom was characteristic. (d)the dispersed particles were (e)fragmented with a stringy graphitic tube, (f)CNT deemed to grow from the spindle-shaped heads.

Plenary Venue Poster

P006 **Mo 19:00 - 21:00**

Field emission property of bilayer graphene edges under an external electric field

Yanlin Gao[1], Susumu Okada[1]

[1]*University of Tsukuba, Tsukuba, 305-8571, Japan*

Graphene acts as an excellent field emission source with remarkable emission efficiency, owing to its high structural aspect ratio, high mechanical stiffness, high chemical stability, and high electron conductivity arising from its sp^2 covalent network. Experimentally synthesized graphene exhibits rich variation in its morphologies around its edges. In this work, we aim to provide the theoretical insight into the field emission property of bilayer graphene nanoribbons (GNRs) and folded GNRs, using the density functional theory combined with the effective screening medium method. Our calculations showed that field emission property of the bilayer GNR depends on the edge shape and the lateral displacement. Armchair bilayer GNRs have higher field emission current than zigzag ones due to their lower potential barriers for the emission. In addition, for wrinkled graphene, we consider the folded armchair and zigzag GNRs as the structural model, and found that the field emission property is sensitive to the atomic arrangements in the folded moiety. Folded zigzag GNRs have lower potential barrier, producing higher field emission current compared with folded armchair GNRs due to the absences of the dangling bond and edge states.

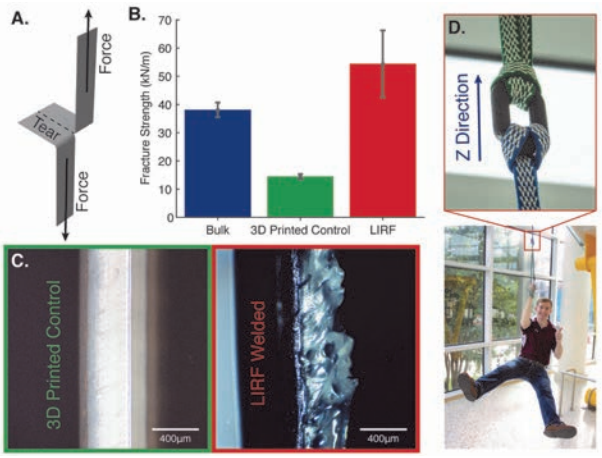
P008 **Mo 19:00 - 21:00**

Heating, Curing, and Welding of 3D Printed Carbon Nanotube-Polymer Systems by Locally Induced RF Heating

Micah Green[1]

[1] *Texas A&amp*
[2] *M University, College Station, TX, USA*

A key obstacle facing 3D-printed plastic parts in engineering applications is the weak weld between successive filament traces, which often leads to delamination and mechanical failure. This is the chief obstacle to the use of thermoplastic additive manufacturing. We have recently demonstrated a novel concept for welding 3D-printed thermoplastic interfaces using intense localized heating of carbon nanotubes (CNTs) by electromagnetic irradiation. We apply CNT-loaded coatings to 3D printer filament; after printing and microwave exposure, this is shown to improve the weld fracture strength. These remarkable results open up entirely new design spaces for additive manufacturing and also yield new insight into the coupling between dielectric properties and electromagnetic field responses for nano-filled materials. Further study has shown that low-frequency RF fields can couple with CNT networks, allowing for a variety of rapid scanning techniques without any need for shielding. We have demonstrated that such techniques can be used to induce rapid localized heating in a range of technologies, including thermoset 3D printing and automotive thermoset curing.



(A) Tear tests determine that (B) the fracture strength of 3D-printed PLA coupons is increased by 275% when nanotube coatings and RF welding are applied, as shown by the (C) fracture surfaces. (D) A nanotube-coated, welded PLA chain link.

Plenary Venue Poster

P010 **Mo 19:00 - 21:00**

Enhancement of CNT Textiles through Bundle Alignment and Catalyst Sweating by Photonic Post-Processing

Thurid Gspann[1], John Bulmer[2], Joe Stallard[3], Adarsh Kaniyoor[1], Jennifer Mizen[1], James Elliott[1]

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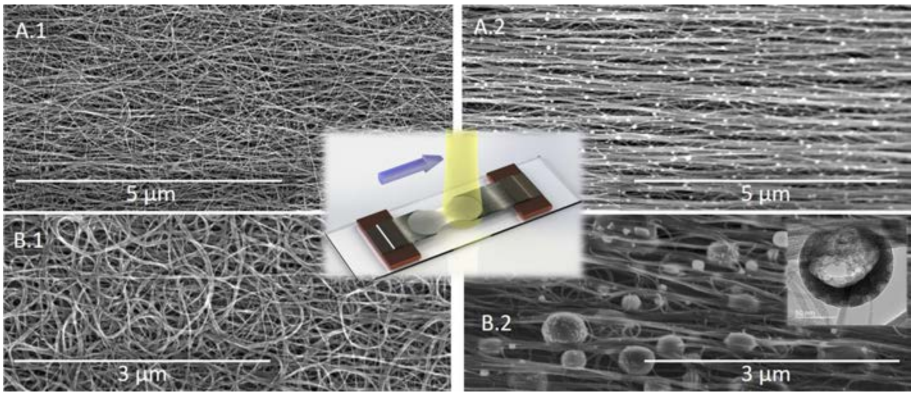
[2]*B. Institute for Manufacturing, University of Cambridge, CB3 0FS, UK*
[3]*C. Engineering Department, University of Cambridge, CB2 1PZ, UK*

Photonic post-processing of FC-CVD spun CNT textiles results in selective sorting of the CNTs present. Defective, thermally non-conductive or unconnected CNTs burn, leaving behind a highly crystalline, highly conductive network [1]. But further to the mere decomposition of undesirable CNTs, there are crucial side-effects depending on the sample's material composition and geometry: Even where no significant G:D improvement is observed, pulse irradiation – not only by laser but also camera flashes – leads to a major improvement in alignment, as well as sweating of molten catalyst beads to the surface which facilitates their removal.

Macroscopically, the irradiated samples show an hourglass shape, if the laser spot exceeds the sample width. We postulate that the laser induces strong currents, thereby generating Lorentz forces that compact the network within the constraints imposed by external geometry. In wider samples, central bundles cannot compact as much as those close to the edge, the bundles are pinched together spot-wise, creating an internal waviness. We discuss these beneficial side-effects of photonic processing as a fast, scalable method to enhance a textile's microstructure, independent of its graphenic crystallinity.

[1] Bulmer, Gspann et al., SciRep, 7, 12977 (2017)



Two FC-CVD CNT textile samples (A, B), as-spun (1) and after photonic post-processing (2), illustrating the improvement in alignment and molten catalyst beads sweating to the surface. Inset in B.2: remaining shell of an acid washed catalyst bead

P012 **Mo 19:00 - 21:00**

Ultrafast combinational techniques revealing reduction mechanisms of graphene oxide via photoexictation and heating

Masaki Hada[1], Kiyoshi Miyata[2], Satoshi Ohmura[3], Shin-ya Koshihara[4], Yasuhiko Hayashi[5], Ken Onda[2], Yuta Nishina[5]

[1] University of Tsukuba
[2] Kyushu University
[3] Hiroshima Institute of Technology
[4] Tokyo Institute of Technology
[5] Okayama University

The high popularity of graphene oxide can be ascribed to the facts that the atomic framework and physical properties of its reduced form are similar to those of graphene, and that graphene oxide is highly dispersible in water and polar organic solvents enabling functionalization by chemical transformations. However, the structure of graphene oxide and the nature of processes occurring during its reduction have remained elusive. We introduce combined use of ultrafast time-resolved electron diffraction, ultrafast time-resolved infrared vibrational spectroscopy, and time-dependent density functional theory calculation for the study of structural dynamics of graphene oxide. This productive cooperation evidently distinguished the reduction mechanisms of graphene oxide via thermal treatments or ultraviolet photoexcitation. Our findings have revealed that the oxygen atoms of epoxy groups are selectively removed from the basal plane of graphene oxide by anti-bonding nature of photoexcitation, in contrast to the behaviour observed for thermal excitation-based reduction of hydroxyl groups.

P014 **Mo 19:00 - 21:00**

Measuring the current–voltage characteristics of isolated carbon nanotubes under transient temperature conditions

Kaori Hirahara[1,2], Michihiro Hashimoto[1]

[1]*Department of Mechanical Engineering, Osaka University, Suita 565-0871, Japan*
[2]*Center for Atomic and Molecular Technologies, Osaka University, Suita 565-0871, Japan*

When a single CNT bridged between two large substances is Joule-heated, it possesses a parabolic thermal gradient described by one-dimensional heat equation. However, most practical cases are complicated. Although CNTs have excellent thermal conductivity, the degree of interfacial heat conductance between CNTs or at the CNT substrate should also be considered. We recently tried to visualize the temperature distribution of a single CNT under Joule heating using a nanomanipulator system in a transmission electron microscope by decorating gold nanoparticles as a thermometer. Monitoring the temperature-dependent structural changes in the gold particles resulted in the temperature map on the CNT with a range 500°C–900°C, showing that rather shorter and thicker CNTs tended to have the highest temperature at the end contacting the electrode. Additionally, CNT's current–voltage (I–V) relation can be measured using the same electrodes used for Joule heating. The I–V curves were measured at a certain period after stopping the Joule heating at the highest temperature of 900°C, revealing that the curves' gradients changed by seconds order interval time. This is probably related to the transient temperature changes of CNT. This work was supported by JST CREST grant number JPMJCR1715 Japan.

P016 **Mo 19:00 - 21:00**

Interaction between layers of single-walled carbon nanotube coated with boron nitride nanotube

Kaoru Hisama[1], Susumu Okada[2], Shohei Chiashi[1], Shigeo Maruyama[1,3]

[1]*The University of Tokyo, Tokyo, 113-8656, Japan*
[2]*University of Tsukuba, Tsukuba, 305-8571, Japan*
[3]*AIST, Ibaraki 305-8564, Japan*

Tubular structures of C or BN allow them to form one-dimensional van der Waals (vdW) heterostructures by coaxially arranging them with appropriate diameter difference. Indeed, a recent experiment demonstrated that a carbon nanotube (CNT) is coated with BN nanotube (BNNT) as an ultimate surrounded gate transistor where CNT and BNNT are conducting channel and dielectric, respectively. This BNNT coated CNT may exhibit interesting variation in their physical properties, which is different from the simple superpose of each constituent. Thus, we aim to provide the energetics and electronic structures of CNT coated with BNNT, using the density functional theory.
Here, we consider double-walled NT consisting of inner (n,0) CNT and outer (m,0) BNNT, as the representative structure of the hybrids. The total energy calculation elucidated that the most stable combination of chirality index is $m=n+9$ where the interwall spacing is 0.35 nm. Under the optimum combinations, the calculated cohesive energies of the NTs are about 10 meV/atom weakly depending on the tube index and interwall atomic arrangements [Fig. 1(a)]. As for the electronic structure, band gaps of inner CNTs are modulated by forming the hybrid structures depending on the interwall stacking arrangements [Fig. 1(b)].

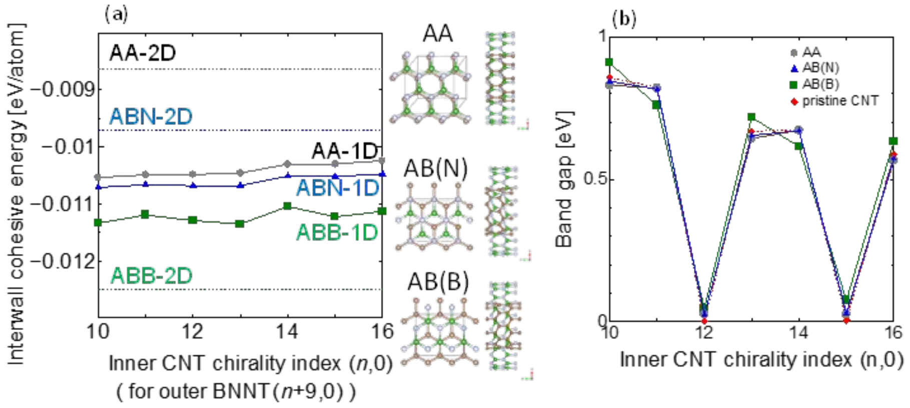


Figure 1 (a) Interwall cohesive energy and (b) band gap of CNT(n,0)@BNNT(n+9,0) as a function of the index n. Dotted lines in (a) indicate the cohesive energy of hBN and graphene with AB(B), AB(N) and AA stacking arrangements.

Plenary Venue Poster

P018 **Mo 19:00 - 21:00**

CO_2 reduction using transition metal decorated phosphorene

Tibor Höltzl[1,2], Endre Faragó[2]

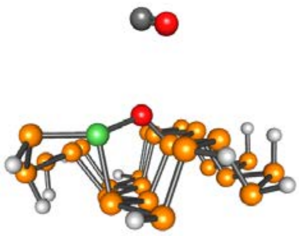
[1]*Furukawa Electric Institute of Technology*
[2]*Budapest University of Technology and Economics*

Reduction of CO_2 to organic compounds is in the frontier of interest with great potential application as well as many interesting chemical phenomena.

Transition metal surfaces, clusters and even single atoms were shown to catalyze the CO_2 reduction, while due to its favorable band gap, phosphorene is an excellent co-catalyst e.g. for photochemical hydrogen evolution reaction.

In our work, we investigate the CO_2 reduction with transition metal decorated phosphorene using Density Functional Theory computations. We found that both CO_2 and H_2 binds weakly to copper atom atom decorated phosphorene, but carbon-monoxide can be formed in the process. Nevertheless the weak binding of phosphorene leads to low catalyst activity. Therefore we screened the first row transition metals to understand the effect of the dopant atom on the reaction mechanism.

We hope our work will facilitate the synthesis of novel, single metal atom based phosphorene catalysts for carbon-dioxide reduction.



P020 **Mo 19:00 - 21:00**

Scalable and Continuous Production of Small Diameter Single-Walled Carbon Nanotubes with Narrow Chirality Distribution

Aqeel Hussain[1], Er-Xiong Ding[1], Saeed Ahmad[1], Yongping Liao[1], Mohammad Tavakkoli[1], Qiang Zhang[1], Hua Jiang[1], Kimmo Mustonen[2], Esko I. Kauppinen[1]

[1]*Department of Applied Physics, Aalto University School of Science, FI-00076 Aalto, Finland*
[2]*Faculty of Physics, University of Vienna, Boltzmanngasse 5, 1090 Vienna, Austria*

We report a scalable floating catalyst CVD (FCCVD) production of single-walled carbon nanotubes (SWCNTs) with controlled chirality distribution. The SWCNTs are synthesized using 0.75 ccm ethylene as carbon source along with 40 ccm $H_2$and iron as a catalyst in the inert environment of 300 ccm N_2at 1050 °C. For the first time, we used water as the growth promoter in the FCCVD process to modulate the growth of SWCNTs. At an optimum water concentration of ca. 115 ppm, we have succeeded in producing SWCNTs having small diameters, especially with extremely narrow chirality distribution. In particular, the contents of (9,8) and (8,7) tubes have been dramatically enhanced up to 45% with 27% of the (9, 8) tube in the product. Water-assisted the growth of 76% semiconducting nanotube in the sample measured with electron diffraction. We believe that the addition of water has affected the nucleation and formation of nanoparticles thus resulted in the growth of small diameter SWCNTs with the narrow chirality distribution. Our direct and continuous water assisted FCCVD process can lead SWCNTs one step closer to their commercial applications in nanoelectronics.

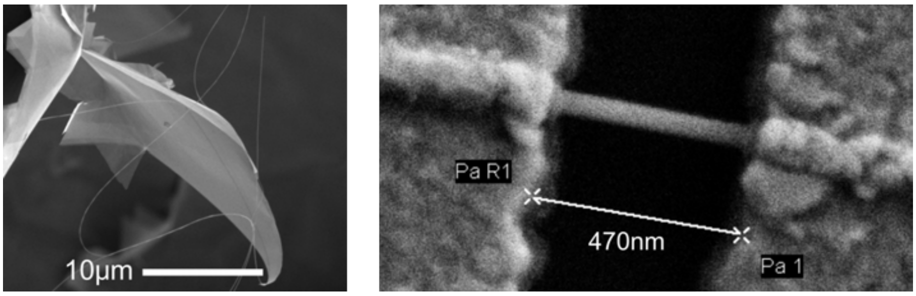
P022 **Mo 19:00 - 21:00**

Quantum transport measurements of MoS_2 nanotubes

Andreas K. Hüttel[1], Simon Reinhard[1], Luka Pirker[2], Christian Bäuml[1], Maja Remškar[2]

[1]University of Regensburg, 93040 Regensburg, Germany
[2]Solid State Physics Department, Institute Jožef Stefan, Ljubljana, Slovenia

While synthesis procedures for nanotubes based on layered materials other than graphene are well-known, their quantum transport properties are so far largely unexplored. Here, we introduce transition metal dichalcogenide (TMDC) nanotubes as a new material platform for low temperature transport spectroscopy. We present results on optimized nanotube synthesis, first device fabrication, and electronic characterization. MoS_2 nanotubes are synthesized using a chemical transport reaction. Optimized growth parameters lead to thin nanotubes with diameters down to 7nm, lengths up to several millimeters, and an extremely low number of structural defects. Field effect transistor devices based on individual nanotubes are characterized in low temperature transport measurements. They display the typical behavior of Coulomb blockade systems, with clear indications of discrete quantum levels.



Scanning electron microscope images of TMDC nanotubes, as-grown (left panel) and lithographically contacted (right panel).

P024 **Mo 19:00 - 21:00**

Third-order nonlinear optical properties in photo-reduced graphene oxide

Masao Ichida[1], Yuto Hosomi[1], Kazunari Matsuda[2], Hiroaki Ando[1]

[1] *Department of Physics, Konan University, Kobe, 658-8501, Japan*
[2] *Institute of Advanced Energy, Kyoto University, Uji, 611-0011 Japan*

Nonlinear optical properties in nano-carbon systems such as single-walled carbon nanotubes are interesting topics for both fundamental material science and application of new optical devices. Many theoretical and experimental works have been done in nonlinear optical properties for single-walled carbon nanotubes. For graphene oxide, nonlinear optical properties in graphene oxide have been reported by several groups. However, because of the change in absorption spectra due to the reduction by photo-irradiation, it is difficult to obtain precise values of optical nonlinearity. In this study, we have measured third-order nonlinear susceptibility of graphene oxide by a combination of Z-scan and saturation power density method around the absorption edge. The absolute value of imaginary part of third-order nonlinear susceptibility increases with increasing photon energy. On the other hand, the figure of merit of nonlinearity (the ratio of third-order nonlinear susceptibility to absorption coefficient) increases with decreasing photon energy. After photo irradiation to graphene oxide sample, the values of figure of merit decrease and approach that for graphene dispersion sample. These result can be explained by the decrease of lifetime in graphene nanodisc embedded in graphene oxide.

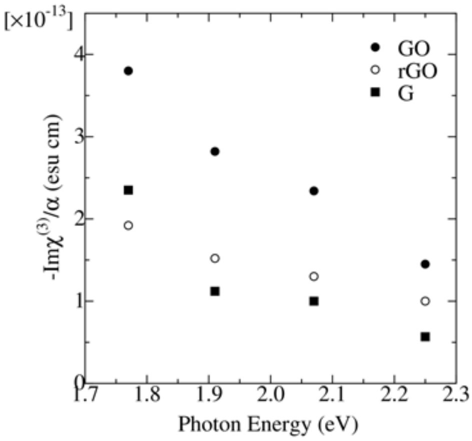


Figure of merit of nonlinearity (the ratio of third-order nonlinear susceptibility to absorption coefficient) of graphene oxide (solid circles), photo-reduced graphene oxide (open circles), and graphene dispersion (solid squares).

P026 **Mo 19:00 - 21:00**

Atomic Scale Structural Identification and Evolution of Co-W-C Ternary SWCNT Catalytic Nanoparticles: HR-STEM imaging on SiO_2

Rong Xiang[1], Akihito Kumamoto[2], Rong Xiang[1], Yan Li[3], Yuichi Ikuhara[2], Shigeo Maruyama[1,4]

[1]*Department of Mechanical Engineering, The University of Tokyo, Tokyo 113-8656, Japan*
[2]*Institute of Engineering Innovation, The University of Tokyo, Tokyo 113-8656, Japan*
[3]*College of Chemistry and Molecular Engineering, Peking University, Beijing 100871, China*
[4]*Energy NanoEngineering Laboratory, AIST, Tsukuba 305-8564, Japan*

Recently W-based catalyst has provided a promising route to synthesize SWCNTs with specific chirality, but the mechanism of the growth selectivity is still vaguely understood and under intensive discussion. Here we propose a strategy to identify the atomic structure, as well as the structure evolution of Co-W-C ternary catalyst. The key is to use a thin SiO_2 film as the catalyst support and observation window. As the catalyst can be uniformly prepared on this high-temperature stable film and directly used for SWCNT synthesis. With this technique, we illustrate that Co-W-C ternary catalyst form junctions of metallic W and η carbide Co6W6C after reduction. But as the CVD starts, the catalyst undergoes a W loss, which finally results in a precipitation of pure hexagonal close packed (hcp) phase metallic Co. This precipitated Co phase is fully coherent to the parent crystal, having a strict crystal orientation to Co_6W_6C. As a method, the current TEM imaging directly on SiO_2 serves as a powerful and versatile tool to investigate nanocrystals and high temperature reactions; for synthesis of SWCNTs, this work successfully visualizes the structure and evolution of catalyst, and illuminates the possible nucleation sites of chirality specific growth.

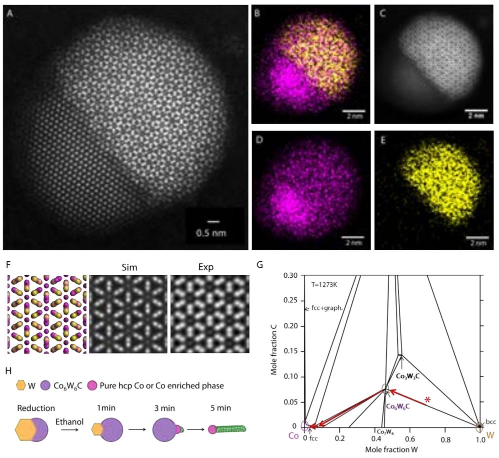


Figure Atomic resolution images of Co-W-C catalyst.

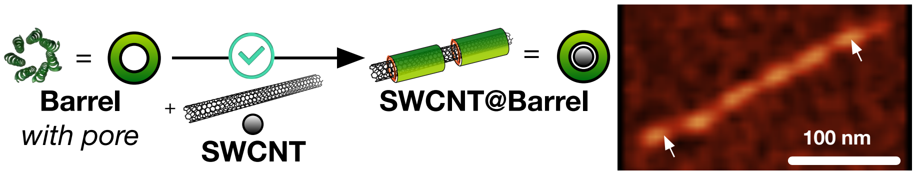
P028 **Mo 19:00 - 21:00**

Peptide-barrel encapsulated carbon nanotubes

Florian A. Mann[1], Jan Horlebein[1], Franziska Thomas[2], Sebastian Kruss[1]

[1] *Institute for Physical Chemistry, Göttingen University, 37077, Germany*
[2] *Center for Biostructural Imaging of Neurodegeneration, Göttingen, 37075, Germany*

Single-walled carbon nanotubes (SWCNT) are a highly interesting material for optoelectronic applications due to their non-bleaching fluorescence in the near-infrared tissue transparency window. To use them in aqueous environments, however, one has to mask their highly hydrophobic surface.
Here, we present a novel strategy for SWCNT functionalization based on de novo designed ????-helical coiled-coil peptide barrels. These barrels contain hydrophobic pores of various diameters. For our study, we chose the barrel termed CC-Hept containing a pore of approx. 7.6 Å matching the diameter of (6,5) SWCNT.
Using spectroscopy and microscopy methods, we show that only certain SWCNT species fit right into the peptidic barrel structure. Using Atomic Force Microscopy we observed small, periodic changes in height for the CC-Hept-dispersed SWCNT, which, based on analytical ultracentrifugation and X-Ray crystallography data, could be attributed to the peptidic barrel structure formed around the SWCNT.
In summary, we showed that it is possible to insert SWCNTs into ????-helical peptide barrels containing a pore of appropriate size. Our results are highly encouraging not only from a fundamental point of view, but also for application as a universal functionalization platform for carbon nanotubes.



P030 **Mo 19:00 - 21:00**

Pre-reactor pyrolytic reaction of ethylene to improve growth efficiency of single-walled carbon nanotubes synthesis

Naoyuki Matsumoto[1], Sachiko Ishizawa[1], Michiko Irie[1], Megumi Hirano[1], Kenji Hata[1], Don Futaba[1]

[1]*AIST, Central 5, 1-1-1 Higashi, Tsukuba, Ibaraki, 305-8565, Japan*

The research field of single-walled carbon nanotube (SWCNTs) has shifted to the development of SWCNT-based applications. Many applications benefit from a high aspect ratio of SWCNTs. In additions, the catalysts on a substrate, can grow SWCNTs up to the millimeter-scale, which is leading to the mass production. Therefore, the high efficiency and large throughput synthesis for SWCNT is important for realizing the SWCNT industry.

In this study, we investigated an approach for high conversion efficiency synthesis of SWCNTs using the heterogeneous catalysis of ethylene prior to the substrate (denoted “Pre-Cat”). In this way, this approach separates the heating of the reactor as the primary source of pyrolysis of the ethylene feedstock. Our results showed that the ethylene conversion efficiency as evidenced by CNT forests of 1575 μm height in 10 min while using reduced ethylene concentration. In TEM observation, the CNTs grown in Pre-Cat process were SWCNTs (the average wall number; 1.2 and the diameter; 2.9 nm), whose structures were the same as SWCNTs in normal growth (without Pre-Cat process).

This work was supported by JSPS Grant-in-Aid for Young Scientists (B) Grant Numbers JP17K14091.

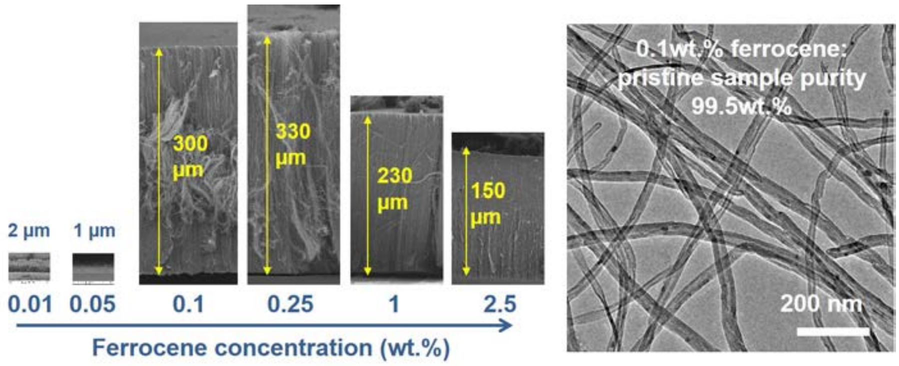
P032 **Mo 19:00 - 21:00**

Effect of ferrocene and hydrogen concentrations on the growth of vertically aligned carbon nanotubes by aerosol-assisted chemical vapor deposition

Martine Mayne-L'Hermite[1], Emeline Charon[1], Mathieu Pinault[1], Martine Mayne-L'Hermite[1]

[1]*CEA-Saclay, Université Paris-Saclay, NIMBE, 91191 Gif/Yvette France*

Aerosol-assisted catalytic chemical vapor deposition is a powerful one-step method to synthesize forests of vertically aligned multiwalled carbon nanotubes (VACNTs) of high quality at industrial level at temperature about 800-900°C. Continuous injection of both catalyst and carbon precursors (ferrocene/toluene) enables long duration synthesis at performing growth rate without growth promoter and catalyst poisoning. However, samples contain iron-based by-products that can affect VACNT intrinsic properties and high temperature stability in air, which is restrictive in terms of applications. It is therefore of the greatest interest to reduce the iron content in pristine VACNTs. Here, we show that adding H_2 in the precursor flow affects considerably the kinetics of ferrocene decomposition and leads to the deposition of a higher number density of catalytic particles on the substrate. Consequently, the ferrocene concentration threshold allowing the growth of a self-organized VACNT forest is drastically reduced and iron content drops to 0.5wt.%, while maintaining high quality and growth rate. The pristine VACNT samples display an increased oxidation temperature which depends only on iron content. Finally, a new methodology to control forest density is made possible and presented.



P034 **Mo 19:00 - 21:00**

Chiral structure dependence of the strength of single-walled carbon nanotubes

Yuhei Miyauchi[1,2], Akira Takakura[1,2], Ko Beppu[3], Taishi Nishihara[1,2], Akihito Fukui[3], Takahiro Kozeki[4], Takahiro Namazu[3], Kenichiro Itami[2]

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Single-walled carbon nanotubes (SWNTs) theoretically possess ultimate intrinsic tensile strengths in the 100–200 GPa range. However, experimentally reported values are considerably lower than the theoretical predictions; furthermore, the considerable degree of scatter among the measured samples poses a critical problem regarding their practical use in macroscopic structural materials. The lack of the structural information of the measured samples complicates the detailed discussion on the fracture mechanism. Here we report the experimental measurements of the ultimate tensile strengths of structure-defined individual SWNTs using home-made microelectromechanical system device [1]. The ultimate tensile strengths of the sixteen measured SWNTs depend on the chiral structure; near-armchair SWNTs with small diameter exhibit the highest tensile strengths. This observed structural dependence is comprehensively understood via the structure-dependent inter-atomic stress and its concentration at structural defects. In the presentation, we will discuss the fracture mechanism and an empirical formula predicting the ultimate tensile strength of real SWNTs.

[1] A. Takakura et al., under revision.

P036 **Mo 19:00 - 21:00**

Tuning the carbon single wall nanotube growth with carbon solubility of NixPt1-x catalysts

Cora Moreira Da Silva[1], Armelle Girard[1, 2], Frédéric Fossard[1], Vincent Huc[3], Annick Loiseau[1], Costel-Sorin Cojocaru[4]

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CVD synthesis on catalytic NPs suffers from a lack of control of tube diameter and chirality. This non-selectivity is due to an insufficient knowledge of the parameters controlling the growth mechanisms. Our research path focuses on the NPs role and its carbon solubility, which has been identified to be a key parameter for the NTs growth mode [1,2]. We have studied the CNTs growth from Ni_xPt_{1-x} alloyed NPs. Ni being known to be an efficient catalyst for the SWCNTs growth thanks to its ability to solubilize carbon, unlike Pt, the alloy composition is expected to tune the NP carbon solubility. A key point was to set NPs synthesis conditions leading to alloyed NPs with no segregation effect to take advantage of this property. We used successfully colloidal route to the synthesis Ni_xPt_{1-x} catalysts NPs, with size, shape control and homogeneous compositions [3]. We performed HFCVD synthesis on fully characterized NPs, at various temperatures, for each composition Ni, Ni_3 Pt, NiPt, $NiPt_3$ and Pt NPs using CH_4 as the feedstock gas [4]. Carbon solubility's influence on SWCNTs growth will be discussed.

[1] M. He et al Carbon 113 (2017) 231-236 [2] M. He et al Nanoscale 10 (2018) 6744-6750 [3] C. Moreira Da Silva et al under preparation (2019) [4] A. Castan et al Carbon 123 (2017) 583-592

P038 **Mo 19:00 - 21:00**

Observation in situ of carbon nanotubes growth catalyzed by nickel-platinum nano-alloy

Cora Moreira Da Silva[1], Mounib Bahri[2], Ileana Florea[3], Frédéric Fossard[1], Ovidiu Ersen[2], Armelle Girard[1,4], Annick Loiseau[1]

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[2]*IPCMS, CNRS, Université de Strasbourg, Strasbourg, 67034, France*
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CVD on catalytic NPs is the most studied and promising method for SWCNT synthesis. However, this process suffers from a lack of control of tube diameter and chirality. This non-selectivity is due to an insufficient knowledge of the parameters controlling the growth mechanisms. One of the research path focuses on the NPs role, and notably its carbon solubility[1,2]. We have studied the CNTs growth from Ni_xPt_{1-x} alloyed NPs. Ni was known to be an efficient catalyst for the CNTs growth thanks to its ability to solubilize carbon, unlike Pt. We used the colloidal route to synthesize Ni_xPt_{1-x} catalysts, with size, shape control and homogeneous compositions[3]. Structure and chemical composition of the NPs are characterized before CNTs growth (TEM, EDX, Electron diffraction). We performed in situ analyses of the growth process of CNT catalyzed by Ni_xPt_{1-x} NPs using an environmental TEM equipped with different gases supply (CO/CH_4). The structural modifications of the dual nanotube/NPs system and the general dynamics of the involved processes have been followed during the growth, in real time and at the atomic scale and will be discussed[4].

[1]M. He et al, Carbon 2017 [2]M. He et al, Nanoscale 2018 [3]C. Moreira Da Silva et al, under preparation 2019, [4]M. Bahri et al, Nanoscale 2018

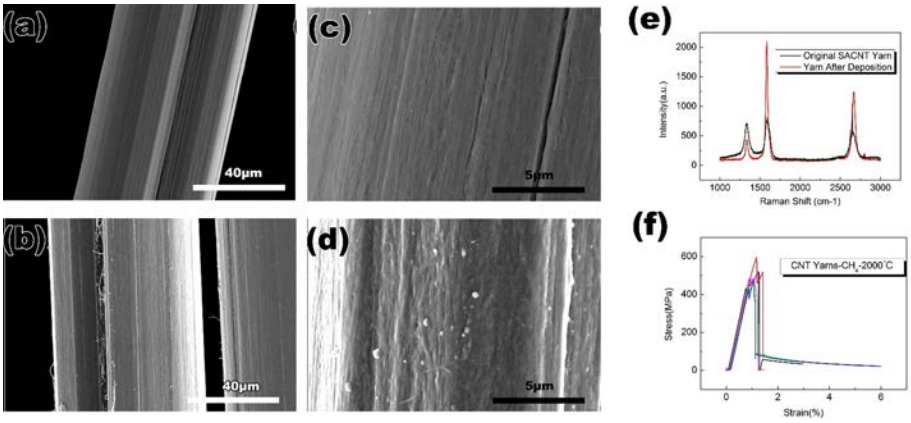
P040 **Mo 19:00 - 21:00**

High Temperature Epitaxial Growth of Aligned Graphitic Fiber by using Super-aligned Carbon Nanotubes as Seeds

Wen Ning[1], Peng Lei[1], Wen Ning[1], Shiwei Lv[1], Yufeng Luo[1], Wei Zhao[1], Xinhe Yang[1], Qingwei Li[1], Duanliang Zhou[1], Peng Liu[1,2], Qi Cai[1], Liang Liu[1], Lina Zhang[1,2], Jiaping Wang[1,2], Qunqing Li[1,2], Shoushan Fan[1,2], Kaili Jiang[1,2]

[1] *Tsinghua University, Beijing 100084, China*
[2] *Collaborative Innovation Center of Quantum Matter, Beijing 100084, China*

By using super-aligned carbon nanotube as seed, the homoepitaxial growth of graphitic fiber has been achieved in a homemade experimental setup at a temperature as high as 2500°C. The high temperature homoepitaxy strategy has been applied to three kinds of structures, the super-aligned carbon nanotube yarn, super-aligned carbon nanotube film, and super-aligned carbon nanotube array. This approach shows the advantage of simple, high throughput and energy efficient. The samples after high temperature homoepitaxy show increased G/D ratio in the Raman spectra. The mechanical properties are also generally enhanced. This approach shows great promise in making high performance carbon fiber in the near future.



The SEM images,Raman spectra comparison and mechanical properties test results of the original super-aligned carbon nanotube yarn and that after high temperature homoepitaxy.

P042 **Mo 19:00 - 21:00**

An insight into Single-walled carbon nanotube growth onto graphene crystals using Ir as a catalyst

Kamal Prasad Sharma[1,2], Takuya Okada[1], Aliza K Sharma[1], Takahiro Maruyama[1,2]

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[2] *Meijo University/Nanomaterials research center, Nagoya, 468-8502, Japan*

Graphene and single-walled carbon nanotubes (SWCNT), sp^2 hybridized honeycomb structures of carbon, are realized as the promising materials to use in wide ranges of application due to their high carrier mobility, high electrical and thermal conductivity, and large surface area [1, 2]. A high quality 3D hybrid structure of graphene and SWCNT is highly desirable to further enhance their properties so as to use in large volume
application [3,4]. Here we attempt to address this issue by growing narrow diameter SWCNT onto graphene crystals.

Graphene crystals were synthesized on Cu by chemical vapor deposition (CVD) technique and transfer onto SiO_2/Si as reported elsewhere [5]. Samples with 1.2nm Ir catalyst layer deposited onto graphene were utilized as growth substrate. SWCNT growth was carried at optimized condition using ethanol gas as carbon source in ultra-high vacuum CVD (UHV-CVD) system [6]. Optical microscope (OM), Raman spectrometer, FESEM, and XPS were employed for the characterization.

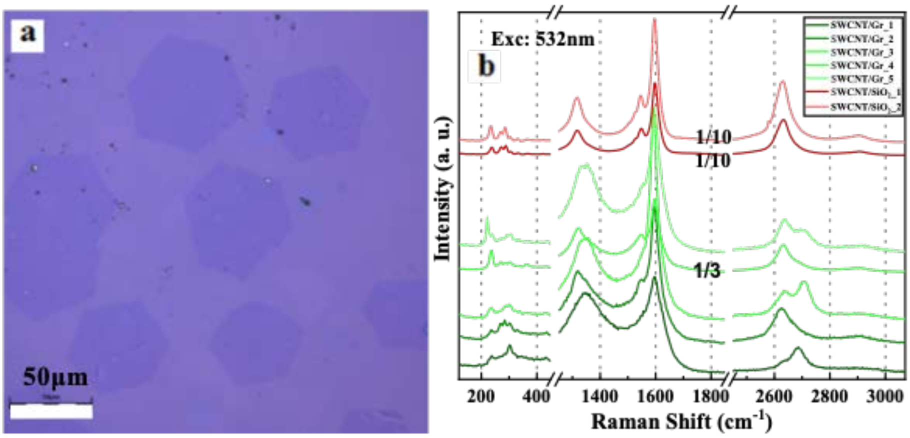


Fig. 1. (a) OM images of SWCNT grown on graphene crystals. Circular structures with dark contracts represent graphene crystals. (b) Raman spectra highlighted in different color represents as listed in inset.

P044 **Mo 19:00 - 21:00**

Doping of collapsed carbon nanotubes by filling of edges cavities

Emmanuel Picheau[1], Ferdinand Hof[1], Hassan Saadaoui[1], Alain Pénicaud[1]

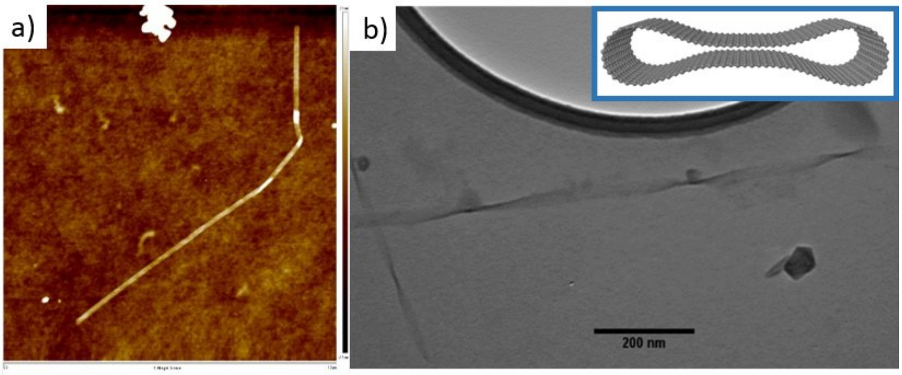
[1]*Centre de Recherche Paul Pascal, UMR5031 CNRS - Bordeaux University*

Due to their extremely good transport properties, carbon nanotubes and graphene are strong candidates to build the electronic of the future. To make electronic components out of a material, it has to be semi-conductive and easy to doped. The gap opening by confinement in graphene nano ribbons, the sorting of carbon nanotubes, and their doping still remain challenging.

The Edgefiller project proposes to use collapsed carbon nanotubes, also called "dogbones" as basic elements for electronic components. Dogbones, which can be seen as bilayer graphene nano ribbons, are predicted to be a semi conductive materials[1]. Moreover, the edges cavities (see insert fig.1) can be filled with various atoms and molecules, useful to reach specific doping.

Dogbones can be obtained from highly crystalline multi walls carbon nanotubes (MWCNTs), by extracting tubes from each other[2]. The high fraction of large single wall carbon nanotubes obtained from MWCNTs extraction, collapse naturally. Dogbones can be recognised because of the twists and folds they form, see fig.1. The presentation will focus on the extraction, the study and the filling of dogbones obtained from MWCNTs sample.

[1] Giusca, C. E. et al. Phys. Rev. B 76, 35429 (2007).
[2] Choi, D. H. et al. Sci. Rep. 3, 1617 (2013).



a) AFM image of folded and twisted dogbone (height). b) TEM image of twisted dogbone. Insert : scheme of a dogbone.

P046 **Mo 19:00 - 21:00**

Floating catalyst CVD synthesis of single-walled carbon nanotubes from carbide catalyst

Liu Qian[1], Ying Xie[1], Jin Zhang[1]

[1]*Peking University, Beijing, 100871, China*

Floating catalyst CVD (FCCVD) is a manageable and cost-effective strategy for the production of CNT aerogels, which can further be deposited or transferred onto specific substrates. However, in traditional FCCVD, iron is the most widely used catalyst. The liquid state of iron under growth temperature made it a challenge to control the diameter and chirality of nanotubes. An appropriate and narrow diameter and property distribution of SWCNTs is critical to achieve the desired performances of final products. In this work, we introduce several carbide catalysts into FCCVD system for the first time. The high melting point of carbide provides a rigid catalyst template for the CNT growth and is beneficial for the control of CNT structures. The carbides, typically TiC and Mo_2C, were obtained from the thermal decomposition of corresponding metallocene. The concentration of catalyst particles in gas phase was adjusted through the change of driving temperature and the flow rate of carrier gas. The size of catalyst particles after thermal decomposition was selected through an electrical strategy. Finally, relatively large amount of single-walled carbon nanotubes (SWNTs) were synthesized through FCCVD from carbide catalysts. We also studied the relationship between obtained SWCNTs and catalyst crystals. The further controlled growth of SWNTs through FCCVD can be realized by more precise design of these solid catalysts.

P048 **Mo 19:00 - 21:00**

Vertically-Aligned Carbon Nanotubes directly grown on transparent substrates as potential dark matter target

Ilaria Rago[1], Maria Grazia Betti[1], Carlo Mariani[1], Francesco Pandolfi[2], Andrea Goldoni[3], Loredana Casalis[3], Denis Scaini[3], Gianluca Cavoto[1]

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An important challenge in the field of CNTs research is the possibility to control the engineering of ordered CNTs-based architectures having predefined alignments, such as vertically aligned carbon nanotubes (VA-CNTs). Recently, large arrays of VA-CNTs have been proposed as potential targets for directional detection of dark matter by exploiting their clear anisotropic behavior. Here, we present an easy, low cost and reproducible synthesis method for growing VA-CNTs on transparent substrate (i.e. fused silica) following an iron nanoparticle-catalyzed Chemical Vapor Deposition process (CVD). Notably, in our synthesis method, although no metal other than iron has been used as catalyst layer and even if the growth time was limited to merely 4 minutes, the yield, reproducibility, and density of the produced CNTs are comparable to similar structures found in the literature, grown by using more sophisticated and time-consuming techniques. The low cost and high versatility of the here presented CVD-based synthesis process open up new opportunities in the perspective of adopting them as potential targets in novel detection schemes for dark matter particles.

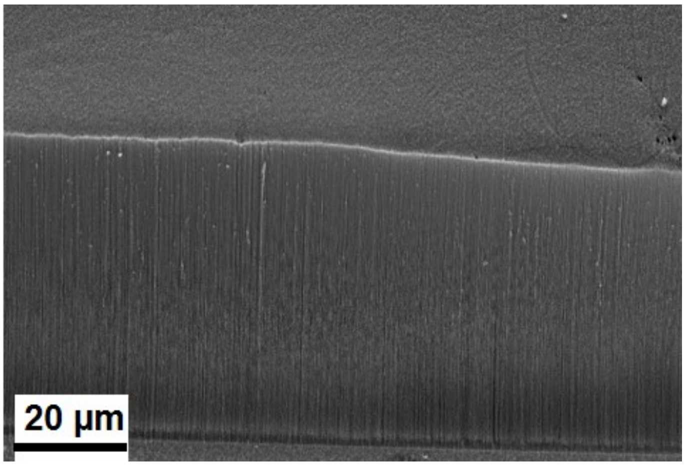


Figure 1. SEM image showing a fused silica surface covered by a thick layer of aligned CNTs, oriented perpendicularly to the surface substrate

P050 **Mo 19:00 - 21:00**

Controlling nanoscale architectonics of natural graphene-like carbon

Natalia Rozhkova[1], Anna Kovalchuk[1], Sergey Rozhkov[1]

[1] *Institute of Geology Karelian Research Center RAS, Petrozavodsk 185910, Russia*

The most attractive properties of carbon materials are associated with the ability to form new nanoscale architectonic forms. Therefore, the study of shungite carbon (ShC) as a natural graphene-like material and its structural modifications is of scientific and practical interest.

Clustering of non-planar graphenes of ShC is a key process of a multilevel structural organization scenario and of structural transformations in systems of various physico-chemical nature. ShC favorably differs from all synthetic objects by fixed lateral dimensions ~ 1 nm and amphiphilicity of graphene fragments. Water contributes into the formation of structural hierarchy of ShC at the nanolevel, in fractal structure and porosity of bulk ShC. The reverse process of releasing of graphene fragments was realized through preparation of stable aqueous dispersions of ShC nanoparticles. Such processing and further condensation of the dispersion guarantee reproducibility of structural peculiarities of basic element and its clustering at all levels up to 3D-net formation.

ShC heat treatment led to the formation of polyhedral particles, spatially arranged fractals of curved, mono- or stacked graphene layers and nanographite. The factors responsible for structural rearrangements are discussed.

P052 **Mo 19:00 - 21:00**

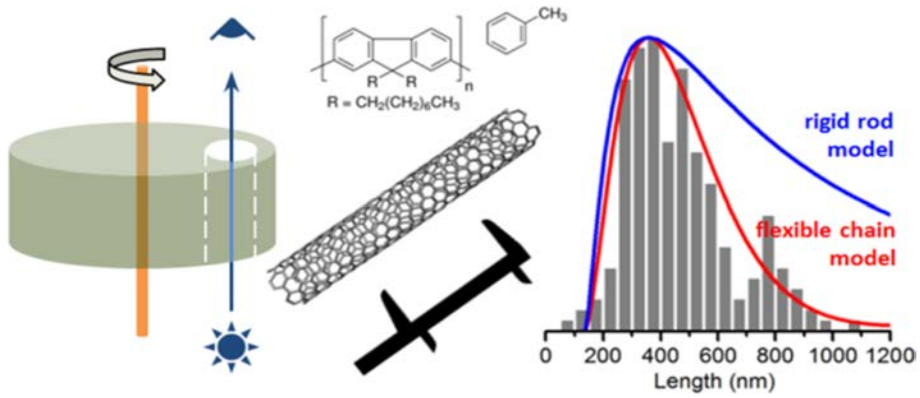
Measuring in Situ Length Distributions of Polymer-Wrapped Monochiral SWCNTs Dispersed in Toluene with Analytical Ultracentrifugation

Pranauv Balaji Selvasundaram[1,2], Rainer Kraft[1], Wenshan Li[1,2,4], Regina Fischer[3], Manfred M Kappes[1,3], Frank Hennrich[1], Ralph Krupke[1,2]

[1]Institute of Nanotechnology, Karlsruhe Institute of Technology, Karlsruhe, 76344, Germany
[2]Institute of Materials Science, Technical University Darmstadt, Darmstadt, 64287, Germany
[3]Institute of Physical Chemistry, KIT, Karlsruhe, 76131, Germany
[4]Cambridge Graphene Centre, University of Cambridge, Cambridge, CB3 0FA, UK

The length of a CNT is an important dimension that has to be adjusted to the requirements of an experiment. So far, AFM has been the method of choice for measuring length distributions, despite being an ex-situ method with apparent shortcomings. In this work, we explore analytical ultracentrifugation (AUC) as an in situ method for measuring the length distribution of polymer-wrapped (7, 5) SWCNTs dispersed in toluene, the nowadays preferred media for nanotubes used in device fabrication. In AUC, the resulting sedimentation curves can be deconvoluted with a standard data processing procedure (SEDFIT), to yield the sedimentation coefficient distribution. However, the conversion of the sedimentation coefficient distribution into a length distribution requires finding a suitable model for the nanotube friction coefficient. Also, since AUC is based on optical absorption, it yields a volume distribution and not a number distribution as obtained from AFM reference data. By meeting these challenges and finding a surprisingly simple empirical flexible-chain-like model to describe the sedimentation, we suggest AUC as a viable method for measuring in situ nanotube length distributions of nonaqueous dispersions [1].

[1] Selvasundaram et al., Langmuir 2019, DOI: 10.1021/acs.langmuir.9b00005



P054 **Mo 19:00 - 21:00**

Real-time mechanistic study of carbon nanotube anion functionalisation through open circuit voltammetry.

Pichamon Sirisinudomkit[1,2], Adam Clancy[1,3], David Anthony[1], Aaron Thong[2], Jake Greenfield[1], Maniesha Sigh[1], Milo Shaffer[1,2]

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[2]*Department of Materials, Imperial College London, SW7 2AZ, UK*
[3]*Department of Chemistry, University College London, WC1E 7JE, UK*

The mechanism of the functionalisation of reduced single walled carbon nanotubes with organobromides was monitored by open circuit voltammetry throughout the reaction and further elucidated through a series of comparative reactions. In contrast to the previously assumed reduction/homolytic cleavage mechanism, the reaction was shown to consist of a rapid association of carbon–halide bond to the reduced nanotube as a complex, displacing surface condensed countercations, leading to an initial increase in the net nanotube surface negative charge. The complex subsequently slowly degrades through charge transfer from the reduced single-walled carbon nanotube to the organobromide, utilizing charge, and the carbon–halide bond breaks heterolytically. Electron density on the C–Br bond in the initial reagent is the best predictor for degree of functionalisation. [1]

References

1. Clancy, A. J.; Sirisinudomkit, P.; Anthony, D. B.; Thong, A. Z.; Greenfield, Jake L.; Salaken Singh, M. K.; Shaffer, M. S. P., Real-time mechanistic study of carbon nanotube anion functionalisation through open circuit voltammetry. Chemical Science 2019.

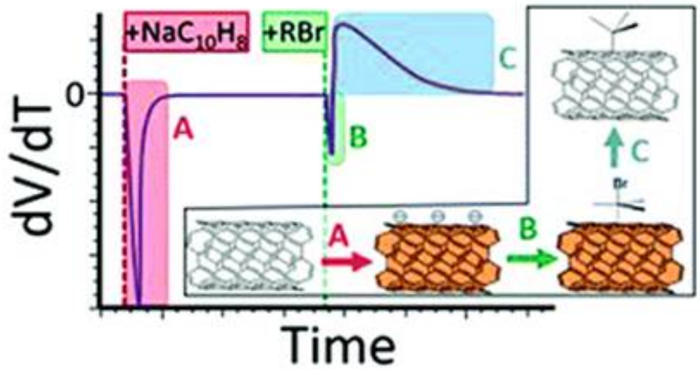


Figure: Scheme of derivative OCV versus time of a buckypaper working electrode during addition of sodium naphthalide solution (pink), and addition of organobromide (green). [1]

P056 **Mo 19:00 - 21:00**

Fundamental parameters for direct-spinning of carbon nanotube aerogels

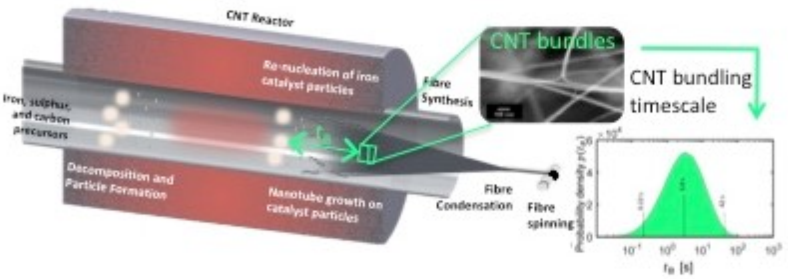
Fiona Smail[1], Adam Boies[1]

[1] *University of Cambridge, Department of Engineering*

The direct spinning of CNT aerogels from a FC-CVD reactor starts from simple precursors for Fe, S, and C. Recent studies using aerosol sampling methods have shown insights into the chemistry driving the process. The product is mainly synthesised from pyrolytic carbon species, not the C precursor. Also, the product CNTs are made by re-nucleation of catalyst nanoparticles. highlighting a new role of sulphur in stimulating the catalyst particle nucleation process.

Understanding of CNT collision timescales necessary for aerogel formation is crucial to process scale-up. Stochastic calculation, accounting for parameters such as CNT length, diameters and number of CNTs per bundle gave a typical bundling time of 3s, agreeing well with experiments.

Further, the interdependence of variables (e.g. alteration in reactant flows changing both concentrations and residence times) means that few publications provide quantitative correlations between precursor input rates and product quality or yield. A parameter-space mapping exercise, correlating published atomic input rates with product outputs reveals metrics spanning several orders of magnitude. The resulting trends demonstrate the key process parameters necessary for direct spinning and relationships between them.



Direct Spinning of CNTs showing aerogel formation from sulphur-driven re-nucleation of catalyst nanoparticles, CNT bundles and the characteristic time for CNT bundle formation

P058 **Mo 19:00 - 21:00**

Molecular Layer Deposition of Crosslinked Single-walled carbon nanotube films

David Stringer[1], Milo Shaffer[1]

[1] *Imperial College London*

Single-walled carbon nanotubes (SWCNTs) have a multitude of remarkable properties including high strength and stiffness, surface area and thermal and electrical conductivity. Unlocking these superlative properties requires exfoliation of the SWCNT bundles and dispersion in a suitable solvent. Reductive dissolution is an effective route to individualised nanotubes that preserves the high aspect ratio and retains the sp^2carbon framework whilst providing a handle for subsequent functionalisation.[1]

We present herein, a method for the molecular layer deposition of SWCNTs thin films by the sequential dip coating of these SWCNT polyanion layers and a dielectrophile covalent crosslinking species. A combination of UV-Vis spectroscopy and atomic force microscopy reveal a high degree of individualisation in the resultant solid film. Through this method we demonstrate tight control over the thin film properties, with each additional layer exhibiting a uniform increase in thickness and electrical conductivity, with a decrease in optical transparency. Films of this kind show promise in various applications from sensors and catalysts to conductive inks and coatings.

1. A. J. Clancy, J. Melbourne, M. S. P. Shaffer. J. Mater. Chem. A,2015, 3,16708–16715

P060 **Mo 19:00 - 21:00**

Impact of Experimental Parameters on Solution-Processed Semi-transparent Conductive Films of Carbon Nanotubes and Ethylene-Vinyl Acetate

Bernd Sturdza[1], Giulio Mazzotta[1], Moritz K. Riede[1], Robin J. Nicholas[1]

[1] *University of Oxford, Dept. of Physics, Clarendon Laboratory, Oxford, OX1 3PU, UK*

Aggregation of Carbon Nanotubes (CNT) poses a major obstacle towards their large scale application in optoelectronic devices. A common approach to produce stable dispersions of separated CNTs is solubilisation in organic solvents via non-covalent wrapping with conjugated polymers. Recently, solubilisation of CNTs has been demonstrated for the non-conjugated insulating polymer Ethylene-Vinyl Acetate (EVA) which allows fabrication of conductive, semi-transparent films for not only single-, but also multi-walled CNTs with high uniformity by spray coating (1). Here, we present a study of the impact of film treatment, varying concentrations and using different kinds of CNTs on the optical and electronic properties of the CNT:EVA films.

(1) G. Mazzotta et al. Solubilization of Carbon Nanotubes with Ethylene-Vinyl Acetate for Solution-Processed Conductive Films and Charge Extraction Layers in Perovskite Solar Cells. ACS Appl. Mater. Interfaces 2019, 11, 1185–1191.

P062 **Mo 19:00 - 21:00**

Macroscopic Separation of Multi-Species Single-Chirality Enantiomers of Single-Wall Carbon Nanotubes

Xiaojun Wei[1,2], Jiaming Cui[1], Linhai Li[1,3], Dehua Yang[1,3], Weiya Zhou[1,2,3], Sishen Xie[1,2,3], Hiromichi Kataura[4], Huaping Liu[1,2,3]

[1]*Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China*
[2]*Songshan Lake Materials Laboratory, Dongguan, Guangdong 523808, China*
[3]*School of Physics Science, UCAS, Beijing 100049, China*
[4]*Nanomaterials Research Institute, AIST, Tsukuba 3058565, Japan*

The fundamental and applied researches of single-wall carbon nanotubes (SWCNTs) enantiomers are still in the bottleneck stage to date due to the great difficulty in the macroscopic preparation of multi-species single-chirality carbon nanotubes enantiomers. In this work, we improved our previous gel chromatography method by combining temperature selective adsorption with stepwise elution [1]. First, the semiconducting SWCNTs with different narrow chirality distributions were selectively adsorbed into gel by controlling temperature [2]. Second, these adsorbed SWCNTs were then separated individually into single-chirality enantiomers by using stepwise elution [1]. As a result, 14 different single-chirality SWCNTs and their enantiomers were successfully separated with high purity. Furthermore, the amount of most samples increased by more than 10 times compared with previous work, indicating that the current method is more suitable for macroscopic production of multi-species single-chirality enantiomers.

This work is financially supported by the National Key R&D Program of China (Grant 2018YFA0208402), NSFC (51472264, 11634014, 51820105002, 51872320, 51561022), and CAS (QYZDBSSW-SYS028).

[1] Nature Commun. 7, 12899 (2016).
[2] Nano Lett. 14, 6237 (2014).

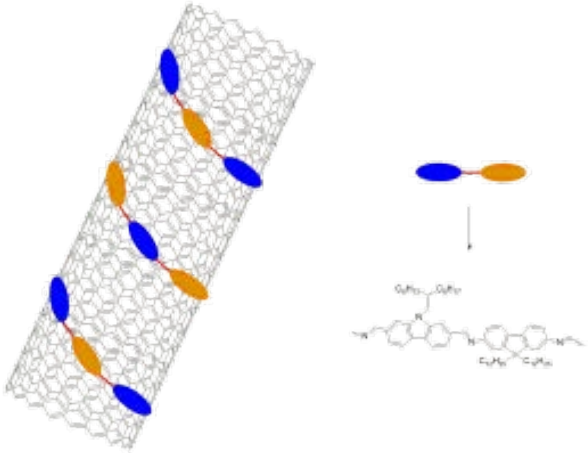
P064 **Mo 19:00 - 21:00**

RECYCLABLE FLUORENE-CARBAZOLE COPOLYMER FOR HIGHLY SELECTIVE DISPERSION OF SEMI-CONDUCTING SINGLE-WALLED CARBON NANOTUBES

Liang Xu[1], Michal Valášek[1], Frank Hennrich[1], Marcel Mayor[1,2]

[1]*Institute of Nanotechnology, Karlsruhe Institute of Technology, P. O. Box 3640, D-76021 Karlsruhe, Germany*
[2]*Department of Chemistry, University of Basel, St. Johannsring 19, CH-4056 Basel, Switzerland*

Semi-conducting single-walled carbon nanotubes (sc-SWNTs) with high purity is of great importance to their application in electronics, optoelectronics and photonic devices1. Herein, we present the selective dispersion of sc-SWNTs by acid-degradable conjugated copolymers. To harvest sc-SWNTs with a wide range of chiral angles and high yield we introduced carbazole subunits into the backbone of polyfluorene. The bridging imine bond in each repeat unit ensures the complete removal of the polymer upon acid triggering. After the wrapping and cleavage of copolymers, the intrinsic properties of the naked sc-SWNTs are well preserved and they are ready for further measurement and processing. The pre-sorted sc-SWNTs containing several pairs of indices (n,m) are a racemic mixture of left- and right-handed enantiomers (n,m) and (n+m,-m). For further separation of the pre-sorted sc-SWNTs according to their handedness, we designed and synthesized chiral polyfluorenes. The handedness of rewrapped tubes is currently under investigation.



Polymer@SWNT

P066 **Mo 19:00 - 21:00**

SWCNT synthesis by promoter-assisted floating catalyst CVD

Qiang Zhang[1], Esko Kauppinen[1]

[1]*Department of Applied Physics, Aalto University School of Science, Espoo, Finland*

Due to scalability, low-cost and good control of Single-walled carbon nanotube (SWCNT) synthesis, floating catalyst chemical vapor deposition (FCCVD) keep attracting intense attention in both academic and industrial fields. In FCCVD, the growth promoters as well as carbon sources and catalysts, play a critical role in the controllable preparation of SWCNTs. Recently, tremendous progress of promoter-assisted FCCVD in mass production, controllable synthesis and CNT architectures, has been achieved. According to the composition, there are four categories of promoters, i.e. oxygen-containing promoter, sulfur-containing promoter, nitrogen-containing promoters and other promoters, utilized in FCCVD, as shown in Fig 1. Herein, we systematically review the role of various promoters in FCCVD SWCNT synthesis and specifically show the effect of sulfur, water and carbon dioxide as promoters on yield, morphology, quality and structure of FCCVD grown-SWCNTs. Moreover, few items related to promoter-assisted FCCVD grown-SWCNTs, i.e. SWCNTs with narrow chirality distribution, transparent electrodes, high-performance fibres, colourful CNT films, will be discussed in detail.

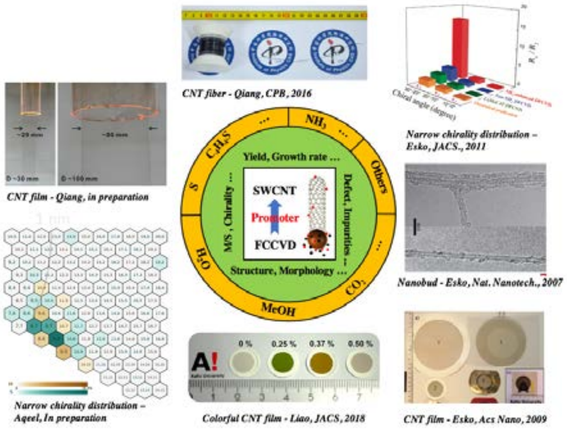


Fig 1. Four categories of promoters in FCCVD for SWCNT synthesis.

P068 **Mo 19:00 - 21:00**

Solid catalyst synthesis for direct growth of chirality controlled SWCNTs

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Single-walled carbon nanotubes (SWCNTs) with controlled chirality are believed to have a wide range of applications and could be the key to significant advancements in many fields of technology. Despite the need, after decades of research growing SWCNTs with a narrow distribution is still challenging. Recently, it has been reported that catalysts which remain solid during the growth process can maintain their crystalline structure, and that controlling SWCNT chirality can be achieved through catalyst size and crystalline symmetry. Therefore, a method of preparing these catalysts which results in a narrow particle size distribution is paramount.

Here, using an aerosol method we demonstrate the synthesis of high melting point metal nanoparticles with nearly monodisperse size distributions for diameters in the range of 1~5 nm. Catalyst particles can then be deposited on a variety of substrates from which random and aligned SWCNTs with controlled chirality were successfully grown from chemical vapour deposition of ethanol. Based on this catalyst production and SWCNT growth method, chirality control from nanoparticles with different symmetries and diameters were further explored to extend our understanding of chirality selection mechanisms for solid catalysts.

P070 **Mo 19:00 - 21:00**

Length selective growth of highly pure aligned semiconducting carbon nanotubes

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Carbon nanotubes (CNTs) are the promising candidates for the novel integrated electronics. Whereas, it's a challenge to mediate their bandgap or chiral structures from a vapor-liquid-solid growth process. Here, we demonstrate the self-purified ultralong semiconducting CNT (s-CNT) arrays based on an interlocking between the atomic assembly rate and bandgap of CNTs. Rate analysis verified the Schulz-Flory (SF) distribution6 for both metallic (m-) and s-CNTs, indicating their different decay rates as length increased. Quantitatively, a nearly ten-fold faster decay rate of m-CNTs, led to a spontaneous purification of 99.9999% s-CNTs at a length of 154 mm and the longest CNT can be 650 mm through an optimization of the reactor. Transistors fabricated on them delivered a high current of 1.4 mA/um with an on/off ratio around 10^8 and mobility over 4000 cm^2/V·s. Our self-purification strategy offers more freedom to in-situ control the CNT purity and provides a robust method to synthesize perfectly entangled condensate over a wide length scale.

P072 **Mo 19:00 - 21:00**

Efficient n-Doping of SWCNT Network Transistors

Jan Gotthardt[1], Severin Schneider[1], Maximilian Brohmann[1], Roxana Lorenz[2], Eric Sauter[1], Michael Zharnikov[1], Hans-Jörg Himmel[2], Jana Zaumseil[1]

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For the practical application of semiconducting single-walled carbon nanotubes (SWCNTs) networks in field-effect transistors (FETs) and integrated circuits efficient p- and n-doping is necessary. Achieving unipolar n-type transistors with SWCNTs using air-stable electrodes (e.g. gold) is still challenging. Recently, guanidino-functionalized aromatic compounds (e.g. ttmgb) have been shown to be efficient n-dopants for FETs with (6,5) SWCNT networks. These devices show unipolar electron transport with high carrier mobilities, complete suppression of hole currents, excellent on/off current ratios and steep subthreshold swings, and almost no hysteresis. Here, we investigate the effects of electrode materials with different work functions on charge injection, contact resistance and the overall performance of SWCNT FETs with or without ttmgb-doping by gated and temperature-dependent four-point probe measurements. Furthermore, we apply ttmgb-doping not only to large bandgap (6,5) SWCNTs but also mixed networks based on polymer-sorted HipCo nanotubes and large diameter, small bandgap plasma torch SWCNTs.

P074 **Mo 19:00 - 21:00**

Dense electrolyte-gated single-walled carbon nanotube networks as artificial synapses

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The conductivity of dense films of purified semiconducting single-walled carbon nanotubes (SWNT) can be varied over many orders of magnitude by electrochemical doping as demonstrated in a variety of lateral and vertical electrolyte-gated SWNT network transistors (Rother et al., ACS Appl. Nano Mater. 2018, 1, 3616). The associated doping of the nanotubes also leads to characteristics bleaching of the main absorption features as shown recently in electrochemical cells (Berger et al., ACS Appl. Mater. Interfaces 2018, 10, 11135) with very thick (6,5) SWNT layers and large optical density. A number of different absorption levels could be achieved that were stable for hours under open circuit conditions by simply applying short voltage pulses due to the slow movement of electrolyte ions through a dense nanotube network. Here, we utilize the combination of fast charge carrier and slow ionic movement in an analogous SWNT/iongel system to create a type of artificial synapse where the channel (postsynaptic) conductance is determined and varied by presynaptic potential pulses (i.e. gate voltage pulses). We investigate the device parameters that enable such operation using aerosol-jet printed and spray-coated carbon nanotube films and iongels.

P076 **Mo 19:00 - 21:00**

Flexible, lightweight carbon nanotube sponge with high performance electromagnetic interference shielding

Dongmei Hu[1], Qingwen Li[1]

Flexible, low-density, desirable corrosion susceptibility high-performance electromagnetic interference(EMI) shielding performance-materials are urgently required in aerospace and integrated electronics devices. Due to the high aspect ratio , electrical conductivity and excellent mechanical, carbon nanotubes (CNTS) has been considered as one of the most promising candidates for excellent EMI shielding performance. Here, we report a flexible carbon nanotube sponge via chemical vapor deposition (CVD) method, with a density of 10 mg/cm^3, thickness of 1 mm shows high EMI shielding effectiveness(SE) and specific SE(SSE) of 70 dB and 6448 dB cm^3/g in x-band, respectively. the possible mechanism of the high performance EMI shielding was attribute to their enhanced microwave absorption via the internal hierarchical porous structure and high electrical conductivity. Moreover, the EMI SE of carbon nanotube sponge is almost unchanged after repeated compression or bending for 100 cycles. The results indicate that the lightweight porous film with outstanding magnetic and electrical properties could be used as multifunctional high-performance EMI shielding materials.

P078 **Mo 19:00 - 21:00**

Soft Aerogels supported by 1 mass% carbon nanotubes for thermal interface material

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Thermal interface materials (TIMs) are used for enhancing heat transfer between solid surfaces by creating thermal paths. Their important characteristics are high thermal conductivity and softness for filling the air gaps. However, many conventional TIMs consist of thermal conductive fillers dispersed in polymer matrix, which has disadvantages of low thermal conductivity and poor thermal stability.

Here we propose aerogel TIM replacing polymer matrix with air matrix. Air matrix is released upon pressing and conductive fillers can directly contact each other. Soft, sponge-like self-supporting films can be fabricated using carbon nanotubes (CNTs), and this structure is able to support fillers 100 times larger in mass compared with their own mass [1].

We selected Ag having the highest thermal conductivity among metals as conductive filler. The aerogel TIM was fabricated by hybridizing Ag particles with CNTs. The TIM was self-supporting even when the amount of fillers were 200 times larger than that of CNTs and thermal resistance of 40 mm2 K/W was achieved. Optimization of the structure is now underway, and latest results will be reported.

[1] K. Hasegawa and S. Noda, J. Power Sources 321, 155 (2016).

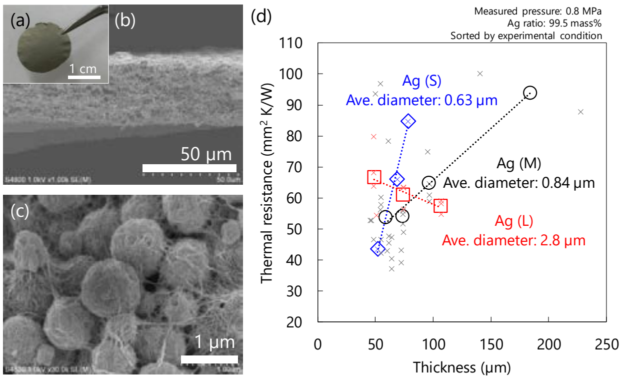

Figure 1. Images of Ag-CNT aerogel TIM and their thermal resistance. (a) Digital image and (b), (c) SEM images. (d) Thermal resistance of Ag-CNT aerogel TIMs.

P080 **Mo 19:00 - 21:00**

The Solar-Thermal Characteristics of Anodic Aluminum Oxide for Solar Selective Absorber Applications

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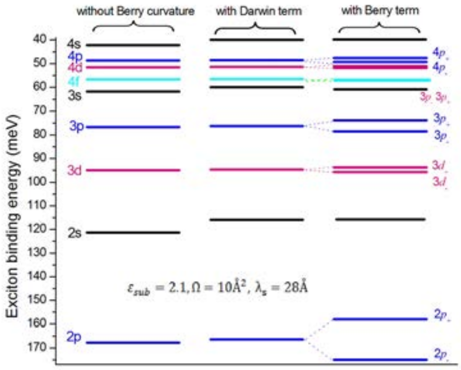
Solar absorbing coating layer which captures heat source from sunlight efficiently is useful for many applications, such as solar thermal electricity generation. This solar selective absorbing film must absorb most of the solar wavelengths and have high solar absorptivity and low thermal emissivity. In our study, the aluminum alloy 6061-T6 after sulfuric acid (0.3M) anodizing process was used to form the nano-porous anodic aluminum oxide (NPAAO) for solar absorbing applications. The SEM results showed that the diameter and thickness of NPAAO increase with increasing anodic temperature. Besides, the increasing of anodizing temperature, which increases the NPAAO film growth, leads to enhancement of absorption over the solar spectra range. Therefore, the solar absorptivity increases with the thickness of the NPAAO film and more penetrated beams are trapped by thicker NPAAO film due to its deeper medium and higher pore density. Moreover, the heating temperatures of NPAAO film were measured by 500W halogen light illumination. The results indicated that the steady heating temperature increases with higher absorptivity of NPAAO film and the spectral reflectance of aluminum alloy sample is greater than 62% and less than 10% before and after anodizing oxidation process, respectively.



The SEM images of NPAAO films at different anodic process temperature (a) 0oC (b) 5oC (c)10oC, and the (d) reflectivity and (e) heating temperature of NPAAO films

P082 **Mo 19:00 - 21:00**

Covalent assembly of nanocarbon frameworks for the support of catalyst/sorbent nanoparticles

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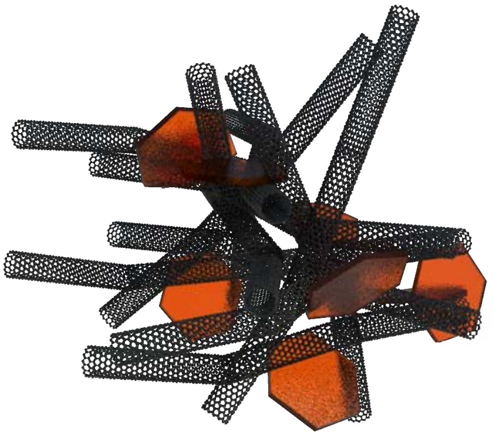
True solutions of single walled carbon nanotubes in organic solvent are cross-linked through covalent interaction for the preparation of low density, high surface area, mesoporous conductive frameworks [1]. Removing the solvent under supercritical conditions produces robust aerogels that can be used for energy storage, environmental applications and as catalyst or sorbent supports amongst others.
The co-precipitation of layered double hydroxides (LDHs) on hybrid powders of oxidised multiwalled carbon nanotubes and graphene oxide improves their CO_2 adsorption and multicycle stability [2]. The chemical functionalisation used in this work allows the preparation of complex hierarchical structures, combining the properties of carbon based structures operating on different length scales into a covalent assembly. The electrical, thermal, and mechanical properties as well as morphology are tailored to the in-situ synthesis of LDHs on the supporting network.

1.De Marco, M. et al. Cross-linked single-walled carbon nanotube aerogel electrodes via reductive coupling chemistry. J. Mater. Chem. A 4, 5385–5389 (2016).
2.De Marco, M. et al. Hybrid effects in graphene oxide/carbon nanotube-supported layered double hydroxides: enhancing the CO 2 sorption properties. Carbon 123, 616–627 (2017).



3D representation of Layered Double Hydroxide platelets supported on Single Walled Carbon Nanotube network.

P084 **Mo 19:00 - 21:00**

Versatile Manipulation of Nanostructured Noble Metal Aerogels for Electrocatalysis and Beyond

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Combining the features of noble metals and aerogels, noble metal aerogels (NMAs) have emerged as a rising star in material science. Sol-gel process is the dominant strategy to fabricate NMAs. To date, quite a few systems (Au, Ag, Pd, Pt, Pd-Pt, etc.) have been demonstrated and diverse applications have been investigated. However, a superficial understanding of gelation mechanism retard the flexible manipulation of NMAs, thus hindering investigating composition/structure-property/performance relationship for material design and optimization.

In this regard, we introduced specific-ion effects to address above issues,1 where a delicate modulation of ion-nanoparticle interactions afford versatile manipulation of NMAs. As a result, NMAs with highly tunable compositions (Au, Ag, Pd, Pt, etc.), ligament size (3.1~142.0 nm), special morphologies are directly produced from dilute nanoparticle solutions. An overall physical picture regarding the gelation process has been proposed by combined experimental and theoretical approaches. Various applications including electro-oxidation of methanol/ethanol and self-propulsion bevavior have been demonstrated.

1. R. Du, Y. Hu, R. Hübner, J.-O. Joswig, X. Fan, A. Eychmüller, Sci. Adv. 2019, accepted.

P086 **Mo 19:00 - 21:00**

Nano-engineering of a hybrid organic-inorganic composite hole-transporting material and its application in perovskite solar cells

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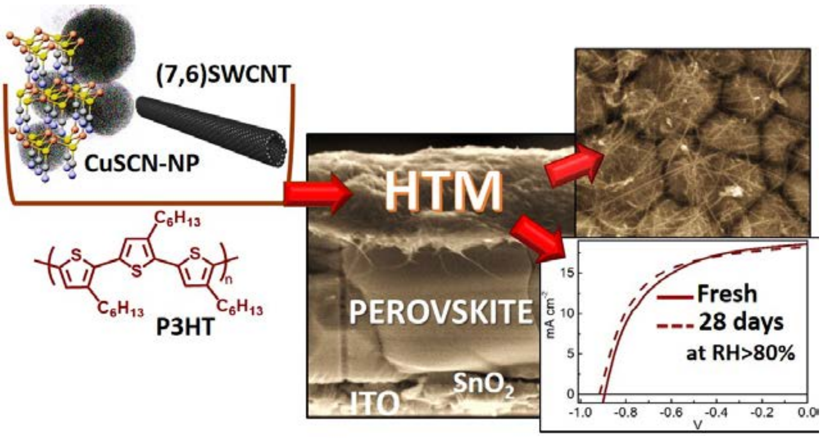
The development of cost-effective hole-transporting materials (HTM) that are capable of providing stable solar cells in environmental conditions is of paramount importance to prospect an effective commercialization of third-generation photovoltaic technology. We report here on a ternary composite HTM based on a semiconducting poly(3-hexylthiophene) (P3HT) matrix used to disperse CuSCN nanoparticles and semiconducting single-walled carbon nanotubes (SWCNT). The choice of this materials combination comes from rational design of the HTM, based on exploiting the ease of processing a polymer-based HTM as P3HT, the electron-blocking ability of a high-band gap semiconductor as CuSCN and the fine-tuning of the layer electronic properties through the addition of SWCNT.
The composite HTM is tested in a standard architecture perovskite solar cell (PSC). Physicochemical and electrical investigations on the bulk HTM, coupled to photophysical probing of the perovskite/HTM interface, unravel the contributions and limitations of each component in the composite. A synergic action of the three species in the HTM occurs, ensuring the maintenance of a stable power conversion efficiency in PSC stored un-encapsulated for almost one month in a high-moisture content atmosphere.



P088 **Mo 19:00 - 21:00**

Highly heat-resistant battery separator based on boron nitride nanotube

Kentaro Kaneko[1], Keisuke Hori[1], Suguru Noda[1]

[1]*Department of Applied Chemistry, Waseda University, Tokyo 169-8555, Japan*

Separator is a key component for safety of batteries. The conventional separator is made of polypropylene (PP), but its fundamental thermal stability is low. We here propose and report highly heat-resistant separator based on boron nitride nanotube (BNNT), which has high chemical and thermal stabilities (air-stable up to 900 °C).

Self-supporting BNNT films (Thickness: 25 µm) were fabricated by dispersion and filtration without using binder. Similarly, self-supporting electrodes based on carbon nanotube (CNT) with lithium cobalt oxide (LCO) and graphite for cathode and anode, respectively, were fabricated. The cathode/separator/anode stack was prepared, heated to and kept at a certain temperature for 10 min. After cooled down, the insulation was checked and coin cell was fabricated using the stack and fresh electrolyte.

Fig. 1a shows the cathode/separator/anode stacks after the heat-resistance test. The PP separator shrank, resulting in short-circuit at 225 °C whereas the BNNT separator showed no change and kept insulation at 500 °C. Fig. 1b shows the charge-discharge curves of the stacks without and with heating. No difference was found between them, showing that BNNT separator as well as the CNT-based electrodes worked without problem after heating at 500 °C.

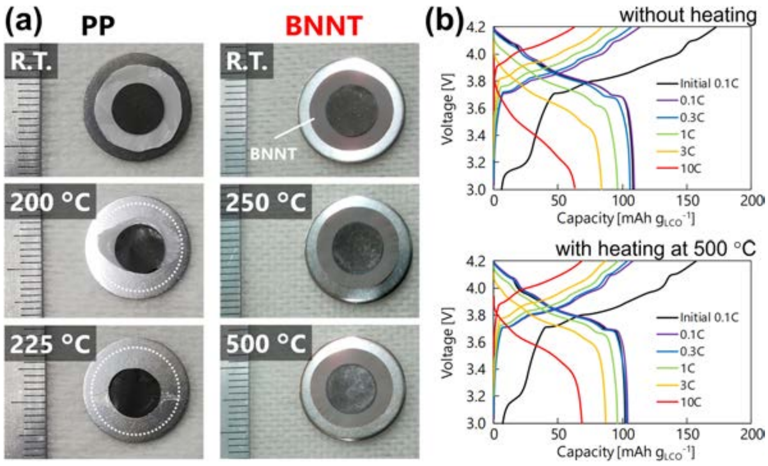


Fig. 1. Heat-resistance test. (a) Optical images of the cathode/PP/anode and cathode/BNNT/anode stacks after heating at various temperatures. (b) Charge-discharge curves of the LCO/BNNT/graphite full cells without and with heating.

P090 **Mo 19:00 - 21:00**

Mechanism of Ferrocene Decomposition and Fe Cluster Formation during Floating Catalyst Chemical Vapour Deposition

Ben McLean[1], Alister Page[1]

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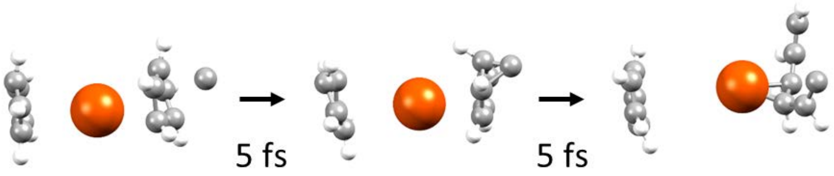
Floating catalyst chemical vapour deposition (FCCVD) using ferrocene provides a simple and effective way of producing high quality single-walled carbon nanotubes (SWCNTs).1 With ferrocene as the floating catalyst, FCCVD has successfully synthesised SWCNTs with carbon monoxide, methane, ethanol, and most recently, ethylene. Ferrocene is observed to dissociate and form catalytic Fe nanoparticles during this process and subsequently catalyse the nucleation and growth of SWCNTs. However, the mechanism of ferrocene decomposition in the presence of ethylene and the nucleation mechanisms of SWCNTs during FCCVD is largely unexplored. Here, using QM/MD simulations, we reveal the mechanism of ferrocene dissociation and Fe nanoparticle formation. We observe the nucleation of sp^2 carbon networks from the reorganisation of polyyne chains akin to those previously observed to form during fullerene formation. We note a competitive process between the formation sp^2 carbon networks and the nucleation of Fe clusters.



The decomposition of ferrocene in the presence of ethylene during FCCVD.

P092 **Mo 19:00 - 21:00**

Nucleation Mechanism of Boron Nitride Nanotubes during Ni-catalysed Chemical Vapour Deposition

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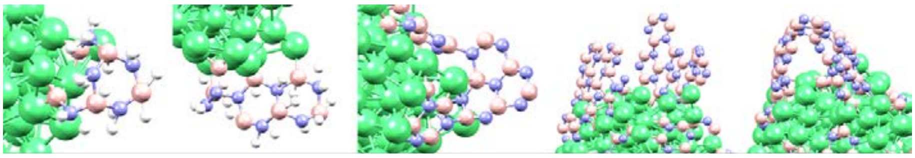
The catalytic chemical vapour deposition (CVD) growth of carbon nanotubes (CNTs) has been studied extensively both experimentally and theoretically, with a well understood growth mechanism. In contrast, boron nitride nanotubes (BNNTs) have been synthesised successfully via CVD though little is known regarding the catalytic pathways to BNNT nucleation and growth. Here we present a CVD mechanism explaining the nucleation and growth of BNNTs during Ni-catalysed CVD from ammonia borane, using ReaxFF molecular dynamics simulations. Our simulations reveal that the Ni catalyst activates B-H bonds to produce H_2, and subsequently frees BN fragments to form BN chains on the Ni catalyst surface. The formation of BN rings is achieved via the Ni catalyst selectively breaking B-B and N-N bonds within BN chains in favour of B-N bonds. Ultimately, these simulations reveal the formation mechanism of BNNT caps, which prior to this work, were assumed to follow similar formation mechanisms to CNT caps. We observe the “clicking together” of adjacent BN ring networks that grow perpendicular to the surface. This mechanism supports experimental evidence of the comparatively sharper caps and wider diameters of BNNTs to CNTs.



0.7 ns 1.5 ns 3.0 ns 17.6 ns 17.7 ns

Mechanism of BN ring nucleation during Ni-catalysed CVD following the production of H2. After significant simulation time, we observe the subsequent growth and “clicking together” of BN ring networks to form a BNNT cap.

P094 **Mo 19:00 - 21:00**

Metadynamics and DFTB: Free energy calculations using density functional tight binding.

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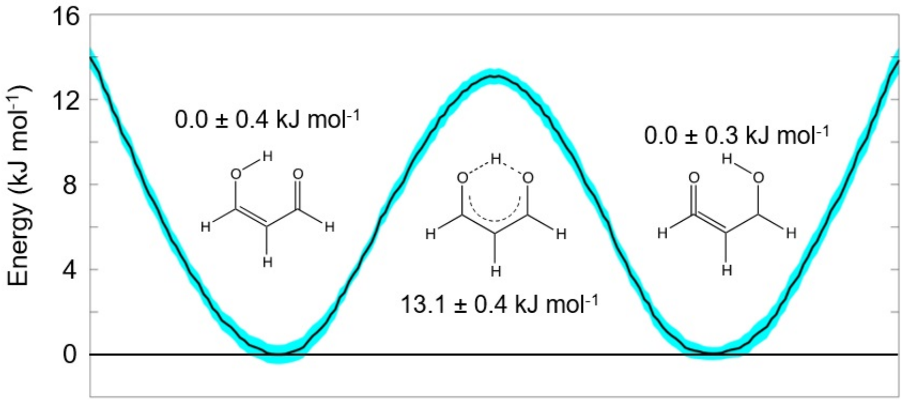
[3] *Bremen Center for Computational Materials Science, University of Bremen, Bremen, 28334, Germany*

Despite extensive advancements in quantum chemical methods in investigating the kinetics of chemical systems at a fundamental level, one of the key remaining barriers to simulating dynamics over long time scales is the presence of high energy barriers in the free energy surface and the rare events. These rare events result in typical simulations such as molecular dynamics and Monte-Carlo calculations being confined to specific low energy minima, unable to sample the larger free energy surface. One promising method for overcoming these high energy barriers is metadynamics. Metadynamics works simply by biasing a molecular dynamics simulation via a memory bias consisting of gaussian functions which prevent or hinder the simulation from revisiting areas of the free energy surface it has already sampled. Further, by summing these gaussians at the end of the simulation an approximation to the free energy surface can be recovered. As such, we have integrated PLUMED2, an analysis and biasing suit capable of implementing metadynamics into the DFTB+ code, a density functional tight binding calculation code capable of molecular dynamics. We then tested this interface on several model systems including epoxide diffusion and Stone-Wales defect healing in graphene.



Malonaldehyde Free energy surface at 300K determined using DFTB-MD with metadynamics.

P096 **Mo 19:00 - 21:00**

Long Carbon Chains Observed in ab initio Molecular Dynamic Simulation of Carbon Nanotube Growth

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[2]Center for Multidimensional Carbon Materials, Institute for Basic Science, Ulsan, 44919, Republic of Korea

Long carbon chains are often observed in many molecular dynamic (MD) simulations during carbon nanotube (CNT) growth, while its role in the cap formation and further elongation process is still beyond our knowledge. In this work, using density functional theory-based molecular dynamics simulation (DFT-MD), we, for the first time, report a complete cap nucleation process of CNT on an iron particle, and reveal the important role of long carbon chains in CNT nucleation. At initial stage, the existence of long chains facilitates CNT growth by triggering the nucleation of the first polygon in CNT cap. However, when there grows more chains, it in turn, interrupts the cap formation by preventing the increasing of more polygons and poisoning the catalyst surface. We found that by breaking the long chains on the particle into pieces, the nucleation could be easily restarted, and subsequently, a complete cap formation was observed. Therefore, we propose that in experiments of growing CNT, such as chemical vapor deposition method, appropriate partial pressure of gases (H_2, and H_2O, etc.) other than the precursor is essential for cutting down the formed long chains and facilitating the cap nucleation.

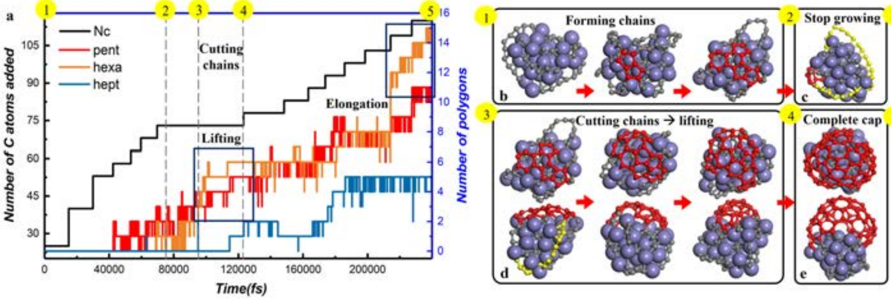

Fig. 1 (a) Number of C and polygons during cap formation on Fe. Four periods in cap formation: (1-2) long chains and 5 polygons grow; (2-3) no new polygons appear; (3-4) by cutting the long chains, cap formation restarts; (4-5) a complete cap forms.

P098 **Mo 19:00 - 21:00**

Necking of carbon nanotubes: a 1D continuum approach

Nicola Rizzi[1], Ginevra Salerno[1], Alessandra Genoese[1], Andrea Genoese[1]

[1] *LIMeS, Department of Architecture, Roma Tre University*

This work exploits a 1D model, proposed previously [1] for graphene sheets, for the analysis of necking in CNTs subjected to tension (see e.g. [2]). Two cases are examined: a) only stretch and angular variation energies are considered; b) also dihedral energy is added. Cauchy-Born procedure is adopted for constructing the continuum model and several interatomic potentials are used. Some cases are studied, involving both armchair and zigzag arrangements. The trivial nonlinear equilibrium path is determined, that exhibits a limit point, and a bifurcation (necking) is determined along it. The postbuckling behaviour is then studied. The numerical results are discussed pointing out relevant questions like the auxetic behavior of the armchair CNTs and the snap-back of the bifurcated path.

[1] H. Aminpour, N. Rizzi, On the Modelling of Carbon Nano Tubes as Generalized Continua, in Generalized Continua as Models for Classical and Advanced Materials, (H. Altenbach and S.Forest, Editors), Springer International Publishing Switzerland 2016, ISBN 978-3-319-31719-9 ISBN 978-3-319-31721-2 (eBook) DOI 10.1007/978-3-319-31721-2

[2] S. Zhang and T. Zhu, Atomic geometry and energetics of carbon nanotube necking, Philosophical Magazine Letters, Vol. 87, No. 8, August 2007, 567-574.

P100 **Mo 19:00 - 21:00**

Molecular dynamics simulations for nuclear magnetic relaxation time of water encapsulated in a carbon nanotube

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[2]*Department of Electrical Engineering, Tokyo University of Science, Tokyo, 125-0051, Japan*

In a solid phase of water encapsulated in a carbon nanotube (CNT), a one-dimensional structure called “ice nanotube’’ is known to be formed, different from that of a hexagonal ice called Ih. The previous works have reported that the solid phase changes to liquid-like phase with increase in temperature. In the liquid-like phase, the motions of water molecules are not as random as the bulk liquid since the water molecules are confined inside the CNT. One of experiments suitable for investigating such motions is the nuclear magnetic resonance (NMR). However, the NMR experiment allows us to measure the characteristic time scale of the motions, while it is difficult to identify the dynamic atomic scale structure. Therefore, we need to relate the results obtained from the atomic scale simulation to the NMR measurement.

In this study, we simulated the motions of water molecules encapsulated in a CNT by using the molecular dynamics method, and then estimated the nuclear magnetic relaxation times according to the procedure in the previous theoretical work. The water model used in our simulations is the SPCE, and the UFF potential is employed for the interaction of the water molecules with the fixed CNT. Moreover, the temperature was controlled with the Nose-Hoover thermostat.

P102 **Mo 19:00 - 21:00**

Molecular Dynamics Simulation of Defect Generation by Irradiation of Platinum Particles on Graphite

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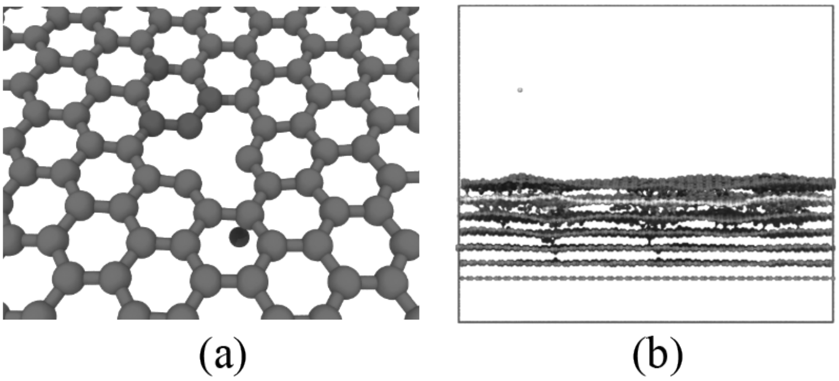
[2]*RIST, Tokyo University of Science, Tokyo 125-8585, Japan*

Arc Plasma deposition (APD) method is focused as a method of producing platinum catalyst, which can reduce a quantity of platinum. Since platinum which is used as catalyst of fuel cell is a valuable resource and costly, it is desired to reduce the amount of platinum used. Therefore, as a solution to this problem, APD method has been proposed.

In the previous study, it was reported that the platinum nanoparticles deposited on graphite by APD method improves catalytic activity. The reason of enhancing is assumed that grain boundaries of graphite deform lattice constant of platinum. Furthermore, in other previous study, the adsorption energy of platinum atoms to graphene with point defect was calculated by the first principle calculation, and it showed the highest adsorption energy at the point defect. From these results, defects formed on the graphite surface are considered to improve the catalytic performance. However, it is not clear how and what defects are generated by APD method.

In this study, we simulate the APD method by molecular dynamics and investigate how and what defects are generated on the graphite surface.

Our calculations show that defect structures and defect size are strongly affected by irradiation position, velocity and angle.



Schematic illustration of simulation, (a)Structure of Defects, (b)Amount of Defects

P104 **Mo 19:00 - 21:00**

Computational simulation of cohesive energy of CNT bundles in the water

Nanami Yamazaki[1], Takahiro Yamamoto[1,2]

[1]*Department of Electrical Engineering, Tokyo University, Tokyo 125-8585, Japan*
[2]*RIST, Tokyo University of Science, Tokyo 125-8585, Japan*

Carbon-nanotube ink (CNT ink) is expected to be a new generation of ink for printed electronics applications, because CNTs are highly conductive and functions better than metals under oxidative conditions. In this application, it is essential to understand and control the dispersibility of CNTs in water. Recently, Homma et al., found experimentally that the water form two hydration layers around a CNT in the water. Thus our purpose of study is to clear the effects of the hydration layers on the dispersibility of CNTs in water.
In this study, we have computationally studied the cohesive energy of CNT bundles in the water using classical molecular dynamics (MD) method. We used SPCE potential as a force field between water, Tersoff potential as a force field between carbons, Lennard-Jones potential as a force field between CNTs and UFF potential as a force field between carbon and water. In this presentation, we explain the influence of giving aggregation between CNTs by two hydration layers around CNT in water.

Program Tuesday

Plenary program Franconia Hall

Session Pl3 Chair: Milo Schaffer

08:30 - 09:15	K2	**Janina Maultzsch** (FAU Erlangen-Nürnberg) *Optical Spectroscopy of Low-Dimensional Semiconductors*
09:15 - 09:40	I5	**Caterina Cocchi** (Humboldt-Universität zu Berlin) *Graphene Modulates the Optical Properties of Low-Dimensional Heterostructures*
09:40 - 10:05	I6	**Shohei Chiashi** (University of Tokyo) *Water Adsorption and Desorption on Single and Suspended Single-Walled Carbon Nanotubes by Spectroscopy*

Coffee break CCW Lobby

Session Pl4 Chair: Boris Yakobson

10:35 - 11:00	I7	**Milo Shaffer** (Imperial College London) *Versatile and Scalable Approaches to Chemical Processing of Nanocarbons*
11:00 - 11:25	I8	**Michael Strano** (MIT) *From Energy Harvesting to Living Plants - Concepts in Living and Synthetic Energy Conversion Enabled by Carbon Nanomaterials*
11:25 - 11:50	C3	**Lei Shi** (Sun Yat-sen University) *Tailoring the Confined One-Dimensional Linear Carbon Chains*
11:50 - 12:15	I9	**Qingwen Li** (Chinese Academy of Sciences) *Sorting and Aligning Single-Chirality Semiconducting Carbon Nanotubes*

Lunch break

Electronics Symposium (CNTFA19) Panorama 11

Chair: Christoph Strunk

14:00 - 14:40	SEI7	**Edward Laird** (Lancaster University) *A Coherent Mechanical Oscillator Driven by Single-Electron Tunnelling*
14:40 - 15:00	SEI8	**Pertti Hakonen** (Aalto University) *Suspended Single-Walled Carbon Nanotubes for Optomechanics and Sensing*
15:00 - 15:20	SEI9	**Andreas K. Hüttel** (University of Regensburg) *Microwave Optomechanics With a Suspended Carbon Nanotube Quantum Dot*

10 minute break

Chair: Edward Laird

15:30 - 15:50	SEI10	**Yuval Yaish** (Technion) *Snap-Through Buckling Bi-Stability in Suspended Carbon Nanotube Resonators*
15:50 - 16:10	SEI11	**Lin Cong** (Tsinghua University) *Realization of the Mixing Excitation and the Coherent Electron-Phonon Coupling in Nanomechanical Resonators*
16:10 - 16:30	SEI12	**Alexis Descombin** (Université Lyon 1 ILM) *Tuning the Mechanical Q-Factor of SWCNT With External Voltage*

Coffee break CCW Lobby

Energy Symposium (NMES19) Franconia Hall

Chair: Sang Ouk Kim

14:00 - 14:40	SEn7	**Fei Wei** (Tsinghua University) *Structure Control, Mass Production of Well Aligned Carbon Nanotubes for Energy Application*
14:40 - 15:00	SEn8	**Christoph Brabec** (FAU Erlangen-Nürnberg) *TBA*
15:00 - 15:20	SEn9	**Esko I. Kauppinen** (Aalto University) *Dry Deposition of Nanocarbon Thin Films for Energy Applications*

10 minute break

Chair: Fei Wei

15:30 - 15:50	SEn10	**Sang Ouk Kim** (KAIST) *Graphene Oxide Liquid Crystal*
15:50 - 16:10	SEn11	**Chang Liu** (Chinese Academy of Sciences) *Single-Wall Carbon Nanotube Films and Their Hybrids for Energy Applications*
16:10 - 16:30	SEn12	**Wei Lyu** (Tsinghua University) *Catalysis in Lithium-Sulfur Batteries*

Coffee break CCW Lobby

2D Materials Symposium (GSS19) Panorama 13

		Chair: Alexander Hoegele	
14:00 - 14:20	S2D7	**Yoke Khin Yap** (Michigan Technological University) *Two-Dimensional Gold With Tunable Bandgaps*	
14:20 - 14:40	S2D8	**Catherine Journet** (Laboratoire des Multimatériaux et Interfaces) *New Atomic Layer Deposition (ALD) of Boron Nitride (BN) Based on Polymer Derived Ceramics Route: Potentiality for Complex Nanostructure Fabrication*	
14:40 - 15:00	S2D9	**Jinbo Pang** (University of Jinan) *Large Area Synthesis of Transition Metal Dichalcogenide for Non Linear Optics and Q Switched Laser Application*	
15:00 - 15:20	S2D10	**Yang Wu** (Tsinghua University) *Effective Growth of Large Scale 2D Single Crystals With High Qualities*	
		10 minute break	
		Chair: Xavier Marie	
15:30 - 15:50	S2D11	**Usman Khan** (Tsinghua University) *Controlled Vapor-Solid Deposition of Millimeter-Size Single Crystal 2D Bi2O2Se for High Performance Phototransistors*	
15:50 - 16:10	S2D12	**Michael Heuken** (AIXTRON) *MOCVD Growth and Characterization of MoS_2 and WS_2*	
16:10 - 16:30	S2D13	**Hyangsook Lee** (Samsung advanced Institute of Technology) *TEM Observation of Dynamic Structural Change in Synthetic MoS_2 Under Electron Beam Irradiation*	
		Coffee break	CCW Lobby

Synthesis Symposium (SPFLD19) Panorama 12

Chair: Ben Flavel

14:00 - 14:20 SSy1 **Wim Wenseleers** (University of Antwerp)
Nanocarbon Structures Synthesized in the One-Dimensional Core of Carbon Nanotubes: Wavelength-Dependent Raman Spectroscopy

14:20 - 14:40 SSy1 **Jeffrey Fagan** (National Institute of Standards and Technology)
Extending the Boundaries of Aqueous Two-Phase Extraction of Single-Wall Carbon Nanotubes Using Surfactants

14:40 - 15:00 SSy2 **Michael Arnold** (University of Wisconsin-Madison)
Bottom-Up Synthesis of Sub-5 Nm Armchair Graphene Nanoribbons via CVD

15:00 - 15:20 SSy3 **Etienne Gauffrès** (CNRS - Lab. Phot. Numérique et Nanosciences)
Optical Properties of Dyes Aggregated Into Carbon and Boron Nitride Nanotubes

10 minute break

Chair: Shigeo Maruyama

15:30 - 15:50 SSy4 **Robert Nißler** (Georg-August-Universität Göttingen)
Chirality Enriched Carbon Nanotubes With Tunable Wrapping via Corona Phase Exchange Purification (CPEP)

Spectroscopy Symposium (NSAP19) Panorama 12

Chair: Leandro Malard

15:50 - 16:30 SSp1 **Steven Doorn** (Los Alamos National Laboratory)
Harnessing Carbon Nanotube Defect States as Quantum Emitters

Coffee break CCW Lobby

Theory Symposium (CCTN19) Panorama 10

Chair: Christophe Bichara

14:00 - 14:20	STh1	**Alister Page** (University of Newcastle) *Etchants, Nucleation and Chirality Control During CVD Growth of CNTs: Insights From Molecular Simulation*
14:20 - 14:40	STh2	**Zhao Wang** (Guangxi University) *Chirality-Dependent Motion Transmission Between Aligned Carbon Nanotubes*
14:40 - 15:00	STh2	**James Elliott** (University of Cambridge) *Dynamics of CNT Aerogel Formation: a Hybrid Langevin and Molecular Dynamics Approach*
15:00 - 15:20	STh3	**Benedetta Flebus** (University of California LA) *Tuning Electronic Properties of Carbon Nanotubes by Graphene Promixity*

10 minute break

Chair: Deborah Prezzi

15:30 - 15:50	STh4	**Ksenia V. Bets** (Rice University) *Carbon Nanotube–Catalyst Interface Segregation and the Quest for Chirality Control*

NanoBio Symposium (CNBMT19) Panorama 10

Chair: Ardemis Boghossian

15:50 - 16:30	SNB1	**Michael S. Strano** (MIT) *Applications of Carbon Nanosensors to Understanding Biochemical Signaling Within the Human Body*

Coffee break CCW Lobby

Poster Sessions CCW Lobby Level

17:00 - 18:30	Poster Session 3 (odd poster numbers)
19:00 - 21:00	Poster Session 4 (even poster numbers)

Abstracts Tuesday
(Oral)

Plenary Venue K2 (keynote)

Franconia Hall **Tu 08:30 - 09:15**

Optical spectroscopy of low-dimensional semiconductors

Janina Maultzsch[1]

[1] *Chair of Experimental Physics, Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany*

Two-dimensional semiconductors, such as transition-metal dichalcogenides, can be stacked vertically into heterostructures, where the individual layers are bound by predominantly van-der-Waals forces. Depending on the band alignment, optical excitation create interlayer-excitons, where electron and hole are spatially separated. Here we present ab-initio calculations, including many-particle interactions, of the electronic band structure of a $MoSe_2$-WSe_2 hetero-bilayer [1]. Our calculations of the optical absorption confirm the existence of interlayer excitons with substantial binding energy. Furthermore, we show that the fundamental band gap of this heterostructure is indirect in k-space, while it is indirect in real space as well. The polarization selection rules are predicted to depend on stacking order, which may be used for optical characterization of twisted heterostructures.

[1] R. Gillen and J. Maultzsch, Phys. Rev. B 97, 165306 (2018); https://arxiv.org/abs/1801.06310

Plenary Venue I5 (invited)

Franconia Hall **Tu 09:15 - 09:40**

Graphene modulates the optical properties of low-dimensional heterostructures

Caterina Cocchi[1]

[1] *Physics Department and IRIS Adlershof, Humboldt-Universität zu Berlin, Germany*

The ability of graphene to effectively interact with molecular adsorbates and other layered materials can be exploited to modulate the electronic and optical properties of the resulting hybrid systems. Ab initio methods like density-functional theory and many-body perturbation theory are ideally suited to disclose and analyze these effects. In this talk, I will discuss how the graphene substrate impacts the optical response of a physisorbed monolayer of azobenzene molecules via two counteracting mechanisms. Substrate-induced polarization reduces the band-gap while enhanced dielectric screening weakens the electron-hole attraction. As a result, intramolecular (intermolecular) excitations are blue- (red-)shifted and dark excitations in the isolated azobenzene monolayer are activated by the graphene substrate [1]. As a second example, I will illustrate how the controlled intercalation of graphene and hexagonal BN layers can significantly enhance light-matter interaction in the resulting heterostructure and lead to new excitations [2] that are sensitive to the stacking arrangement [3].

[1] Q. Fu, et al., Phys. Chem. Chem. Phys. 19, 6196 (2017)
[2] W. Aggoune, et al., J. Phys. Chem. Lett. 8, 1464 (2017)
[3] W. Aggoune, et al., Phys. Rev. B (R) 97, 241114 (2018)

Franconia Hall **Tu 09:40 - 10:05**

Water Adsorption and Desorption on Single and Suspended Single-walled Carbon Nanotubes by Spectroscopy

Shohei Chiashi[1], Yoshikazu Homma[2]

[1] *Dept. of Mechanical Engineering, The University of Tokyo, Bunkyo, Tokyo 113-8656, Japan*
[2] *Dept. of Physics, Tokyo University of Science, Shinjuku, Tokyo 162-8601, Japan*

Though the interaction between a water molecule and graphitic surface is weak, water often plays an important role in the properties of carbon materials. In the case of single-walled carbon nanotubes (SWCNTs), water exhibit adsorption and desorption phenomena on the outer surface of SWCNTs [1,2]. Moreover, the inner space of SWCNT is also adsorption site of water [3]. Water in SWCNTs at lower temperature forms ice-nanotube and the melting point of ice-nanotubes sensitively depends on SWCNT tube diameter [3,4]. In this study, we investigated the various behaviors of water surrounding SWCNTs by using optical spectroscopy measurements to single and suspended SWCNTs. The structure of suspended SWCNTs is ideal and it veiled the details of the water effects on SWCNT properties.

[1] Y. Homma, S. Chiashi, T. Yamamoto, K. Kono, D. Matsumoto, J. Shitaba, S. Sato, Phys. Rev. Lett., 110, (2013) 157402.
[2] S. Chiashi, K. Kono, D. Matsumoto, J. Shitaba, N. Homma, A. Beniya, T. Yamamoto, Y. Homma, Phys. Rev. B, 91 (2015) 155415.
[3] S. Chiashi, T. Hanashima, R. Mitobe, K. Nagatsu, T. Yamamoto, Y. Homma, J. Phys. Chem. Lett., 5,(2014) 408.
[4] S. Chiashi, Y. Saito, T. Kato, S. Konabe, S. Okada, T. Yamamoto, Y. Homma ACS Nano, 19 (2019) 1177.

Plenary Venue I7 (invited)

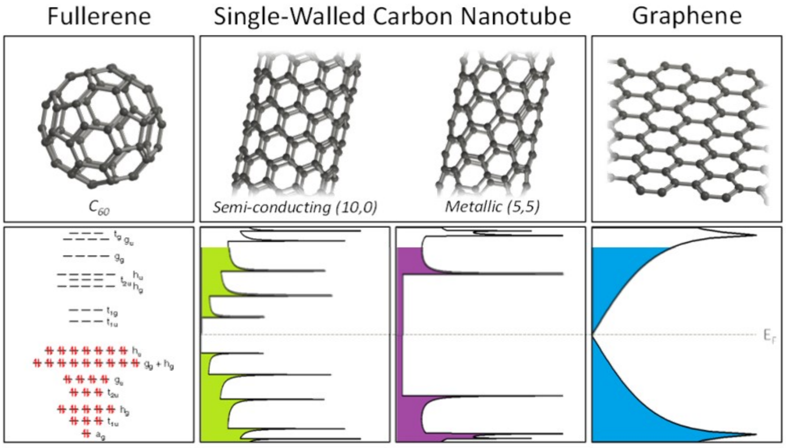
Franconia Hall **Tu 10:35 - 11:00**

Versatile and scalable approaches to chemical processing of nanocarbons

Milo Shaffer[1]

[1]*Deptartments of Chemistry and Materials, Imperial College London, UK*

Individual perfect nanocarbons have exceptional properties; the challenge is often how to exploit their potential in real macroscopic systems. Filled SWNTs access intriguing new elemental allotropes. However, external chemical functionalisation is critical to a wide range of nanocarbon technologies. Existing approaches tend to rely on liquid phase reactions, often requiring damaging sonication or lengthy work up through filtration or centrifugation.
An alternative uses reductive charging to form pure nanotubide (nanotube anion) solutions. This simple system is also effective for MWCNTs, ultralong SWCNTs, carbon blacks, graphenes, and nitrides. The resulting ions can be modified chemically with organic functional groups, polymers, or inorganic components for a variety of applications. The mechanism involves a surprising, complex intermediate, revealed by open circuit voltammetry. Dispersed nanocarbon materials can be assembled, by electrophoresis, cryogel formation, or direct cross-linking to form Joule heatable networks, protein nucleants, supercapacitor electrodes, and catalyst supports . Comparative studies allow the response of nanocarbons with different dimensionalities to be assessed to identify fundamental trends and the most appropriate form for specific situations.



Adding (or removing) electrons from the band structure of nanocarbons creates discrete molecular ions that can retain a continuum density of state. See Chem. Rev., 2018, 118 (16), 7363 (DOI: 10.1021/acs.chemrev.8b00128) for a comprehensive review.

Plenary Venue I8 (invited)

Franconia Hall **Tu 11:00 - 11:25**

From Energy Harvesting to Living Plants - Concepts in Living and Synthetic Energy Conversion enabled by Carbon Nanomaterials

Michael Strano[1]

[1] *MIT, Department of Chemical Engineering, Cambridge, MA 02139-430, USA*

Our lab at MIT has been interested in how the 1D and 2D electronic structures of carbon nanotubes and graphene respectively can be utilized to advance new concepts in molecular detection, as well as energy generation. By taking advantage of the exceptional electronic properties of these nano-structures, we continue to discover potential application spaces where carbon can play an important role. I will highlight our recent efforts in initiating an endeavor we call “Plant Nanobionics”. There we use techniques to deliver and transport functional nanoparticles into living plants to grant them non-native functions. Our goal is to engineer plants to take over many of the functions now performed by electrical devices. I will introduce the nanoparticle co-localization mechanism in a plant, and highlight some of our recent nanobionic plant prototypes including a light-emitting plant. Two-dimensional (2D) materials can uniquely span the physical dimensions of a surrounding composite matrix in the limit of maximum reinforcement. However, the alignment and assembly of continuous 2D components at high volume fraction remain challenging. We use a stacking and folding method to generate aligned graphene/polycarbonate composites with as many as 320 parallel layers spanning 0.032 to 0.11millimeters in thickness that significantly increases the effective elastic modulus and strength at exceptionally low volume fractions of only 0.082%. An analogous transverse shear scrolling method generates Archimedean spiral fibers that demonstrate exotic, telescoping elongation at break of 110%, or 30 times greater than Kevlar. Additionally, we present a theory, experimentally validated, of how fluid phase equilibria is significantly altered when confined to nanometer scale dimensions, creating the potential to embed tunable phase change materials, as well as unique liquid or solid properties encapsulated within new matricies. Our theory, based on the Turbull number, can predict the solid/liquid coexistence for any fluid and any Nanoconfined system down to approximately 4 nm. Below this limit, we show remarkable departures experimentally. Fluid phase transitions inside isolated nanotubes deviate substantially from classical thermodynamics and also allow the study of ice nanotube (ice-NT) properties. The results reveal both an exquisite sensitivity to diameter and substantially larger temperature elevations of the melting transition than theoretically predicted by as much as 100°C. Dynamic water filling and reversible freezing transitions were marked by 2 to 5cm-1 shifts in the radial breathing mode (RBM) frequency, revealing reversible melting at 138°C and 102°C for 1.05 and 1.06nm single and double-walled CNTs, respectively. These new fabrication and thermodynamic concepts promise fundamentally new materials with unique combinations of properties. Lastly, I will briefly describe several applications of carbon nanomaterials in the energy space that have come out of our lab. We have introduced carbon materials for what we call thermal resonators that make use of thermal storage elements with high effusivity – the product of the thermal conductivity and heat capacity to the one half power. Thermal resonators base on carbon can harvest energy indefinitely from ambient thermal fluctuations of various frequencies, opening new possibilities for remote power applications.

Plenary Venue C3 (contributed)

Franconia Hall **Tu 11:25 - 11:50**

Tailoring the confined one-dimensional linear carbon chains

Lei Shi[1,2], Sofie Cambré[3], Wim Wenseleers[3], Ryosuke Senga[4], Kazu Suenaga[4], Takeshi Saito[4], Alejandro Pérez Paz[5,6], Angel Rubio[5], Paola Ayala[2], Thomas Pichler[2]

[1]*Sun Yat-sen University, School of Materials Science and Engineering, China*
[2]*University of Vienna, Faculty of Physics, Austria*
[3]*University of Antwerp, Experimental Condensed Matter Physics Laboratory, Belgium*
[4]*AIST, Nanomaterials Research Institute, 305-8565 Tsukuba, Japan*
[5]*Nano-Bio Spectroscopy Group, Universidad del País Vasco, Spain*
[6]*Yachay Tech University, School of Physical Sciences and Nanotechnology, Ecuador*

Recently we demonstrated synthesis of confined one-dimensional linear carbon chains (LCCs) inside double-walled carbon nanotubes (DWCNTs) with the shortest chains consisting of around 30 carbon atoms (polyyne) and the longest chains with a record length of more than 6000 carbon atoms (carbyne) [1]. The carbyne formation was confirmed by near-field Raman spectroscopy and its property was much tailored by its nanotube host [2,3]. Later on, we developed a method based on density gradient centrifugation to extract the LCCs and separate the short chains [4]. However, synthesis of specific length of LCCs is still challenging. In this presentation, I will show our recent efforts on tailoring the length of the confined LCCs using different carbon nanotubes as hosts [5]. In addition, I will show another new method to grow different length of LCCs monitored by in-situ Raman spectroscopy [6].

[1] L. Shi, et al. Nature Mater. 15, 634-639 (2016)
[2] S. Heeg, et al. Nano Lett. 18, 5426-5431 (2018)
[3] L. Shi, et al. Phys. Rev. Materials 1, 075601 (2017)
[4] L. Shi, et al. ACS Nano 12, 8477-8484 (2018)
[5] L. Shi, et al. Submitted (2019)
[6] L. Shi, et al. In preparation (2019)

Plenary Venue I9 (invited)

Franconia Hall **Tu 11:50 - 12:15**

Sorting and aligning single-chirality semiconducting carbon nanotubes

Qingwen Li[1], Bing Gao[1], Song Qiu[1], Zhengxia Lv[1], Hehua Jin[1]

[1] *Key Laboratory of Nanodevices and Applications, Suzhou Institute of Nanotech and Nano-bionics, Chinese Academy of Science, Suzhou, 215123, PR China*

Abstract: Semiconducting single-walled carbon nanotubes (s-SWCNTs) have shown potential promise in fabricating high-performance nanodevices for biosensors, broadband IR detectors and flexible TFTs etc. due to their unique one-dimensional confinement of electronic and phonon states. SWCNT with specific chiralities are highly desirable not only for fundamental research but also for designing optoelectronic and room-temperature quantum devices. We demonstrated a simple method by designing conjugated polymers with suitable conformation and energy level to selectively sort high-purity chiral s-SWCNTs with excellent device characteristics. Meanwhile, we also designed an assembly method for preparing a wafer-scale aligned array of s-SWCNT via the combination of introduced inter-tube electrostatic repulsion and an improved "bi-phasic" dip-coating. The inter-tube repulsion can significantly inhibit the agglomeration of s-SWCNT in the formation process of the aligned SWCNT films. Significantly, the aligned thin film can be fabricated with desired chiralities, excellent orientation and surface coverage.

Key words: s-SWCNT thin films, chirality, aligned, inter-tube electrostatic repulsion, dip-coating.

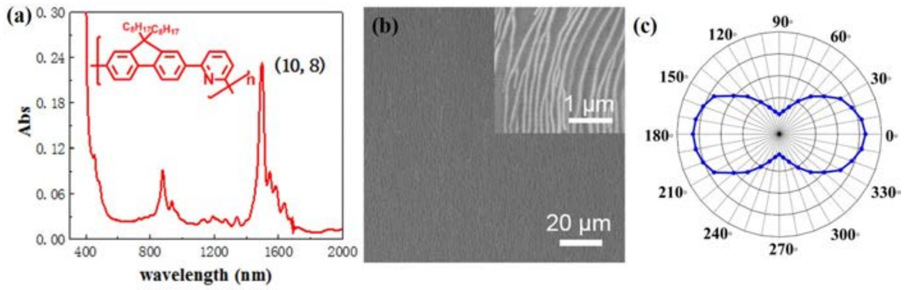


Figure (a) Absorption spectrum of high-purity chiral sc-SWCNTs; (b) SEM images of the aligned SWCNT films; (c) Polar plot of G band intensity under 532 nm laser excitation vs. laser polarization.

Panorama 11 **Tu 14:00 - 14:40**

A coherent mechanical oscillator driven by single-electron tunnelling

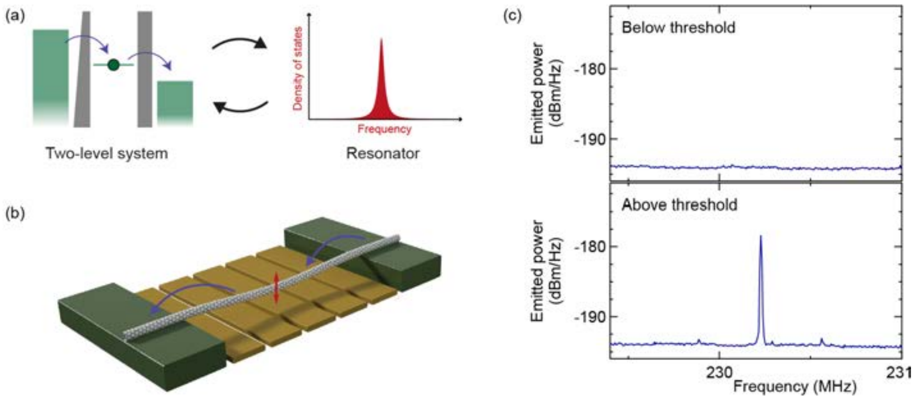
Edward Laird[1]

[1] Department of Physics, Lancaster University, United Kingdom

Suspended carbon nanotubes are mechanical resonators with low mass, high compliance, and high quality factor, which make them sensitive electromechanical detectors for tiny forces and masses. These same properties are favourable for studying the effects of strong measurement backaction. This talk will describe fast electrical measurements of a vibrating nanotube in which electron tunnelling excites spontaneous mechanical oscillations.

Our device consists of a clean carbon nanotube, spanned across a trench. A pair of tunnel barriers defines a single-electron transistor, whose conductance is proportional to the displacement. With low coupling, the single-electron transistor is a sensitive transducer of driven mechanical vibrations. At intermediate coupling, electrical backaction damps the vibrations. However, at strong coupling, the resonator can enter a regime where the damping becomes negative; it becomes a self-excited oscillator.

This electromechanical oscillator has many similarities to a laser, with the population inversion provided by the electrical bias and the resonator acting as a phonon cavity. We characterize the resulting coherence and demonstrate other laser characteristics, including injection locking and feedback narrowing of the emitted signal.



(a) Oscillator schematic. (b) Realization in a vibrating carbon nanotube. (c) Radio-frequency emission for device configurations below and above threshold, showing onset of self-exited oscillations.

Panorama 11 **Tu 14:40 - 15:00**

Suspended single-walled carbon nanotubes for optomechanics and sensing

Pertti Hakonen[1], Kaikkonen Jukka-Pekka[1], T.S. Abhilash[1], Marco Will[1], Igor Todoshchenko[1], Masahiro Kamada[1]

[1]*Low Temperature Laboratory, Department of Applied Physics, Aalto University, Finland*

Substantial supercurrents can be induced into high quality single walled carbon nanotubes (SWCNT) using contacts made of large gap superconducting material, such as MoRe. The supercurrents are strongly dependent on the gate charge and, consequently, these SWCNTs provide gate-tunable inductive components. In conjunction with microwave cavities, one can construct optomechanical settings which can reach charge, force, and displacement sensitivity approaching the limits set by quantum mechanics.

In suspended, 300-nm-long SWCNT devices with MoRe leads we have reached supercurrents up to 50 nA. In our SWCNT devices we find mechanical resonances around 1.5 GHz, while the Q factors amount up to 15000. We have investigated the superconducting phase dynamics in these Josephson junctions both under DC and AC bias, as well as under resonant coupling of mechanical and superconducting degrees of freedom.

Recently, we have employed our suspended SWCNT sensors for studies of atomically thin layers of 3He adsorbed on the tubes. Even though the van der Waals interaction is weak, clear indications of a phase transition are observed in the adsorbed layers at temperatures below 0.5 K.

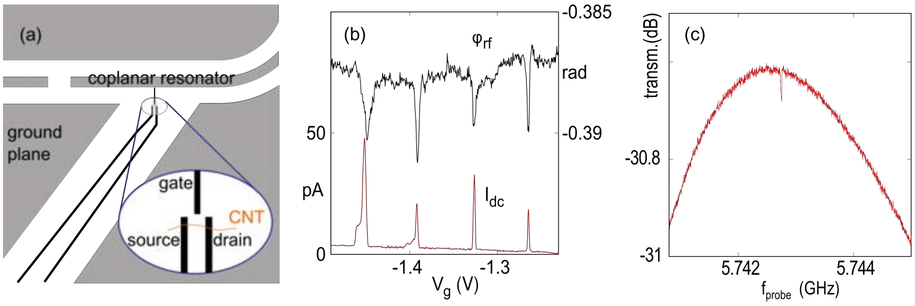
Panorama 11 **Tu 15:00 - 15:20**

Microwave optomechanics with a suspended carbon nanotube quantum dot

Andreas K. Hüttel[1]

[1] *University of Regensburg, 93040 Regensburg, Germany*

A clean, suspended single wall carbon nanotube is the ultimate limit of a nanomechanical beam resonator, where the fundamental transversal vibration mode reaches resonance frequencies on the order of 100MHz – 1GHz and mechanical quality factors up to 10^6. We have implemented a transfer technique to insert such nanotubes into coplanar superconducting circuitry, and present first results on quantum dot optomechanics at millikelvin temperatures. A GHz signal resonant to the microwave cavity probes the quantum capacitance of the attached nanotube, allowing us to characterize its charge response. In addition, however, nanotube vibration and microwave cavity form a dispersively coupled optomechanical system. With an optomechanically induced transparency (OMIT) experiment, we demonstrate that the intrinsic nonlinearity of Coulomb blockade enhances the coupling by several orders of magnitude, reaching high values of up to $g_0 = 50$ Hz. With this, the carbon nanotube - coplanar waveguide resonator system becomes attractive for many types of quantum-nanomechanical experiments.



(a) Schematic device, coupling a suspended nanotube to a coplanar GHz resonator. (b) Coulomb oscillations in dc current and resonator transmission phase. (c) OMIT signal in resonator transmission.

Electronics Symposium SEI10 (invited)

Panorama 11 **Tu 15:30 - 15:50**

Snap-Through Buckling Bi-Stability in Suspended Carbon Nanotube Resonators

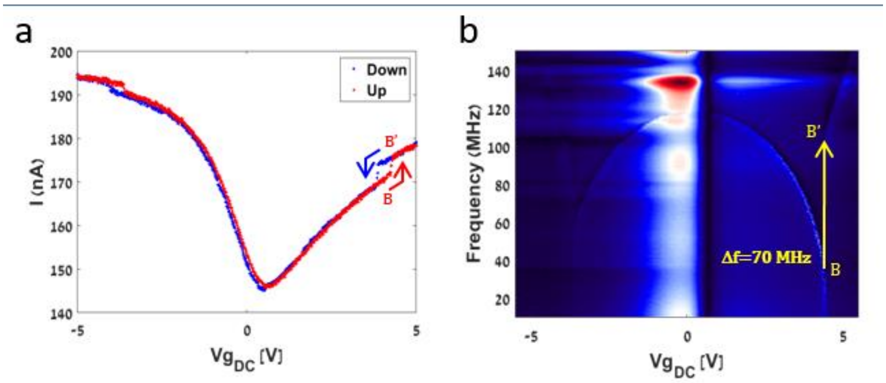
Yuval Yaish[1], Tal Tabachnik[1], Sharon Rechnitz[1], Michael Shlafman[1], Shlomo Shlafman[1]

[1] *Electrical Engineering, Technion, Haifa, 32000, Israel*

Mechanical bi-stability based on snap-through (ST) buckling is a well-known phenomenon in micro-electromechanical systems (MEMS) which serves as the underlying mechanism for many practical applications such as switches, actuators, sensors, filters, and memory elements, to name a few.

Here, we report the first realization of a suspended carbon nanotube (CNT) based bi-stable resonators exhibiting ST buckling phenomena. Both the static and dynamic responses of the system were obtained through conductance and resonance frequency measurements, respectively. In both measurements, non-linear effects such as jumps, hysteresis, softening and hardening, and super and sub-harmonic excitations were observed. Apart from these resonators being the smallest bi-stable electromechanical system based on ST buckling to date, our devices could also serve as excellent sensors with ultrahigh sensitivities, reaching electrostatic tunability values beyond 100MHz/V, which are also attractive for realization of mechanical quantum-bits.

Finally, we developed a comprehensive theoretical model based on the Euler-Bernoulli curved beam equation, and obtained excellent agreement with the experimental results.



Conductance (a) and resonance frequency (b) measurements of a typical device exhibiting snap-through behavior. The large abrupt mechanical ST transition results in a change in the conductance and a jump in the resonance frequency in the device.

Electronics Symposium SEI11 (contributed)

Panorama 11 **Tu 15:50 - 16:10**

Realization of the mixing excitation and the coherent electron-phonon coupling in nanomechanical resonators

Lin Cong[1], Xinhe Wang[2], Dong Zhu[3], Jiangtao Wang[1], Guoping Guo[3], Wenjie Liang[4], Kaili Jiang[1]

[1]*Department of Physics, Tsinghua University, Beijing, 100084, China*
[2]*Beihang University, Beijing, 100084, China*
[3]*University of Science and Technology of China, Hefei, 230022, China*
[4]*Institude of Physics, Chinese Academy of Sciences, Beijing, 100190, China*

The realization and regulation of dynamic coupling based on high-performance mechanical resonators is an extremely important topic in the research of nanomechanical resonators. We study the multimode resonators based on the quantum dot measurement scheme. The harmonic response of different vibration modes and the mechanism of achieving the mixing excitation are clarified through the experiments combined with the model simulation. In the nonlinear resonant region, the coherent coupling between the phonon state of the nanomechanical resonators and the single-electron state of the quantum dot is demonstrated, as well as the regulation of the coupling, which will open up burgeoning opportunities to study the multi-degree-of-freedom hybrid quantum system with phonons and electrons. On the other hand, we have also achieved an unprecedented comprehensive performance of nanomechanical resonators---high frequency, high tunability as well as high quality factor. All of these progresses will promote the exciting application of nanomechanical resonators, such as in quantum information processing.

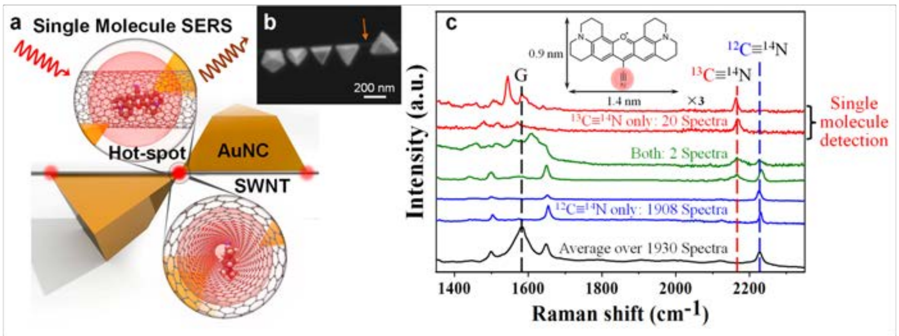
Panorama 11 **Tu 16:10 - 16:30**

Tuning the mechanical Q-factor of SWCNT with external voltage

Alexis Descombin[1], Philippe Poncharal[1], Alina Pascale-Hamri[1], May Choueib[1], Rozenn Diehl[1], Pascal Vincent[1], Steve T. Purcell[1], Anthony Ayari[1], Sorin Perisanu[1]

[1] *Institut Lumière Matière, UMR5306 Université Lyon 1-CNRS, Université de Lyon 69622 Villeurbanne, France*

We have studied the evolution of the mechanical Q-factor of individual Single Wall Carbon Nanotubes (SWCNT) [A. Descombin et al. Nano Letters (2019),19,1534]. Mechanical flexural resonances were excited electrostatically in Ultra High Vacuum in order to minimize dissipation channels, while a voltage VDC is applied on the SWCNT.
The VDC induces a huge axial stress in the SWCNT, increasing the eigenfrequencies (Fig). The novelty here is that it also induces a giant increase of the Q factors (Fig), exceeding 25000 at room temperature, which is two orders of magnitude above values in literature [V. Sazonova et al., Nature (2004),431,284; V. Gouttenoire et al., Small (2010),6,1060]. The same effect was observed on graphene samples, with Q factors over 5400.
This increase in Q factor with axial stress is explained by intrinsic viscoelastic dissipation combined with a non-dissipative "soft clamping" effect due to controlled gradual breaking. Low 300K force noise below 1aN/$\sqrt{Hz}$ is inferred from data. The graphene sample reaches Q/f coherence times (CT) of around 6ms, which is X100 the CT for cryogenic quantum computer demonstrators [www.research.ibm.com/ibm-q/technology/devices/], opening the perspective of mechanical quantum bits [F. Tacchino et al., Phys. Rev. B (2018),20,214302].



Experimental evolution of the eigenfrequency and quality factor with axial electrostatic stress induced by external voltage. A moderate 30% increase in the eigenfrequency is accompanied by an almost one order of magnitude increase in the Q factor.

Energy Symposium SEn7 (overview)

Franconia Hall **Tu 14:00 - 14:40**

Structure control, Mass Production of Well Aligned Carbon Nanotubes for energy application

Fei Wei[1]

[1] *Dept. of Chem. Eng. , Tsinghua University, Beijing 100084, China*

Energy storage in a proper form is an important way to meet the fast increase in the demand for energy. We demonstrate the microscopic bandgap of CNTs versus turnover frequency (TOF) of carbon atom-addition agrees with the uncertainty principle, which governs ~3×106 s-1 atomic assembly during s-CNT formation with a narrower bandgap distribution (~0.1 eV). One magnitude lower TOF of metallic CNTs (m-CNTs) endows the individuals with slower growth rate while the population with higher decay rate, giving rise to a self-purification of 99.9999% aligned s-CNTs at length 154 mm. The detailed strategies for mass production of CNT arrays, super-aligned CNTs, super-long CNTs, as well as CNT/grapheme hybrids were presented. The bulk applications for Li-ion battery, conductive nanocomposites are discussed.

With a tensile strength over 100 GPa, and a Young's modulus over 1 TPa, carbon nanotubes (CNTs) are considered as one of the strongest materials ever found and exhibit overwhelming advantages for storing mechanical energy. The tensile-strain energy density of CNTs is as high as 1125 Wh kg^{-1}. In addition, CNTs also exhibit great potential for fabricating flywheels to store kinetic energy with both high energy density (8571 Wh kg^{-1}) and high power density (2 GW kg^{-1}).

Franconia Hall **Tu 14:40 - 15:00**

TBA

Christoph Brabec

Space for notes.

Energy Symposium SEn9 (invited)

Franconia Hall **Tu 15:00 - 15:20**

Dry deposition of nanocarbon thin films for energy applications

Esko Kaupinnen[1]

[1]Department of Applied Physics, Aalto University School of Science, PO Box 15100, FI-00076 Aalto, FINLAND

We present the direct dry deposition (DPP) manufacturing method of single walled carbon nanotube (SWNT) based transparent conducting films (TCF) with electrical properties on par with those of ITO-on-PET, and with optical as well as mechanical properties i.e. flexibility and stretchability better than those of ITO, metal nanowire and metal mesh. SWNTs have been produced with the floating catalyst chemical vapour deposition (FC-CVD) using Fe nanoparticles as the catalyst and CO, C_2H_4, CH_4 and alcohols as the carbon precursors. SWNT networks consisting of long, clean and highly individualized SWNTs exhibit substantially improved TCF performance. We introduce the novel graphene-SWNT hybrid thin films made via SWNT dry deposition onto the single layer graphene. Also, we present recent results on the simultaneous synthesis of SWNTs and graphene via the FC-CVD method. Finally, we show examples of using SWNT films as the electrodes in solar cells.

Franconia Hall **Tu 15:30 - 15:50**

Graphene Oxide Liquid Crystal

Sang Ouk Kim[1]

[1]*Materials Science & Engineering, Daejeon 34141, South Korea*

Graphene Oxide Liquid Crystal (GOLC) is a newly emerging graphene based material, which exhibits nematic type colloidal discotic liquid crystallinity with the orientational ordering of graphene oxide flakes in good solvents, such as water. Since our first discovery of GOLC in aqueous dispersion, this interesting mesophase has been utilized over world-wide for many different application fields, including liquid crystalline graphene fiber spinning, highly ordered graphene membrane/film production, prototype liquid crystal display and so on. Interestingly, GOLC also allow us a valuable opportunity for the highly ordered molecular scale assembly of functional nanoscale structures. This presentation will introduce our current status of GOLC research particularly focusing on the nanoscale assembly of functional nanostructures in many different structural dimensions. Besides, relevant research works associated to the nanoscale assembly and chemical modification of various nanoscale graphene based materials will be presented particularly focusinig on energy and catalytic applications.

Energy Symposium SEn11 (invited)

Franconia Hall **Tu 15:50 - 16:10**

Single-wall carbon nanotube films and their hybrids for energy applications

Chang Liu[1]

[1] *Institute of Metal Research, Chinese Academy of Sciences*

High-quality single-wall carbon nanotube (SWCNT) films are prepared by a floating catalyst CVD method. As-grown floating SWCNTs were directly deposited onto a porous substrate equipped at the downstream of a CVD reactor without involving any liquid phase process. Therefore, the quality of the SWCNTs obtained is high, evidence by a high G/D ratio of Raman spectra. The thickness of the films can be easily tuned, and the size of the SWCNT films can be in meter-scale [1]. The SWCNT films were used to fabricate silicon heterojunction solar cells, which show desirable power conversion efficiency [2]. We further prepared a SWCNT/Bi_2Te_3 nanocrystal hybrid by megnetron sputtering. This flexible thermoelectric material comprising highly ordered Bi_2Te_3 nanocrystal anchored on SWCNT network showed a maximum thermoelectric figure of merit (ZT) of 0.89 at room temperature [3].

References:

[1] BW Wang et al. Adv. Mater. 2018, 1802057.
[2] XG Hu et al. Nano Energy 2018, 50: 521.
[3] Q Jin et al. Nature Mater. 2019, 18: 62.

Energy Symposium SEn12 (invited)

Franconia Hall **Tu 16:10 - 16:30**

Catalysis in Lithium-sulfur Batteries

Wei Lyu[1], Quan-Hong Yang[2]

[1]*Graduate School at Shenzhen, Tsinghua University, Shenzhen, 518055, China*
[2]*School of Chemical Engineering and Technology, Tianjin University, Tianjin, 300072, China*

Lithium-sulfur (Li-S) batteries are the promising next-generation battery systems with high theoretical energy density. However, the shuttling caused by the soluble lithium polysulfides (LiPSs) formed by the reaction of Li and sulfur causes rapid capacity fading and low sulfur utilization. Normally, carbon materials are tailored to prevent LiPS shuttling because of their abundant porosity and controllable surface chemistry. However, this "passive" strategy becomes less effective with high sulfur loading and ultralong cycling. Herein, we show the "positive" catalysis is a promising way to solve above problem by increasing the conversion rate of soluble long-chain LiPSs to insoluble products. In order to realize a smooth trapping–diffusion–conversion of LiPSs, we proposed a heterostructure design with a highly active interface, and the twinborn TiO_2–TiN, graphene-TiC and MXene-TiO_2 heterostructures are prepared. Moreover, we found the oxidation layer on the TiN surface also affects the catalytic activity, and we built an interface of Ti-S with Ti-O bonds at the atomic level on TiN surface realizing fast conversion of LiPSs.

2D Materials Symposium S2D7 (contributed)

Panorama 13 **Tu 14:00 - 14:20**

Two-Dimensional Gold with Tunable Bandgaps

Yoke Khin Yap[1], Shiva Bhandari[1], Boyi Hao[1], Kevin Waters[1], Chee Huei Lee[1], Juan-Carlos Idrobo[2], Dongyan Zhang[1], Ravindra Pandey[1]

[1]*Department of Physics, Michigan Technological University, USA*
[2]*Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, USA*

Here we describe the discovery of two-dimensional (2D) gold quantum dots (Au QDs) with tunable band gaps. Our results will stimulate further exploration of energetically stable, metal-based 2D semiconductors. 2D Au QDs are synthesized by pulsed laser deposition using BNNTs as the substrates, as we reported for transistors without semiconductor [1]. Our DFT calculation suggests that the bandgap of such a 2D Au QD is controllable by the number of Au atoms forming the QD. Experimentally, the optically transparent and electrically insulating BNNTs enabled the detection of sharp optical band gaps in the visible spectrum range. Atomic imaging by STEM confirms the formation of 2D Au QDs along with isolated gold atoms, dimers, and trimers. We further demonstrate that size and shapes of 2D Au QDs could be atomically trimmed and re-structured by electron beam irradiation. The growth mechanism of these 2D gold on the nano-cylindrically shaped BNNTs will be discussed.

[1]. Lee, C. H. et al, Advanced Materials 2013, 25 (33), 4544-4548.

Y. K Yap acknowledges the support from the U.S. Department of Energy, the Office of Basic Energy Sciences (Grant DE-SC0012762). Part of this work was conducted at the Center for Nanophase Materials Sciences (Projects CNMS2009-213 and CNMS2012-083.)

2D Materials Symposium S2D8 (contributed)

Panorama 13 **Tu 14:20 - 14:40**

New atomic layer deposition (ALD) of boron nitride (BN) based on polymer derived ceramics route: Potentiality for complex nanostructure fabrication

Catherine Journet[1], Wenjun Hao[1], Catherine Journet[1], Arnaud Brioude[1]

[1] *Univ Lyon, Laboratoire des Multimatériaux et Interfaces, UMR CNRS 5615, France*

Fewly investigated, hexagonal BN nanostructures are very attractive materials with various applications such as in environmental domain. ALD technique is an effective approach for surface modification and fabrication of complex nanostructured materials. However, few ALD processes of BN were reported so far and they are mostly based on ammonia and/or halide precursors and no high crystalline quality was yet achieved. Based on polymer derived ceramic (PDCs) chemistry, a new low temperature ALD process of BN, that permits access to various h-BN complex nano- and hetero-structures, was developed.

In the present communication, we report the fabrication of h-BN complex nano-/hetero-structures by a novel two-step ALD approach using trichloroborazine and hexamethyldisilazane. This two-step process consists of the growth layer by layer of a preceramic BN films, onto various substrates, at low temperature, and then to its densification into pure h-BN by annealing process. h-BN thin films were successfully deposited on various substrates/templates, such as carbon nanotubes, polyacrylonitrile fibers, and etc. The present very low deposition temperature ALD approach provides a versatile ammonia free method to fabricate high quality h-BN nano-/hetero-structures promising for water treatment.

2D Materials Symposium S2D9 (contributed)

Panorama 13 **Tu 14:40 - 15:00**

Large Area Synthesis of Transition Metal Dichalcogenide for Non Linear Optics and Q switched Laser Application

Jinbo Pang[1], Qilin Cheng[1], Hong Liu[1,2]

[1] *Institute for Advanced Interdisciplinary Research (iAIR), University of Jinan, Shizhong District, Jinan, Shandong 250022, China*
[2] *State Key Laboratory of Crystal Materials, Shandong University, Shandong 250100, China*

The electronic and optoelectronic properties of 2D materials [1,2] and their stacking heterostructures [3] have inspired enormous interests. WSe_2, with a p-type semiconducting property, represents a foremost building block in the p-n junctions. WSe_2shall possesses the features of large area, homogeneity and precise layer control. To date, there is yet an ideal synthesis method ever reported. Here we present a facile approach to prepare high quality, wafer-scale homogenous WSe_2full films. In brief, we first deposit a thin layer of metal precursor and then do the selenizaition process. With care of the vacuum deposition of metal thin film, we are able to control upon selenization the film thickness of WSe_2, i.e., its layer number. Eventually the high quality of the synthetic film has been reflected on the high performances of saturable transmission in saturable absorbers and the Q switched laser. Our finding may pave the way towards wafer scale integration of transition metal dichalcogenide in the integrated arrays of pulsed laser devices.

[1] Pang, J. et al. ACS nano 2017, 11, 1946-1956.
[2] Hao, Q.; Pang, J.; et al. Advanced Optical Materials 2018, 6, 1700984.
[3] Pang, J. et al. Chem. Soc. Rev. 2019, 48, 72-133.
[4] Pang, J. et al. Adv. Energy Mater. 2018, 8, 1702093

Panorama 13 **Tu 15:00 - 15:20**

Effective growth of large scale 2D single crystals with high qualities

Yang Wu[1,2]

[1]*Department of Physics, Tsinghua University, Beijing, China*
[2]*Tsinghua-Foxconn Nanotechnology Research Center, Tsinghua University*

The discovery of novel materials is not only the frontier of fundamental research, but will trigger the revolution in technology. Lately, 2D materials, as represented by graphene or graphene-like transition metal dichalcogenides (TMDC) have displayed unconventional characteristics, for instance, the emergence of topological quantum states. However, the current research of these novel 2D materials is poorly carried out or restricted in a limited number of known materials due to the lack of effective synthesis and methodology in crystal growth. Furthermore, the top-down approach for 2D materials by the exfoliation from single crystals is believed to result in high quality samples. Therefore, it is critical to explore the potential 2D materials extensively and systematically, with a focus on scientific insights to the controlled chemical synthesis and crystal growth. In this talk, the extensive attempts for growing large-scale 2D single crystals with high quality will be discussed. In addition to their exotic topological electronic structures , the optoelectronic property, based on the measurement of single crystals of TMDC and its derivatives, will be covered as well.

2D Materials Symposium S2D11 (contributed)

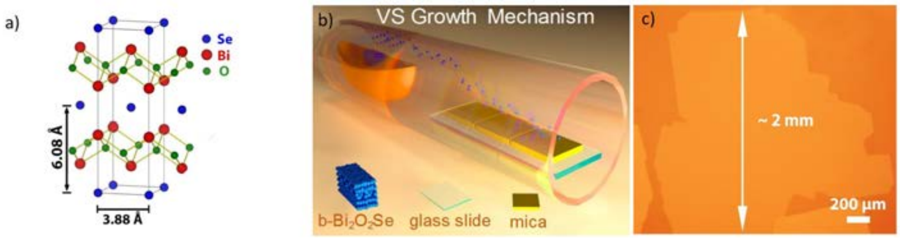
Panorama 13 **Tu 16:10 - 16:30**

Controlled Vapor-Solid Deposition of Millimeter-Size Single Crystal 2D Bi_2O_2Se for High Performance Phototransistors

Usman Khan[1], Yuting Luo[1], Lei Tang[1], Changjiu Teng[1], Jiaman Liu[1], Bilu Liu[1], Hui-Ming Cheng[1]

[1] *Tsinghua-Berkeley Shenzhen Institute, Tsinghua University.*

Atomically thin two-dimensional (2D) materials have received interest both scientific and technological. Bi_2O_2Se is a semiconducting 2D material with high electron mobility and good stability, making it promising for high-performance electronics and optoelectronics. Here we report an ambient-pressure vapor-solid (VS) deposition approach for the growth of millimeter-size 2D Bi_2O_2Se single crystal domains with thicknesses down to a monolayer. The VS-grown 2D Bi_2O_2Se has good crystalline quality, chemical uniformity and stoichiometry. We fabricate field-effect transistors (FETs) using this material and they show a small contact resistivity of 55.2 Ωcm^2 measured by a transfer line method. Upon light irradiation, a phototransistor based on the Bi_2O_2Se FETs exhibits a maximum responsivity of 22,100 AW^{-1}, which is a record among currently reported 2D semiconductors and approximately two orders of magnitude higher than monolayer MoS_2. The Bi_2O_2Se phototransistor shows a gate tunable photodetectivity up to $3.4x10^{15}$ Jones and an on/off ratio up to 10^9, both of which are much higher than phototransistors based on other 2D materials reported so far. Our results indicate a way to grow large 2D Bi_2O_2Se single crystals that have great potential for use in optoelectronic applications.



2D Materials Symposium S2D12 (contributed)

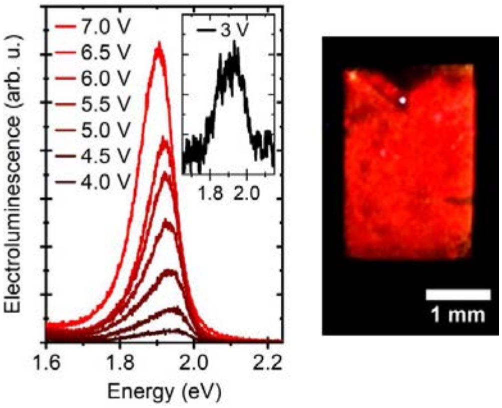
Panorama 13 **Tu 15:30 - 15:50**

MOCVD growth and characterization of MoS_2 and WS_2

Michael Heuken[1,2], Dominik Andrzejewski[3], Henrik Myja[3], Tillmar Kümmell[3], Gerd Bacher[3], Annika Grundmann[2], Holger Kalisch[2], Andrei Vescan[2]

[1]*AIXTRON SE, Herzogenrath, 52134, Germany*
[2]*Compound Semiconductor Technology, RWTH Aachen University, Aachen, 52074, Germany*
[3]*Werkstoffe d. Elektrotechnik and Cenide, Univ. Duisburg, 47057, Duisburg, Germany*

The 2D TMDC $MoS_2$and WS_2 are receiving strong interest due to their exceptional properties and possible application in (opto)electronics. However, material science and device development require a reproducible material basis, i. e. a deposition method providing uniform layers of controlled properties. MOVPE as an established production technology is a perfect choice and can be scaled up to large substrate diameters, volumes and yield. We report on a systematic study of 2D MoS_2 and WS_2 deposition on sapphire using a commercial AIXTRON multi-wafer MOVPE tool. Metal hexacarbonyls (WCO / MCO) and DTBS are used as high-purity MO sources. True 2D growth requires controlled nuclei formation followed by purely lateral growth. The impact of fundamental MOVPE parameters on these processes is discussed, shedding light on nucleation and lateral 2D growth until layer coalescence. The samples are characterized by Raman, SEM, AFM, PL, and reflectometry. A low-damage large-area transfer process was developed to implement the films in optoelectronic devices. Employing organic and hybrid inorganic-organic injection and transport layers, a bright red 6 mm^2-sized WS_2-based LED was fabricated demonstrating the applicability of 2D TMDC for optoelectronic devices.



(Left) EL spectra of the LED with WS_2 monolayer as emitting material in dependence of the operation voltage. (Right) Photograph of a 6 mm^2 LED biased at 7 V.

2D Materials Symposium S2D13 (contributed)

Panorama 13 **Tu 15:50 - 16:10**

TEM observation of dynamic structural change in synthetic MoS_2 under electron beam irradiation

Hyangsook Lee[1,2], Yeonchoo Cho[1], Wonsik Ahn[2], Eunha Lee[1], Hyoungsub Kim[2]

[1] *Samsung Advanced Institute of Technology, Suwon 16678, Republic of Korea*
[2] *Sungkyunkwan University, Suwon 16419, Republic of Korea*

Aberration-corrected low-voltage TEM allows observation of various two-dimensional monolayer materials including MoS_2, while minimizing or avoiding electron irradiation damage. Furthermore, it can also be used to study the dynamic behavior of atomic displacement via electron bombardment during TEM observation. In this presentation, we will present a couple of in-situ observation results for the structural dynamics of synthetic MoS_2 films during electron beam irradiation (TEM observation). Under a high-vacuum condition (in a TEM column), a phase transition of monolayer MoS_2 from 2H to 1T/1T' was induced by weak electron irradiation, which was explained by the electron-delocalization (charge transfer) process originated from the detachment of chemisorbed molecules on the S-vacancy sites by electron bombardment (Hyangsook Lee et al., 2018 2D Mater. 5 041002). The electron irradiation was also used to identify whether the excess Mo ad-atoms in the synthetic bi-layer MoS_2 film were bonded in the interlayer region or physisorbed on the film surface. During this experiment, we observed that the Mo ad-atoms located within the interlayer region produced a change in the stacking sequence from AA' (2H phase) to AB (3R phase) in the bi-layer MoS_2 film.

Panorama 12 **Tu 14:00 - 14:20**

Nanocarbon Structures Synthesized in the One-Dimensional Core of Carbon Nanotubes: Wavelength-Dependent Raman Spectroscopy

Wim Wenseleers[1], Miles Martinati[1], Sofie Cambré[1], Hans Kuzmany[2], Lei Shi[2], Philip Rohringer[2], Paola Ayala[2], Thomas Pichler[2]

[1]*Physics Department, University of Antwerp, Universiteitsplein 1, B-2610 Antwerp, Belgium*
[2]*Faculty of Physics, University of Vienna, 1090 Wien, Austria*

Carbon nanotubes are ideal templates for ordering 1D arrays of molecules and for the controlled synthesis of 1D carbon nanostructures. E.g., we previously demonstrated that in this way dipolar dyes can be aligned in an ideal head-to-tail arrangement to yield a giant total nonlinear optical response,[1] and that the optical properties of dye molecules encapsulated in SWCNTs can be strongly modulated by the CNT diameter, indicating highly diameter-dependent stacking and interactions of the molecules.[2] By thermal conversion also well-defined carbon structures such as long 1D carbon chains (carbyne) or graphene nanoribbons can be synthesized inside the CNTs. Here we show that structure and properties of such 1D carbon chains are strongly modulated by the interaction with the host tube, greatly modifying the chains' bond-length alternation.[3] Also, the band-gap and electronic spectrum of the carbon structures is measured in detail, even in heterogeneous mixtures, by extensive resonance Raman excitation spectroscopy, disentangling the vibrational and electronic spectra of the different structures.

[1] S. Cambré, J. Campo et al., Nature Nanotechnol. 10, 248 (2015)
[2] S. van Bezouw, D. H. Arias et al., ACS Nano 12, 6881 (2018)
[3] L. Shi et al., Phys. Rev. Mater. 1, 075601 (2017)

Synthesis Symposium SSy9 (invited)

Panorama 12 **Tu 14:20 - 14:40**

Extending the Boundaries of Aqueous Two-Phase Extraction of Single-Wall Carbon Nanotubes using Surfactants

Jeffrey Fagan[1]

[1]*NIST, Gaithersburg, MD USA*

Aqueous two-phase extraction is unique among SWCNT separation techniques in its ability to target any (n,m) or (m,n) structure, whether metallic or semiconducting, across potentially the entire breadth of possible diameters. The key to this ability is the fine tunability of each separation in a multistage cascade through the control of the nature and concentrations of surfactants and additives. However, workflow and practical considerations can vastly affect the ease and success of ATPE separations. In this talk I will present my up to date understanding of the factors affecting the types of ATPE separation, including workflow effects, as well as developments in separations within my labs. Particularly results for alkane-filled and empty SWCNTs in both the small and large diameter ranges will be presented.

Panorama 12 **Tu 14:40 - 15:00**

Bottom-up synthesis of sub-5 nm armchair graphene nanoribbons via CVD

Michael Arnold[1]

[1] *University of Wisconsin, Madison, 53562, U.S.A.*

We have discovered how to drive graphene crystal growth with a large shape anisotropy through control of kinetics on the surface of Ge(001) single crystal wafers via CH_4 chemical vapor deposition.[1-5] This discovery enables the direct synthesis of narrow, long, smooth, and oriented graphene nanoribbons that are semiconducting. The nanoribbons have faceted armchair edges, have transport properties exceeding nanoribbons synthesized by other methods, and are grown directly on group-IV wafers, creating the possibility of hybrid carbon nanoelectronics.

This talk will detail the synthesis of these ribbons (including seeded arrays of ribbons), the mechanisms underpinning their anisotropic growth kinetics, the elucidation of their structure, and the characterization of their promising charge transport properties.

[1] Nature Comm. (2015); ACS Nano (2017); Nano Lett. (2018); Nanoscale (2019); Submitted (2019).

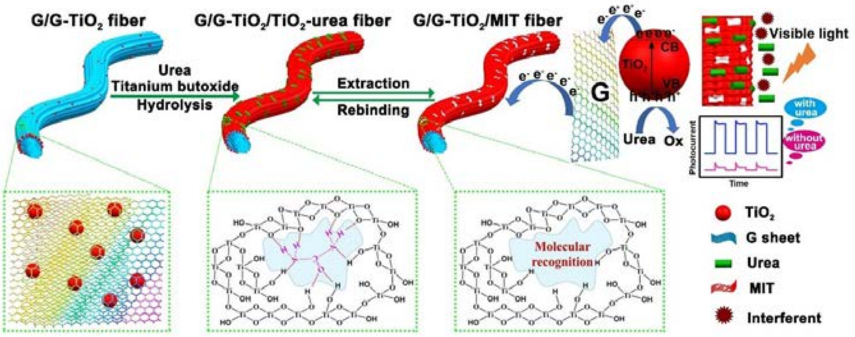


Figure. (A) Self-orienting ribbons spontaneously formed on Ge(001). (B) STM image. Surrounding particles are GeOx species due to ex situ transfer. (C and D) Current and dI/dV maps, respectively, of 5 nm nanoribbon on Ge epilayer on Si(001).

Synthesis Symposium SSy11 (invited)

Panorama 12 **Tu 15:00 - 15:20**

Optical properties of dyes aggregated into carbon and boron nitride nanotubes

Etienne Gauffrès[1,4], Charlotte Allard[2], Raffaela Nascimento[3], Frederic Fossard[4], Leonard Schué[3], Emmanuel Flahaut[5], Annick Loiseau[4], Patrick Desjardins[2], Richard Martel[3]

[1]*Institut d'Optique & CNRS, LP2N UMR 5298, F-33400 Talence, France*
[2]*Regroupement Québécois sur les Matériaux de Pointe (RQMP) and département de génie physique, Polytechnique Montréal, Montréal, Québec H3C 3A7, Canada*
[3]*Regroupement Québécois sur les Matériaux de Pointe (RQMP) and département de chimie, Université de Montréal, Montréal, Québec H3C 3J7, Canada*
[4]*Laboratoire d'Etude des Microstructures, ONERA-CNRS, UMR104, Université Paris-Saclay, BP 72, 92322 Châtillon Cedex, France*
[5]*CIRIMAT, Université de Toulouse, CNRS, INPT, UPS, 5085, 118, route de Narbonne, 31062 Toulouse cedex 9, France*

The confinement of organic molecules inside the vicinity of the nanotube forms a class nanoheterostructure with properties driven by 1D confinement. (1-3) Here we show that boron nitride nanotubes (Eg~5 eV) having inner diameters between 1 nm to 5 nm provide 1D confinement effects similar to those offered by carbon nanotubes with the difference that they preserve the luminescence of the dyes. Experiments on individual dyes@BNNT demonstrate that the BNNT protect efficiently the dyes against photobleaching. Polarized luminescence imaging experiments and High Resolution Transmission Electron Microscopy on dyes@BNNT show ordering states of molecules inside BNNTs that depends on the dyes geometry and the inner diameter of the BNNTs. Preliminary results on Daphnia Pulex colored with dyes@BNNT suggest that these dye@BNNT nanoprobes have reduced toxicity for multimodal imaging based on Raman and luminescence to study biological materials in the NIR I biological window. (4)

[1] E. Gaufrès et al Nature Photon. 8, 72-78 (2014)
[2] S. Cambré et al Nature Nano. 10, 248-252 (2015)
[3] E. Gaufrès et al ACS Nano, 10, 11 (2016)
[4] C. Allard et al, submitted and ChemRxiv (2019),
https://doi.org/10.26434/chemrxiv.8011268.v1

Panorama 12 **Tu 15:30 - 15:50**

Chirality enriched carbon nanotubes with tunable wrapping via corona phase exchange purification (CPEP)

Robert Nißler[1], Florian A. Mann[1], Niklas Herrmann[1], Helen Preiß[1], Sebastian Kruss[1,2]

[1]*Institute of Physical Chemistry, Göttingen University, Germany*
[2]*Center for Nanoscale Microscopy and Molecular Physiology of the Brain, Göttingen, Germany*

Single-walled carbon nanotubes (SWCNTs) have unique photophysical properties. For many applications it is crucial to use chirality enriched SWCNTs. Purification procedures such as wrapping in certain polymers, phase separation, density gradient centrifugation or chromatography yield distinct SWCNT chiralities wrapped in a specific polymer or surfactant. However, many applications such as biosensing require a different organic corona phase around the SWCNTs.

Here, we present a straightforward approach to gain nearly chirality pure SWCNTs by using polymers of the PFO polymer family to 1) enrich certain chiralities 2) remove the polymer and 3) exchange it to a desired organic phase. We demonstrate this concept by using PFO-BPy, which is known to preferentially solubilize (6,5)-SWCNTs, followed by the exchange to surfactants, polymers or ssDNA. This corona phase exchange purification (CPEP) was also extended to other PFO variants to enrich (7,5)-SWCNTs. CPEP purified samples such as (GT)10-(6,5)-SWCNTs are functional as shown by fluorescence changes in response to the neurotransmitter dopamine or by introducing sp^{3}defects in SDBS-(6,5)-SWCNTs. In summary, CPEP provides simple access to chirality enriched SWCNTs functionalized in any desired polymer.

Panorama 12 **Tu 15:50 - 16:30**

Harnessing Carbon Nanotube Defect States as Quantum Emitters

Stephen Doorn[1], Sehmus Ozden[1], Xiaowei He[2], Yue Luo[2], Stefan Strauf[2], Jeffrey Blackburn[3], Younghee Kim[1], Han Htoon[1]

[1]*Los Alamos National Laboratory, Los Alamos, NM 87545, USA*
[2]*Stevens Institute of Technology, Hoboken, NJ 07030, USA*
[3]*National Renewable Energy Laboratory, Golden, CO 80401, USA*

Photoluminescent defect states introduced by low-level covalent functionalization of single wall carbon nanotubes (SWCNTs) have emerged as a route to new functionality. In particular, exciton localization at the defect sites gives rise to single photon emission at room temperature that is tunable to telecom wavelengths. Control over defect-state emission properties is essential for advancing potential applications of these unique light emitters. We present an overview of new developments in defect functionalization and surface chemistry and their role in photonic integration. Selectivity over defect binding configuration will be discussed within the framework of a quantum chemistry model. Surface modification to enable integration approaches will also be presented and demonstrated as a route to establishing intrinsic PL dynamics. Strategies for manipulating PL dynamics via integration into plasmonic cavities will be discussed and demonstrated as a pathway to defect-based quantum photonics. The talk will conclude with a perspective on open questions in defect-state chemistry and photophysics and their potential for future quantum photonic circuits.

Panorama 10 **Tu 14:00 - 14:20**

Etchants, Nucleation and Chirality Control during CVD Growth of CNTs: Insights from Molecular Simulation

Alister Page[1]

[1] *The University of Newcastle, Australia*

The mechanism of graphene and CNT growth during CVD is now well established. Carbon nanotube and graphene growth begin with the precipitation/aggregation of carbon atoms on a catalyst surface to form extended carbon chains, which quickly combine and oligomerise to form "islands" of sp^2-hybridized carbon. Larger nanostructures then form via the coalescence of these structures on the catalyst surface, which are stabilised through strong carbon-catalyst σ-bonding.

I will discuss recent simulations showing how this mechanism is influenced by chemical etchant species commonly used in CVD growth (e.g. H_2[2] H_2O [3] NH_3[4-6] MeCN [7] etc.). Our simulations demonstrate how each of these parameters can potentially be exploited towards controlling growth. Importantly, we show that chemical etchants play key roles regarding growth control and kinetics, despite being overlooked in popular growth models to date

References
1. I. Mitchell et al., Carbon 128 215 (2018).
2. Kimura, R. et al., J. Comp. Chem. 40, 375 (2019).
3. C. A. Eveleens et al., Nanoscale 9 1727 (2017).
4. C. A. Eveleens et al., J. Phys. Chem. C 120 19862 (2016).
5. C. A. Eveleens et al., J. Phys. Chem. C In press (2019).
6. C. A. Eveleens et al., Carbon In press (2019).

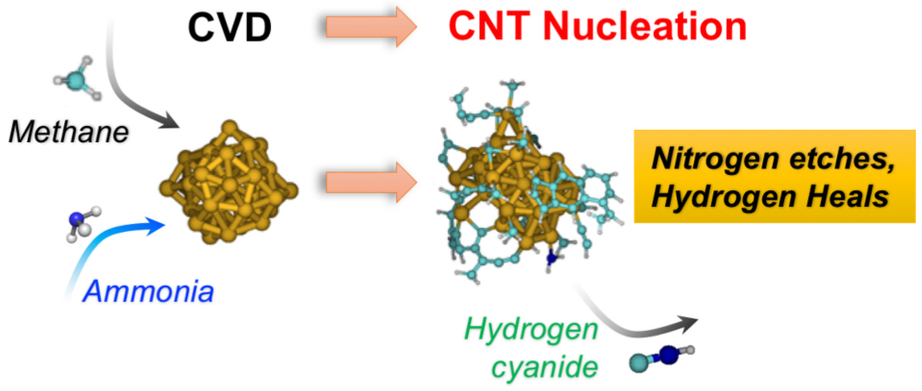


Figure 1. QM/MD simulations reveal etching mechanisms during catalytic CVD

Theory Symposium STh8 (contributed)

Panorama 10 **Tu 14:20 - 14:40**

Chirality-Dependent Motion Transmission between Aligned Carbon Nanotubes

Zhao Wang[1,2]

[1] *Institut fur Materialchemie, Technische Universitat Wien, A-1060 Vienna, Austria*
[2] *Department of Physics, Guangxi University, Nanning 530004, P. R. China*

Taming the mechanical motion of devices at the nanoscale is one of the major challenges in taking the miniaturization technology envisioned by Richard Feynman. The lack of the motion-transmission system remains critical for the design of nano-machines inspired by their macroscopic-world counterparts. Here we demonstrate the motion-transmission behavior of aligned carbon nanotubes (CNTs) using atomistic simulations. The network of overlapping pi orbitals at the interface act as gear teeth to translate the sliding motion of a CNT into a rotating motion of the adjacent CNT, or viceversa. The efficiency of this orthogonal motion transmission strongly depends on the tube chirality, by which the interfacial stacking configuration of the atoms is determined.

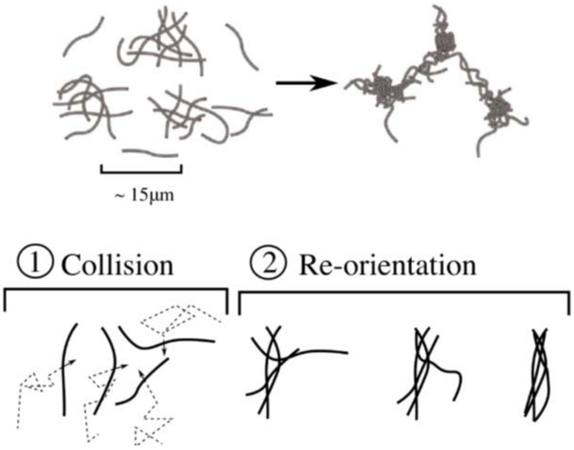
Panorama 10 **Tu 14:40 - 15:00**

Dynamics of CNT aerogel formation: a hybrid Langevin and Molecular Dynamics approach

James Elliott[1], Philipp Kloza[1], Mabel Chao[2], Nicholas Kateris[2], Hoecker Christian[2], Adam Boies[2]

[1]*Department of Materials Science and Metallurgy, University of Cambridge, CB3 0FS, UK*
[2]*Department of Engineering, University of Cambridge, CB2 1PZ, UK*

Aerogel formation within carbon nanotube (CNT) reactors enables continuous production of a self-assembled material with hierarchical structure which is of significant academic and industrial interest. Despite the discovery of the phenomenon over a decade ago, there remains no detailed description of the criteria for aerogel onset or dynamics of formation. In this presentation we report on the dynamics of 1-D materials undergoing Brownian motion, collisions and re-orientation. By employing both adaptive molecular dynamics and Langevin dynamics modelling, we demonstrate that under typical conditions the time-scale for collision is much longer than the time-scale for re-orientation of individual CNTs. The results of simultaneous modelling of both long-range CNT collisions and short-range bundling dynamics enables the timescale of each process to be investigated in detail. These findings are applied to the continuous gas phase process for the bulk production of CNTs, to identify the critical length and number concentration of CNTs required for gelation. Our results show that CNT bundle formation occurs at time scales typical of CNT aerogel reactors for CNT lengths and mass densities found experimentally.



Individual CNTs collide to form bundles in a two-step process that involves (i) collision and (ii) re-orientation.

Theory Symposium STh10 (invited)

Panorama 10 **Tu 15:00 - 15:20**

Tuning electronic properties of carbon nanotubes by graphene promixity

Benedetta Flebus[1]

[1]*University of California, Los Angeles*

Allotropes of carbon, such as carbon nanotubes and graphene, continue to draw attention due to their exceptional physical properties and as promising platforms for understanding the physics of electrons in low dimensions. Recent research has shown that graphene bilayers can display tunable gaps and even superconducting phases, spurring an outburst of interest in carbon-allotropes heterostructures. However, the idea of combining systems with different dimensionality is relatively unexplored. Here, we address the electronic structure of a carbon nanotube deposited on top of graphene. We find that a rigid displacement of the nanotube with respect to the graphene layer has a surprisingly strong impact on the electronic properties of carbon nanotubes.

Our findings suggest that coupling nanotubes with graphene might represent a novel direction for tuning nanotube properties and unveiling new phenomena.

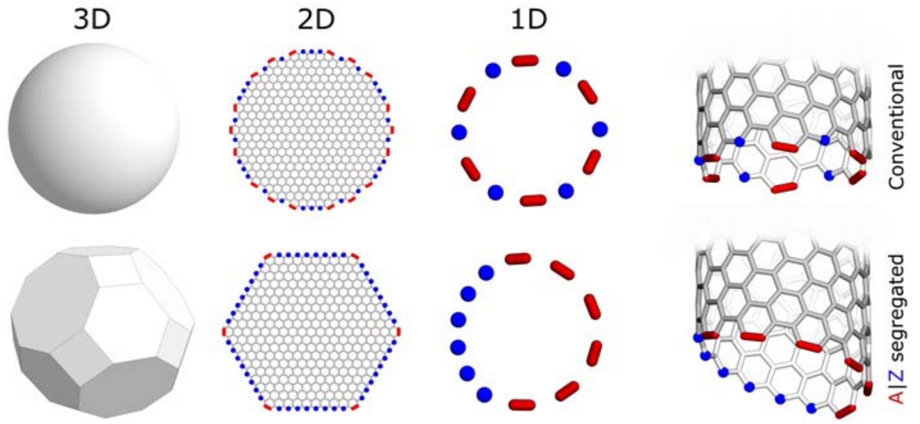
Panorama 10 **Tu 15:30 - 15:50**

Carbon nanotube–catalyst interface segregation and the quest for chirality control

Ksenia V. Bets[1], Evgeni S. Penev[1], Boris I. Yakobson[1]

[1] *Rice University, Materials Science and NanoEngineering Department, Houston, 77005, USA*

The structure of the carbon nanotube-catalyst interface during catalytic synthesis controls both thermodynamics and kinetics of the growth process that in turn prescribe chirality distribution of the growing nanotube (CNT). Despite its importance, the structure of such interface was never investigated but rather assumed to be a minimal-length circle, which is analogous to postulating spherical shape of 3D particles or circular shape of 2D flakes, clearly contradicting faceted Wulff construction in both cases (Fig.1). We present a systematic analysis of the CNT-catalyst interface energetics revealing a drastic change in the interface structure with the solidification of the catalyst. A circular edge is weakly preferred in contact with a liquid catalyst, but interface with rigid catalyst shows a strong preference towards the segregation of the CNT edge into two segments (Fig.1). This trend is further confirmed with the first-principles calculations for a set of representative catalysts (Co_7W_6, WC, Ni, Co). A|Z-segregation lowers the energy of the chiral tubes, largely enhancing their nucleation probability. Kinetics is also greatly influenced, as we demonstrate on the example of selective (2m,m) growth on solid Co_7W_6 catalyst exemplifying the importance of the interface structure.



Minimal-surface versus faceted shapes in 3D (generic nanoparticle), 2D (graphene flake), and 1D (carbon nanotube edge, also shown in side view, demonstrating conventional circular and A|Z-segregated edges).

Panorama 10 **Tu 15:50 - 16:30**

Applications of Carbon Nanosensors to Understanding Biochemical Signaling Within the Human Body

Michael S. Strano[1]

[1]*MIT, Department of Chemical Engineering, Cambridge, MA 02139-430, USA*

The human body is a vast network of biochemical signaling pathways dictating physiological and pathological processes. To probe this network, we have pioneered a novel technique called Corona Phase Molecular Recognition, or CoPhMoRe, for discovering synthetic, heteropolymer corona phases that form molecular recognition sites at the nanoparticle interface. By screening libraries of synthetic heteropolymers chemically adsorbed onto single-walled carbon nanotubes (SWNT), we have engineered new optical biosensors that exhibit high selective recognition for bio molecules, such as riboflavin, L-thyroxine, dopamine, nitric oxide, sugar alcohols, estradiol, and fibrinogen. These results have significant potential for using SWNT-based sensors to interface to biological systems, allowing monitoring pathways at the sub-cellular, cellular, tissue, and whole-animal scale. With deep tissue penetration, we demonstrated our nanosensors in vitro with no photobleaching, and in vivo with no fluorescence degradation (400+ days). Engineering the nanoparticle corona in this way offers significant potential to translate sensor technology to previously inaccessible environments. We recently demonstrated real-time label-free detection of individual proteins from Escherichia coli and Pichia pastoris immobilized in a microfluidic chamber, by non-covalent conjugation of an aptamer-anchor polynucleotide sequence to SWNTs. We further demonstrated protein detection from T7 bacteriophage infection of E. coli, illustrating real-time single-cell analysis of proteins from cells. We recently demonstrated the use of a SWNT array for the detection of dopamine release from PC12 neuroprogenitor cells at a resolution exceeding 20,000 sensors per cell. These nanosensor arrays allow the high-resolution spatiotemporal dynamics of dopamine release, following K+ stimulation. The results illustrate how directionality of chemical signaling is shaped by the cell membrane morphology. For diabetes, we have recently synthesized an insulin sensor sensitive down to 20 µg/mL. The sensor was tested against and proved to be nonresponsive against a panel of human blood proteins and 7 short amino acid fragments of the insulin peptide. The insulin recognition and the concentration quantification were demonstrated in buffer and in blood serum. Interfacing insulin sensors with continuous glucose monitors may revolutionize diabetes management and control using a tightly controlled close-looped system.

Abstracts Tuesday
(Poster)

P001 **Tu 17:00 - 18:30**

Lattice models to study chirality selective growth of SWNTs

Christophe Bichara[1,2]

[1] *CNRS and Aix-Marseille University, Marseille - France*

Recent progress towards an efficient and selective synthesis of carbon nanotubes should be complemented with an improved understanding of their growth mechanisms. We recently proposed a thermodynamic modeling of the interface [1] showing that, at low temperature, only zigzag or armchair tubes are stable. Chiral tubes become stable at higher temperature because of the configurational entropy of the tube edge in contact with the catalyst, that is a key element of the model. This enables us to link the catalyst interfacial properties and the temperature with the resulting equilibrium chiral distribution.

Here, we study the growth of SWNTs using Monte Carlo simulations performed on a simple lattice-gas model for each tube chirality. This enables us to directly study the tube/catalyst interfaces, assess the validity range of our analytic approach [1], and to improve the link between interfacial energies and the resulting SWNT chiral distribution.

[1] Magnin et al., Science 362, 212–215 (2018)

P003 **Tu 17:00 - 18:30**

One-dimensional thermoelectric properties of high-purity single-chirality single-wall carbon nanotube films

Yota Ichinose[1], Kengo Fukuhara[1], Akari Yoshida[1], Yohei Yomogida[1], Takahiro Yamamoto[2], Junichiro Kono[3,4,5], Kazuhiro Yanagi[1]

[1] *Tokyo Metropolitan University/Department of Physics, Tokyo, 192-0372,Japan*
[2] *Tokyo University of Science/Department of Liberal Arts, Tokyo, 125-8585, Japan*
[3] *Rice University/Department of Electrical and Computer Engineering, Texas, 77005, USA*
[4] *Rice University/Department of Physics and Astronomy, Texas, 77005, USA*
[5] *5 Rice University/Department of Materials Science and NanoEngineering, Texas, 77005, USA*

One-dimensional materials have potential to exhibit extremely high thermoelectric performance [1]. One of suggested approaches to achieve the high performance is to tune the Fermi level of the 1D materials with sharp van Hove singularity (vHS). Single-wall carbon nanotubes (SWCNTs) is an ideal model for 1D system with sharp vHS. And thus, we have investigated the thermoelectric properties of SWCNTs as a function of Fermi-level using an electrolyte gating technique [2]. Last year, we found that high-purity (>99%) single-chirality SWCNT (6,5) (Fig. 1) showed relatively large Seebeck coefficient (>1mV/K), which is comparable to theoretical predictions. However, the physical background of the increase was not revealed in detail. Therefore, in this study, we focused on thermoelectric conductivity (called as L12 term) [3] to reveal the background and we investigated L12 of high-purity (6,5) as a function of Fermi level.

As shown in Fig. 2, we observed the unique behavior expected only in 1D materials. High-purity (6,5) showed a sharper peak around vHS. We found that high-purity singe-chirality SWCNT films have an obvious 1D property in L12.

[1] Hicks et al., PRB 47, 16631 (1993)
[2] Yanagi et al., Nano lett. 14 (11), 6437 (2014).
[3] Yamamoto et al., JPSJ 87, 114710 (2018)

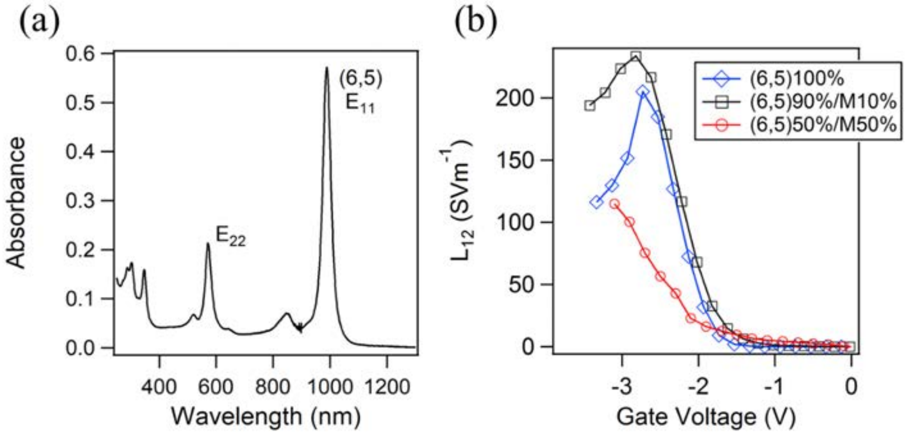


Fig 1. Absorbance spectrum of high-purity (6,5) (99%). Fig 2. Purity-dependence of thermoelectric conductivity (L12) as a function of Fermi-level.

P005 **Tu 17:00 - 18:30**

Substituting silicon in graphene and carbon nanotubes through intermittent vacancies

Heena Inani[1], Kimmo Mustonen[1], Alexander Markevich[1], Erxiong Ding[2], Mukesh Tripathi[1], Aqeel Hussain[2], Clemens Mangler[1], Esko I. Kauppinen[2], Toma Susi[1], Jani Kotakoski[1]

[1]*Faculty of Physics, University of Vienna, Boltzmanngasse 5, 1090, Vienna, Austria*
[2]*Department of Applied Physics, Aalto University of Sciences, FI-00076, Aalto, Finland*

The band structure of single-walled carbon nanotubes (SWCNTs) is entirely determined by the cutting direction and the dimensions of the graphene slab the tubule is constructed from. Synthesizing nanotubes with a desired configuration has proven immensely difficult and alternative routes to tune the properties are still being sought for. One promising approach is substitutional doping by impurity elements. Here, by simultaneous plasma and laser irradiation of a SWCNT-graphene van der Waals heterostructure, we incorporate silicon heteroatoms in both materials. The vacancies thus created are primarily healed by thermally diffusing carbon and Si atoms, the latter of which we directly identify in the lattice by using atomic resolution scanning transmission electron microscopy. In SWCNTs, these atoms are found in 3-coordinated, 4-coordinated and not identifiable configurations with recurrence of ~61%, ~36% and ~3%, respectively and thus in good agreement with earlier theoretical predictions for single and double vacancies. These 1D-nanostructures doped with Si heteroatoms may show up as a promising candidate for water splitting, gas sensing and drug delivery applications.

Plenary Venue Poster

P007 **Tu 17:00 - 18:30**

Growth process of individual single-walled carbon nanotubes analyzed by isotope labelling

Taiki Inoue[1], Bunsho Koyano[1], Shun Yamamoto[1], Shota Hiraoka[1], Keigo Otsuka[2,3], Rong Xiang[1], Shohei Chiashi[1], Shigeo Maruyama[1,4]

[1]*Department of Mechanical Engineering, The University of Tokyo, Tokyo 113-8656, Japan*
[2]*Riken Center for Advanced Photonics, Wako, 351-0198, Japan*
[3]*Riken Cluster for Pioneering Research, Wako, 351-0198, Japan*
[4]*Energy NanoEngineering Lab, AIST, Tsukuba, 305-8564, Japan*

Toward the efficient production and controlled synthesis of single-walled carbon nanotubes (SWCNTs) for practical applications, a deeper understanding of their growth mechanism is needed. While the growth process of entangled SWCNTs has been studied in many ways, it has been more challenging to examine that of individual SWCNTs. We have recently proposed a method for analyzing growth process of individual SWCNTs by means of controlled introduction of isotope labels and revealed the base-growth mode, monotonic growth rates with sudden growth termination, and variations in growth rates even among SWCNTs with the same chirality [1]. In this study, we further investigated the SWCNT growth in a wide range of growth temperatures using Fe or Co as the catalyst by the isotope label technique. Compared with Fe catalyst, Co catalyst resulted in more uniform distributions of growth rates and incubation time. We also conducted the SWCNT growth with intentional pause of carbon feeding and revealed the importance of hydrogen for enabling the regrowth of SWCNTs after reintroducing a carbon source.

[1] K. Otsuka et al., ACS Nano 12, 3994 (2018).

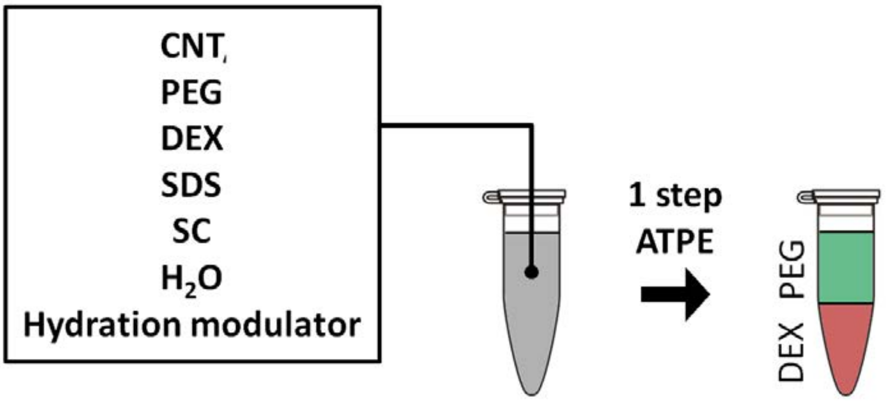
P009 **Tu 17:00 - 18:30**

Simple separation of carbon nanotubes

Dawid Janas[1], Blazej Podlesny[1], Edyta Turek[1]

[1] *Department of Chemistry, Silesian University of Technology, Gliwice, Poland*

The fact that carbon nanotubes come in a wide range of types is not always beneficial because it creates significant processing difficulties if one wants to use just a particular type of them. To tackle this problem, many sorting methods have been recently developed and so obtaining carbon nanotubes of a desired type is not a dream about a distant future but this has become a reality already. Unfortunately, many of the sorting methods either require expensive chemicals or they are very elaborated. In this presentation, we would like to share our recent results how we compacted the aqueous two-phase extraction method to a single step to isolate carbon nanotubes of particular electronic type or light-emission characteristics.



Simple separation of carbon nanotubes

P011 **Tu 17:00 - 18:30**

Have an idea for a new project? Sketch it here.

P013 **Tu 17:00 - 18:30**

Ohmic and voltage-actived transport of ions through single-walled carbon nanotubes

Vincent Jourdain[1], Khadija Yazda[1], Saïd Tahir[1], Thierry Michel[1], Bastien Loubet[2], Manoel Manghi[2], Jeremy Bentin[3], Fabien Picaud[3], John Palmeri[1], Mohamed el Amine Kribeche[1], Jin Cui[1], Adrien Noury[1], François Henn[1]

[1]*Laboratoire Charles Coulomb (University of Montpellier / CNRS)*
[2]*Laboratoire de physique théorique (IRSAMC) CNRS-UPS, Université de Toulouse, France*
[3]*LNIT, Université de Bourgogne Franche-Comté, UFR ST & CHU Médecine, France*

We report studies of ion transport through SWCNTs with diameters of 1.2 to 2 nm showing a ohmic or, unexpectedly, a voltage-activated I-V dependence [1-3]. Transition from an activated to a linear behavior and stochastic fluctuations between different current levels were notably observed. For linear devices, the high conductance confirmed with different chloride salts indicates that the nanotube/water interface exhibits both a high surface charge density and flow slippage. In addition, the sublinear dependence of the conductance on the salt concentration points toward a charge-regulation mechanism. Theoretical modelling and computer simulations show that the voltage-activated behavior can be accounted for by local energy barriers at the ends of the nanotube. Raman spectroscopy reveals strain fluctuations along the tubes but insufficient doping or variations of doping to account for the apparent surface charge density and energy barriers revealed by ion transport measurements. Chemical moieties at the nanotube mouths are proposed to be responsible for the voltage-activated transport of ions through SWCNTs within this diameter range.

1) Yazda et al, MRS Advances, 1(28), 2085.
2) Yazda et al, MRS Advances, 1(28), 2079
3) Yazda et al, Nanoscale (2017), 9, 11976

P015 **Tu 17:00 - 18:30**

Targeted tuning of optoelectronic properties of single-walled carbon nanotube films

Eldar Khabushev[1], Dmitry Krasnikov[1], Yulia Kolodyaznaya[1], Alexey Tsapenko[1], Orisia Zaremba[1], Anastasia Goldt[1], Albert Nasibulin[1]

[1]*Skolkovo Institute of Science and Technology, Moscow, Russia*

Single-walled carbon nanotubes (SWCNTs) are still attracting large attention: current technological advances are aimed at utilizing their unique properties in novel optoelectronic devices. Currently, aerosol CVD is a well-established technique to produce SWCNTs of high quality. But this technique is still lacking formation mechanisms conception that hampers precise control of output parameters.

This work is devoted to SWCNT growth by ferrocene aerosol CVD based on Boudouard reaction. We inspected the influence of synthesis conditions (temperature, carbon dioxide and ferrocene partial pressure) on SWCNT parameters by four-probe technique, Raman and UV-vis-nIR spectroscopy, SEM and TEM, and etc. Adjusting synthesis conditions, we obtained SWCNTs with mean diameter tunable in the range from 0.9 to 2 nm. Raman spectra represented high quality of the synthesized films with IG/ID up to 500, corresponding to 10 μm average size of a non-defect area that correlates with electron microscopy. As a result of optimization we obtained pristine films with low equivalent sheet resistance R90=158 Ω/□. Moreover, this value dropped down to 39 Ω/□ after $AuCl_3$ doping providing one of the most advanced results achieved so far.

This work was supported by Russian Science Foundation No. 17-19-01787

P017 **Tu 17:00 - 18:30**

Toward fabrication of hybrid perovskite – semiconducting single-walled carbon nanotube (s-SWNT) systems

Simon Kießling[1], Pascal Kunkel[1], Friedrich Schöppler[1], Tobias Hertel[1]

[1] *Julius-Maximilians-Universität, Würzburg, 97074, Deutschland*

Hybrid organic-inorganic perovskites (HOIPs) are of interest for their expected versatility in applications such as lasers or photodetectors. Here, we explore opportunities that may arise from the fabrication of HOIPs nanocrystals s-SWNT hybrids which are synthesized by the ligand-assisted reprecipitation (LARP) method. To prevent agglomeration and growth, the nanoplatelets are encapsulated by the common capping agent oleic acid (OA) and oleylamine (OAm). Furthermore, poly(9,9-di-n-octylflourenyl-2,7-diyl)-bipyridine (PFO-BPy) stabilized s-SWNT have been investigated as potential capping agents to elucidate perovskite-s-SWNT interactions. Optical and topographical characterization of the colloidal suspensions were carried out by using absorption and photoluminescence spectroscopy, and field emission scanning electron microscopy (FE-SEM), respectively. We show that the LARP method allows synthesizing colloidally dispersed nanocrystals which reveal excitonic behaviour at the band edge but undergo a relatively fast agglomeration and degradation process. HOIPs nanocrystals grown in the presence of PFO-BPy/s-SWNTs exhibit red shifted emission wavelength indicating a greater diameter of the nanocrystals but, unlike with OA and OAm as capping agent, an increased stability over time.

P019 **Tu 17:00 - 18:30**

Reference Material for N_2 Adsorption to Carbon Nanotubes

Kazufumi Kobashi[1], Hideaki Nakajima[1], Takahiro Morimoto[1], Toshiya Okazaki[1]

[1] *AIST, CNT-Application Research Center, Tsukuba, 305-8565, Japan*

A wide variety of commercialized CNTs have been available in recent years. Their industrialization is starting to bloom, however, facing obstacles to characterize diverse CNT structures. For the characterization, a reference material for CNTs is essential. However, one for gas adsorption has not been investigated, which enables us to precisely measure specific surface areas and pore structures.

Here we inspected the reference material for N_2 adsorption to CNTs. Regarding a reference material of gas adsorption, it has been known that preferable ones possess nonporous, flat surfaces and surface compositions similar to measured samples. A monolayer formation of N_2 molecule occurs on a flat, graphite surface at the relative pressure 10^{-5} to 10^{-5}. To clarify surface flatness, we focused on N_2 adsorption curves of various carbon materials like activated carbon, activated CF, CB, graphite, mesoporous carbon, carbon nanohorn, and diverse CNTs. These adsorption curves showed that VGCF and graphitized CB had higher slopes in the N_2 monolayer formation range, suggesting less porous, flatter surfaces than others (Fig. 1). To see surface compositions of the carbon materials, XPS analysis was done. Based on these results, we would like to discuss the suitable reference materials to CNTs.

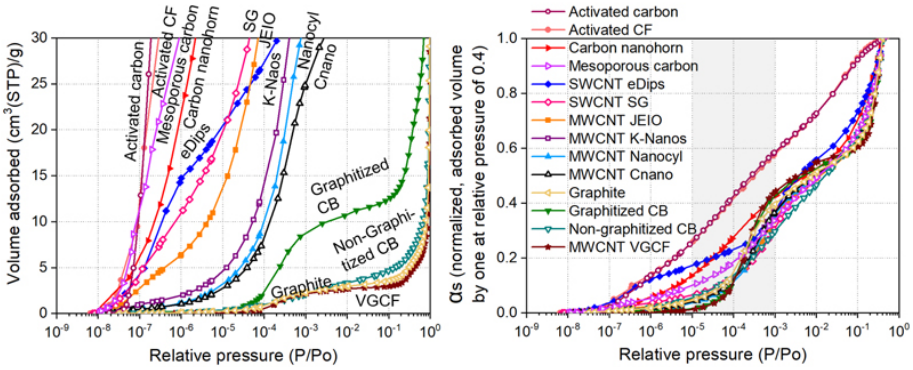


Fig. 1 N_2 adsorption isotherms at 77K for various carbon materials.

P021 **Tu 17:00 - 18:30**

One-pot exctraction of semiconducting single-walled carbon nanotubes with a thermoresponsive polymer

Shota Kuwahara[1], Eriko Shimura[1], Toshiki Sugai[1]

[1] *Department of Chemistry, Toho University, Chiba 274-8510, Japan*

The separation techniques for obtaining single-walled carbon nanotubes (SWCNTs) with homogeneous electronic properties is crucial for the promising electronic devices in nanotechnology. In this study, we utilized the thermoresponsive phase transition for the simple extraction method to obtain SWCNTs with the homogeneous electronic properties, and successfully extracted the semiconducting SWCNTs with poly-(N-isopropylacrylamide) (PNIPAM) [1], a well-known thermoresponsive polymer. Above the lower critical solution temperature, PNIPAM forms aggregates, globules, where hydrophobic space is generated inside, and we separated the specific structure of SWCNTs with the solid (globule) and liquid phases. In the case of small-diameter nanotubes, CoMoCAT, the semiconductor SWCNTs were successfully extracted into the liquid phase. The intensity corresponding to metallic SWCNTs reduced in the absorption spectrum of the liquid phase. The result indicated that a part of the semiconducting SWCNTs was selectively transferred to the aqueous phase rather than remaining in the globules of PNIPAM. When the concentration of aqueous PNIPAM solutions was 5 wt%, (6,5) nanotubes were selectively extracted into the liquid phase (see Figure 1).

[1] E. Shimura, et al., Chem. Commun., 54, 3026 (2018).

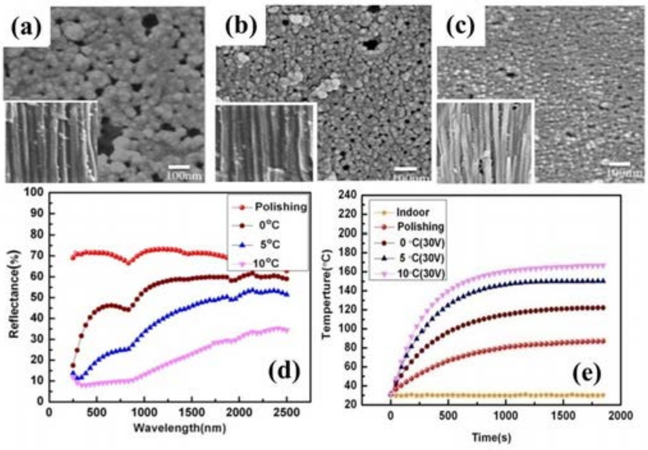


Figure 1. Optical absorption spectra of the pristine SWCNT solution before and after extraction., the liquid phase and the globule phase after extraction.

P023 **Tu 17:00 - 18:30**

Environment Effects on the Charge States of Metallic and Semiconducting SWCNTs during Their Separation by the ELF Method

Yuki Kuwahara[1], Takeshi Saito[1]

[1]*AIST, Tsukuba, 305-8565, Japan*

SWCNTs show metallic (m-) or semiconducting (s-) natures by the difference in the structure rolling a graphene sheet into a seamless cylinder. Since most SWCNTs are synthesized as a mixture of them, therefore, the separation of m-/s-SWCNTs is very important for the use of s-properties. Among various separation methods, we have investigated the ELF method [1]. ELF is quite simple; by applying an electric field in the longitudinal direction to SWCNT dispersion containing the nonionic surfactant, m- and s- SWCNTs are separated into upper and lower layers, respectively. However, the separation mechanism in ELF was unclear. In this study, the effects of the separation-cell environments on the separation process, that is, the effects of pH and surfactant concentration were investigated. The zeta potentials (ZPs) were measured for the m- and s-SWCNTs, as an important property for evaluating the charge state and the influence of the electric field. It has been revealed that both types of SWCNTs are negatively charged in the dispersion, yet the magnitudes of their ZPs are clearly different. On the basis of these results, we have proposed the plausible mechanism of the ELF [2].

[1] K. Ihara et al., JPCC 2011, 115, 22827.
[2] Y. Kuwahara et al., JPCC 2019, 123, 3829.

P025 **Tu 17:00 - 18:30**

A Systematic Study of CO_2-assisted Growth of Single-walled Carbon Nanotubes

Yongping Liao[1], Aqeel Hussain[1], Nan Wei[1], Qiang Zhang[1], Hua Jiang[1], Saeed Ahmad[1], Er-Xiong Ding[1], Esko I. Kauppinen[1]

[1] *Department of Applied Physics, Aalto University School of Science, Aalto, Finland*

The geometric and electronic structure of single-walled carbon nanotubes (SWCNTs) are vital to electronic applications. We find that CO_2 plays a key role in modulating the SWCNT structure during growth in floating catalyst chemical vapor deposition (FC-CVD). By introducing various amount of CO_2 in FC-CVD using CO as carbon source, we have directly synthesized SWCNTs with tunable geometry (diameter, length and bundle size) and chirality distribution 1, 2. As CO_2 concentration increases, both tube diameter and bundle length considerably increases. In particular, the yield of SWCNTs can be significantly promoted at an optimized amount of CO_2. As a result, the transparent conductive films (TCFs) of optimized SWCNTs exhibit excellent sheet resistance as low as 86.8 Ω/sq. at 90% transmittance after $AuCl_3$ doping, about 50% reduced compared to those TCFs without CO_2. Interestingly, for the first time, we have observed that as-synthesized SWCNT films with 0.25 and 0.37 vol% of CO_2 display green and brown colors, respectively. By further optimizing reactor temperature, we achieved much narrower (n,m) distribution clustering around (11,9), giving extremely narrow diameter range (98% between 1.2 and 1.5 nm).

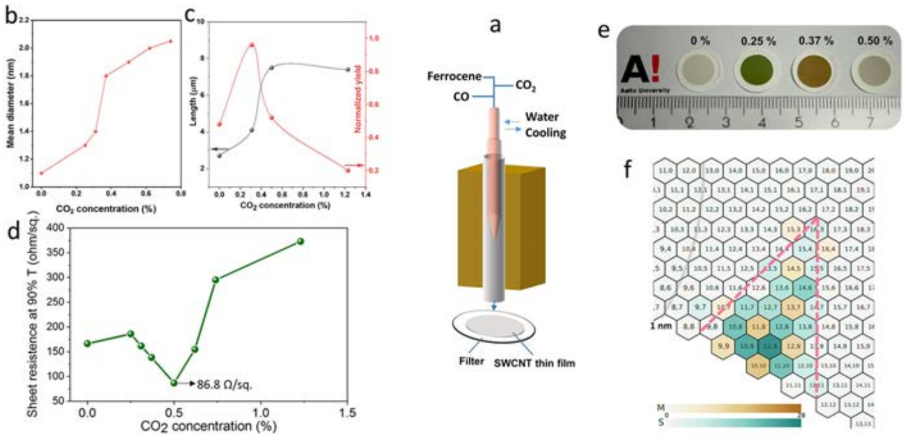


Figure 1. Setup for SWCNT synthesis, the geometric and electronic structure modulated by CO_2.

P027 **Tu 17:00 - 18:30**

Preparation of High-Concentration Carbon Nanotube Dispersion for High-Throughput Production of Multiple Single-Chirality Species

Huaping Liu[1,2,3,4,5], Dehua Yang[1,3,4], Wei Su[1,3,4], Xiaojun Wei[1,3,4], Weiya Zhou[1,3,4,5], Fei Wei[7], Hiromichi Kataura[6], Sishen Xie[1,3,4,5]

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High-throughput separation of multiple single-chirality carbon nanotubes (CNTs) is a critical step for their applications in the fields of electronics, optoelectronics and bio-imaging. Here, we report a method for preparing high-concentration monodisperse CNT solution by re-dispersion. With this technique, we can increase the initial concentration of raw materials from 1mg /ml to 3 mg/ml, resulting in a threefold or higher increase in the CNT concentration in the as-prepared mono-dispersion solution, which distinctly increase the efficiency and throughput of single-chirality separation by several to a dozen folds with gel chromatography. Moreover, we have demonstrated that this technique could be used to macroscopically separate more than ten (n, m) single-chirality species and other large-diameter semiconducting CNTs (diameter >1.2 nm) from the raw nanotubes with wide-diameter distribution, which can be industrially produced at low cost. Our current technique was suitable for the sa variety of CNT raw materials, and promoted the single-chirality separation of CNTs to an important step towards industrialization.

This work is financially supported by NSFC (Grants 11634014, 51820105002, 51872320), and the Key Research Program of Frontier Sciences, CAS (Grant QYZDBSSW-SYS028).

P029 **Tu 17:00 - 18:30**

Developing Strong and Tough Carbon Nanotube Films by Proper Dispersing Strategy and Enhanced Interfacial Interactions

Weibang Lyu[1,2], Shuxuan Qu[1,2], Wenbing Gong[1,2], Qingwen Li[1,2], Xinrong Jiang[1,2]

[1] *Innovation Center for Advanced Nanocomposites*
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A new approach for making carbon nanotube (CNT) films that are both strong and tough is detailed in this paper. Aqueous dispersions of long CNTs were first obtained by dispersing CNT arrays with heights of about 200 μm in deionized water with the help of polyvinylpyrrolidones (PVPs) and polydopamines (PDAs). CNT films were then obtained by vacuum-assisted filtration of CNT dispersions. The tensile strength and toughness of the composite films can be as high as 143.5 MPa and 5.0 MJ/m^3, respectively, which was 330.7 % and 213.8 % higher than CNT films made without using PVPs and PDAs. The underlying mechanism of PVPs and PDAs induced CNT film strengthening and toughening was revealed through preliminary molecular dynamics simulations, which indicated that the hydrogen bonds between the PVPs and PDAs enhanced the strength of the film, and these bonds can cyclically break and reform, making CNT films tougher. The strategy proposed here can also be applied to making other nano-materials based strong and tough macro-assemblies.

Plenary Venue Poster

P031 **Tu 17:00 - 18:30**

Surface protection of austenitic steels by carbon nanotube coatings

Timothy MacLucas[1]

[1] *Saarland University*

In the present study, surface protection properties of multiwall carbon nanotubes deposited on polished austenitic stainless steel are evaluated. Electrophoretic deposition is used as a coating technique. Contact angle measurements reveal hydrophilic as well as hydrophobic wetting characteristics of the carbon nanotube coating depending on the additive used for the deposition. Tribological properties of carbon nanotube coatings on steel substrate are determined with a ball-on-disc tribometer. Effective lubrication can be achieved by adding magnesium nitrate as additive due to the formation of a holding layer detaining CNTs in the contact area. Furthermore, wear track analysis reveals minimal wear on the coated substrate as well as carbon residues providing the lubrication. Energy dispersive x-ray spectroscopy is used to qualitatively analyse the elemental composition of the coating and the underlying substrate. The results explain the observed wetting characteristics of the each coating. Finally, merely minimal oxidation is detected on the CNT coated substrate as opposed to the uncoated sample.

P033 **Tu 17:00 - 18:30**

Unique features of carbon nanotubes: shaping electron wave functions with parallel magnetic field

Magdalena Marganska[1], Daniel Schmid[2], Alois Dirnaichner[2], Peter Stiller[2], Christoph Strunk[2], Milena Grifoni[1], Andreas Hüttel[2]

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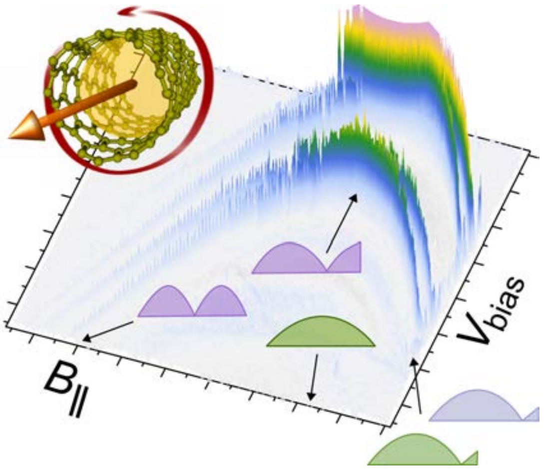
The motion and distribution of charges in almost all known systems is affected only by the transverse components of the magnetic field. Classically, the Lorentz force is perpendicular to B. Quantum mechanically, the parallel component of the vector potential can be gauged away.

In carbon nanotubes, due to their cylindrical topology and bipartite hexagonal lattice, the boundary conditions couple the transverse and longitudinal components of the wave vector. By tuning the former via the Aharonov-Bohm effect, we also affect the latter. The high fields (up to 17 T) in our experiment are sufficient to reshape the electronic wave function from a "quarter-wave resonator" profile with an antinode at one end all the way to a "half-wave resonator" profile with nodes at both ends. These changes cause a distinct dependence of the conductance through our device on the magnetic field.

Using the non-trivial lattice and topology of carbon nanotubes we have discovered a new strategy for the control of the wave functions, using an unexpected agent - the parallel magnetic field.



Differential conductance for one electron tunneling through a carbon nanotube quantum dot as a function of bias and parallel magnetic field. The variation of conductance strength is caused by changes in the profile of the wave function.

Plenary Venue Poster

P035 **Tu 17:00 - 18:30**

Synthesis of Boron Nitride Wrapped Vertically-Aligned Single-Walled Carbon Nanotubes and Boron Nitride Nanotubes Array

Ming Liu[1], Yongjia Zheng[1], Taiki Inoue[1], Shohei Chiashi [1], Rong Xiang[1], Shigeo Maruyama[1,2]

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Boron nitride nanotubes (BNNTs), as a structural analogue of carbon nanotubes (CNTs), exhibit outstanding properties, such as high thermal conductivity, robust anti-oxidation ability, amd non-conducting electrical ability. Synthesizing BNNTs, as well as BN coatings, have attracted much research interest. However, the quality and morphology control of BN coatings and the synthesis of BNNTs array are still challenging tasks. In this work, firstly we demonstrated a new recipe for the efficient synthesis of vertically-aligned single-walled carbon (VA-SWNTs) with controllable diameter distribution. By combining two CVD unfavorable synthesis conditions: low temperature and mono-metallic cobalt catalyst, we were able to obtain approximate 85% of the VA-SWNTs between 1.6 and 2.4 nm. Moreover, as-synthesized VA-SWNTs was using as a template in BN CVD process to form a co-axial structure. The vertically-aligned morphology was maintained after BN CVD process and the quality of BN coating was examined by TEM and spectroscopy characterizations. Furthermore, high quality and small diameter BN nanotubes array is produced after an efficient annealing treatment of the co-axial material. The resulting product was studied by Raman spectroscopy, absorption spectra, and TEM.

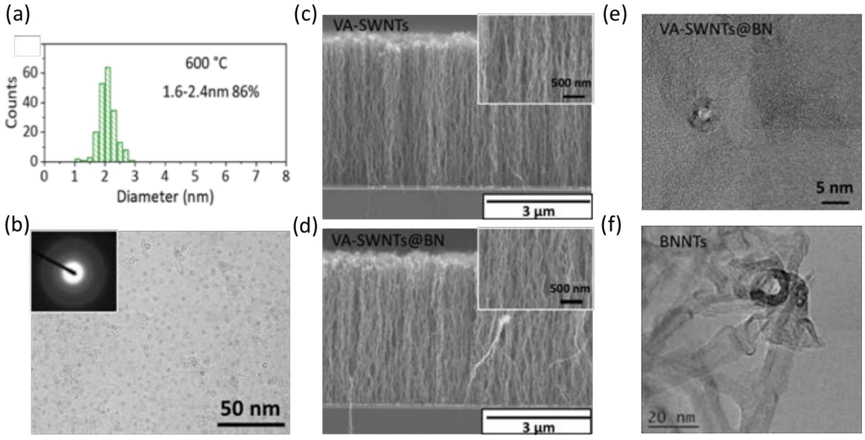


Fig. (a) Diameter distribution of VA-SWNTs; (b) Representative TEM image of VA-SWNTs; Representative SEM images of (c) VA-SWNTs and (d) VA-SWNTs@BN; Representative TEM images of (e) VA-SWNTs@BN and (f) BNNTs.

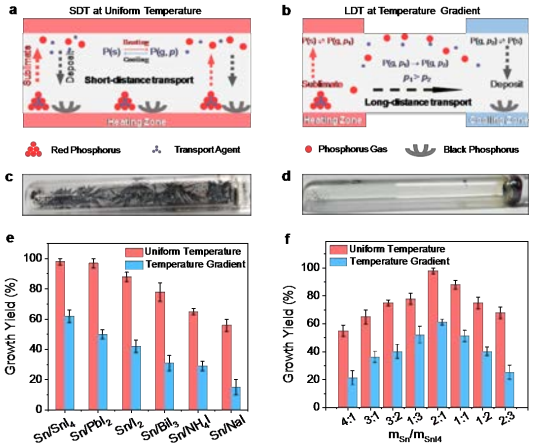
P037 **Tu 17:00 - 18:30**

High Yield Growth and Doping of Black Phosphorus with Tunable Electronic Properties for Ultrasensitive Molecule Sensing

Mingqiang Liu[1]

[1] *Tsinghua-Berkeley Shenzhen Institute (TBSI), Tsinghua University*

Black phosphorus (BP) has recently attracted significant interest due to its unique electronic and optical properties. Doping is an effective strategy to tune a material's electronic properties, however, the direct and controllable growth of BP with a high yield and its doping remain a great challenge. Here we report an efficient short-distance transport (SDT) growth approach and achieve the controlled growth of high quality BP with the highest yield so far, where 98% of the red phosphorus is converted to BP. The doping of BP by As, Sb, Bi, Se and Te were also achieved by this SDT growth approach. Spectroscopic results show that doping systematically changes its electronic properties including band gap and work function. As an example of its use, we used doped BP as an ultrasensitive molecular sensor to detect organic molecules with a concentration down to 1×10^{-11} M, due to its tunable band alignment with target molecules. Our work develops a new method to grow BP and doped BP with tunable electronic properties, and should extend the uses of these class of materials in various areas.



Experimental setup of BP crystal growth with both uniform and gradient temperature furnace and the comparison of BP yield with various growth conditions.

P039 **Tu 17:00 - 18:30**

Metal fibrils embedded in continuous carbon nanotube fibers with high current-carrying capacity

Dong Su Lee[1], Hokyun Lee[1, 2], Min Park[1], Junbeom Park[1], Jiyoon Han[1], Aram Lee[1], Sukang Bae[1], Tae-Wook Kim[1], Seung Min Kim[1], Jun-Seok Ha[2], Sang Hyun Lee[2]

[1]*Korea Institute of Science and Technology, Jeonbuk 55324, South Korea*
[2]*Chonnam National University, Gwangju 61186, South Korea*

With the growth of nanoelectronics, the importance of thermal management in device packaging and the improvement of high-current-carrying interconnects/wires for avoiding the premature failure of devices have been emphasized. The failure mechanism of bulk metal interconnects has been understood in the context of electromigration; however, in nanoscale materials, the effect of the heat dissipation that occurs at the nanointerfaces may play an important role. We report the preparation of continuous carbon nanotube (CNT)–Cu composite fibers that possess Cu nanofibrillar structures with a high current-carrying capacity. Various-shaped CNT-Cu microfibers with different Cu grain morphologies were produced via Cu electroplating on continuous CNT fibers. Cu fibril structures were embedded in the voids inside the CNT fiber during the early stage of electrodeposition. The temperature-dependent and magnetic field dependent electrical properties and the ampacity of the produced CNT-Cu microfibers were measured, and the failure mechanism of the fiber will be discussed. The interconnection of Cu nanograins on the surface of the individual CNTs contributed to the ampacity enhancement.

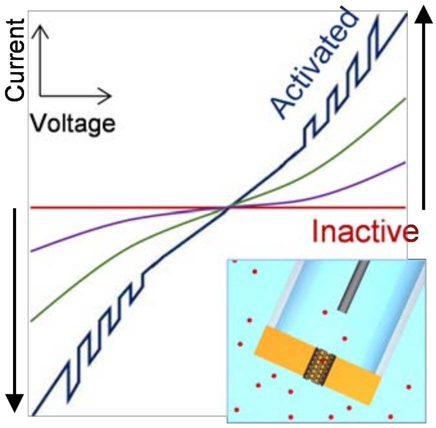
P041 **Tu 17:00 - 18:30**

High-yield fabrication, activation, and characterization of carbon nanotube ion channels by repeated voltage-ramping of membrane-capillary assembly

Hyegi Min[1], Yun-Tae Kim[2], Seung Min Moon[2], Jae-Hee Han[3], Kyungsuk Yum[4], Chang Young Lee[1]

[1]*School of Energy and Chemical Engineering, UNIST, Ulsan 44919, Republic of Korea*
[2]*School of Life Sciences, UNIST, Ulsan 44919, Republic of Korea*
[3]*Department of Energy and IT, Gachon University, Seongnam 13120, Republic of Korea*
[4]*Materials Science and Engineering, University of Texas, Arlington, Texas, USA*

The interior channels of carbon nanotubes are promising for studying transport of individual molecules in a one-dimensional confined space. Here, we developed assembling nanotube membranes on glass capillaries and employing a voltage-ramping protocol. Centimeter-long carbon nanotubes embedded in an epoxy matrix are sliced to hundreds of 10 μm-thick membranes containing essentially identical nanotube channels. The membrane is attached to glass capillaries and dipped into analyte solution. Repeated ramping of the transmembrane voltage gradually increases ion conductance and activates the nanotube ion channels in 90% of the membranes; 33% of the activated membranes exhibit stochastic pore-blocking events caused by cation translocation through the interiors of the nanotubes. Since the membrane-capillary assembly can be handled independently of the analyte solution, fluidic exchange can be carried out simply by dipping the capillary into a solution of another analyte. This capability is demonstrated by sequentially measuring the threshold transmembrane voltages and ion mobilities for K^+, Na^+, and Li^+. Our approach, validated with carbon nanotubes, will save significant time and effort when preparing and testing a broad range of solid-state nanopores.



Attaching a carbon nanotube membrane on a glass capillary enables convenient exchange of analytes when studying the transport of various ionic species in a nanotube. Ramping the transmembrane voltages can activate closed nanotubes with 90% yield.

P043 **Tu 17:00 - 18:30**

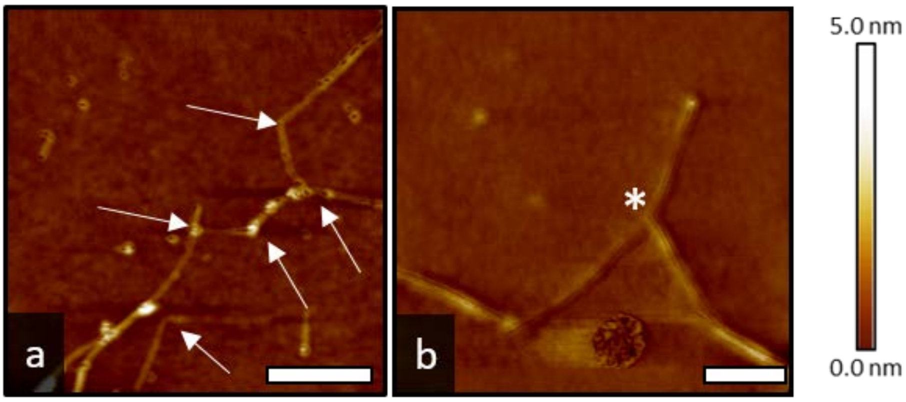
Directed supramolecular assembly of SWCNTs for functional networks

Chris Roberts[1], Hin Chun Yau[1], Milo Shaffer[1]

[1] *Imperial College London/Department of Chemistry, London, SW7 2AZ, UK*

Single-walled carbon nanotubes (SWCNTs) offer exceptional properties relevant to a wide range of applications, but are difficult to organize into well-defined functional architectures. Despite serendipitous examples, rational strategies to build functional metal-semiconductor nanotube junctions are lacking. Directed assembly, with control over SWCNT junction placement and formation is therefore highly desirable, both to form efficient networks, and to address individual nanotube devices.

This work is developing a promising new self-assembly mechanism, exploiting supramolecular nanocarbon chemistry to uniquely identify SWCNT ends for the direct formation of SWCNT junctions with control over multiplicity and geometry. This versatile strategy could generate a range of one- two- and three-dimensional functional networks, incorporating metallic, semiconducting, and insulating links. The underpinning technology is generic and can enable a wide range of applications, of increasing complexity, beginning with sensors and transparent conductors, building up through thin film transistors, ultimately towards nanoelectronics circuitry.



AFM micrographs demonstrating self-assembled a) bis-SWCNT and b) tris-SWCNT junctions (arrows and * respectively) Horizontal scale bars are 500 nm.

P045 **Tu 17:00 - 18:30**

Solid-state integrated capacitors based on carbon nanofibers

Muhammad Amin Saleem[1], R. Andersson[1], M. Bylund[1], M. S. Kabir[1], V. Desmaris[1]

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On-chip fully solid-state 3D integrated capacitors using high aspect ratio vertically aligned carbon nanofibers (CNFs) as electrodes to provide a large 3D surface in a MIM configuration have been manufactured in different sizes (foorprint areas). The CNFs are grown in different textures such as forest form and matrix of individual CNFs using plasma enhanced chemical vapor deposition on a metallic surface at 390 °C temperature. These CNFs are then coated conformally with very thin layer of dielectric material using atomic layer deposition (ALD) technique. A second layer of metal to make it MIM-capacitor is deposited using ALD and physical vapor deposition techniques. The coating with ALD helps to utilize the maximum surface area of the CNFs. The very thin dielectric and high surface area of the CNFs give high capacitance per footprint area. The capacitance density of more than 80 nF/mm2 (footprint area) is achieved from film texture, and higher capacitance is anticipated from matrix texture. The entire manufacturing process of the capacitors is completely CMOS compatible, which along with the low device profile of about 4 μm makes the devices readily available for integration on a CMOS-chip, in 3D stacking, or redistribution layers in a 2.5D interposer technology.

P047 **Tu 17:00 - 18:30**

Autonomous spatial organization in carbon nanotubes for tunable optoelectronic materials

Gustavo A. Zelada-Guillen[1], Martha V. Escarcega-Bobadilla[1]

[1] *School of Chemistry, National Autonomous University of Mexico (UNAM)*

Spatial organization of matter without human intervention has remained a major goal in nanotechnology for two decades. In this sense, bottom-up processes based on spontaneous self-assembly via supramolecular interactions have been exploited as a tool to achieve organized arrays of 0D nanostructures (quantum dots, nanoparticles), thus allowing systems with unprecedented optoelectronic properties.

However, the possibility to apply supramolecular self-assembly principles to achieve self-organization of challenging 1D nanostructures such as carbon nanotubes would represent a great opportunity to overcome many important current processing difficulties in the design of materials with tunable optoelectronic properties.

With this in mind, we designed a modular molecular system able to spatially drive anisotropic self-assembly of carbon nanotubes from the nanoscale to the mesoscale, thus making it possible to simultaneously tailor both electrical and optical properties in transparent conductors. Herein, we present a family of materials with appealing performance parameters (UV-VIS-NIR transparency, semi- to conducting, light polarization, strength), in which auto-organization of the nanostructures proceeds autonomously, using straightforward casting from solution strategies.

P049 **Tu 17:00 - 18:30**

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P051 **Tu 17:00 - 18:30**

Towards single-walled carbon nanotube based sustainable electrocatalysts for hydrogen economy

Tanja Kallio[1], Farhan Ali[1], Taneli Rajala[1], Albert Nasibulin[2]

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[2] *Skolkovo Institute of Science and Technology, 100 Novaya st., Skolkovo, 143025, Russia*

Renewables based energy supply will increase by more than one decade by 2040, which lays foundation for hydrogen economy. Hydrogen utilization as an energy carrier requires, however, introduction of efficient, durable and economically feasible conversion technologies. Electrochemical water splitting and fuel cells are appealing for this purpose but their key components, such as electrocatalysts for hydrogen reactions, must be improved.
Today scarce platinum group metals (PGMs) are utilized for catalyzing the hydrogen reactions. In addition to PGM availability and cost issues, these materials suffer from inadequate durability. Single-walled carbon nanotubes (SWNTs) have several beneficial properties needed for electrochemical applications such as high conductivity and good electrochemical durability. In this study, SWNTs have been used as a support for ultra-low PGM catalysts where their unique morphology contributes to formation of metal nanowires with the aspired properties. The feasibility of PtNW@SWNT is verified, for example, in an electrolyzer. In terms of activity, even with one tenth of Pt mass loading at the cathode, this catalyst accomplishes close to the level of the state-of-the-art Pt/C whereas the durability is confirmed with more than 2,000 h measurement.

Tu 17:00 - 18:30

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P055 **Tu 17:00 - 18:30**

Interwoven carbon nanotubes for supercapacitive wearable energy storage devices

Mihir Kumar Jha[1], Kenji Hata[2], Chandramouli Subramaniam[1]

[1]*Indian Institute of Technology Bombay, Powai, Mumbai 400076, India*
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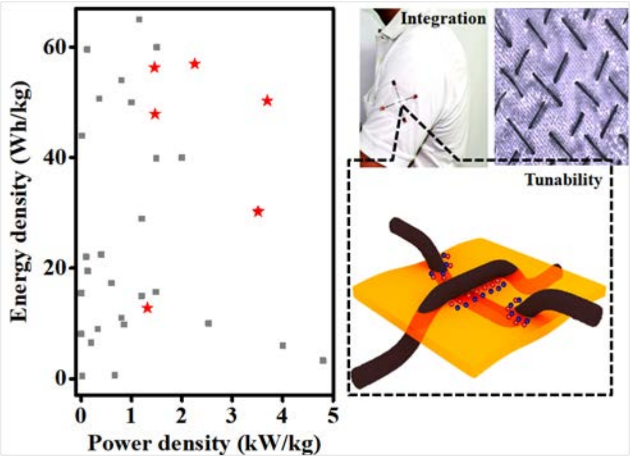
An energy storage device forms the heart of rapidly emerging soft, wearable and conformable electronics and demands high performance, without compromising on mechanical robustness. Driven by this demand, we report a high performing, washable and wearable supercapacitor with high energy density (~60 Wh/kg) and power density (~4 kW/kg) outperforming several similar reports. A facile fabrication strategy, involving interweaving of CNT-immobilized cellulose threads (CNT-wires) onto solid-electrolyte sheets (PVA-KOH and ion-gel), is adopted. Such interweaving produces capacitive junctions. Charge diffusion across such junctions is facilitated by high electrical conductivity (65 S/cm), surface area (614 m^2/g), mechanical tenacity (modulus~160 MPa) and geometry of CNT-wires. Moreover, the compact nature of junctions leads to minimal iRdrop (20 mV) and low relaxation-time constant for ultra-fast charging (1.3 ms). As each junction is capacitive, power-tunability over two orders of magnitude is achieved by creation of numerous junctions, across multiple dimensions. The devices are seamlessly integrated onto textiles as a decorative pattern/patch and can withstand mechanical flexing (360°), impact and harsh laundering, paving way for reliable and self-sustaining wearable technologies.



P057 **Tu 17:00 - 18:30**

Morphology and surface chemistry engineering toward pH-universal catalysts for hydrogen evolution at high current density

Yuting Luo[1]

The large-scale implementation of electrochemical hydrogen production requires several fundamental issues to be solved, especially understanding its mechanism and developing inexpensive electrocatalysts that work well at large current densities. We have addressed these challenges by exploring the roles of morphology and surface chemistry at large current densities in our resent work (Nature Communications, 2019, 10, 269). Three model electrocatalysts, i.e., a flat Pt foil, MoS_2 microspheres made of MoS_2 nanosheets, and MoS_2 microspheres modified by Mo_2C nanoparticles (MoS_2/Mo_2C) were used. We found that the MoS_2/Mo_2C is a highly active catalyst for HER with an activity that is independent of pH, with low overpotentials of 227 mV (in acidic media) and 220 mV (in alkaline media) at a large current density of 1000 mA cm^{-2}. Experimental and theoretical investigations show that the enhanced transfer of mass (reactants and hydrogen bubbles) at the interfaces of MoS_2/Mo_2C, and the fast reaction kinetics due to the surface oxygen formed on Mo_2C during HER are two reasons for the high activity of MoS_2/Mo_2C. Our results pave the way for the rational design of electrocatalysts that work well at large current densities.

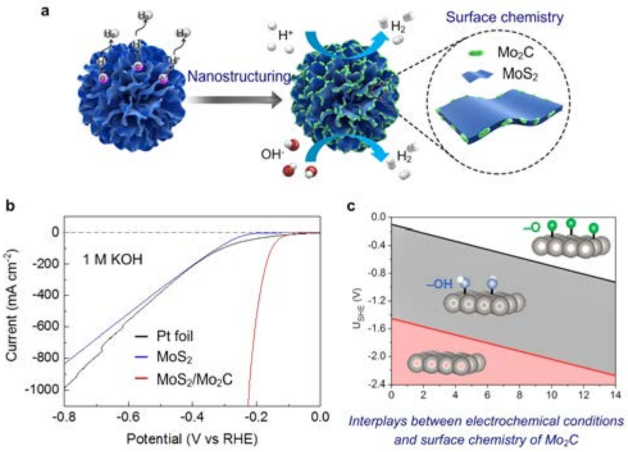


Fig 1. (a) Design of efficient electrocatalysts for large current density HER based on combination of surface chemistry and morphology. (b) Current-potential curves. (c) Interplays between electrochemical conditions and surface chemistry of Mo_2C.

P059 **Tu 17:00 - 18:30**

Vertically aligned carbon nanotube based materials: towards superpacitor devices with tunable performances

Martine Mayne-L'Hermite[1], Fabien Nassoy[1,2], Thomas Vignal[2,3], Cédric Desgranges[2,4], Jérémie Descarpentries[2], Léa Darchy[2], Aurélien Boisset[2], Mathieu Pinault[1], Cécile Reynaud[1], Philippe Banet[3], Pierre-Henri Aubert[3], Fouad Ghamouss[4], François Tran-Van[4]

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[2]*NAWATechnologies, 190, Avenue Célestin Coq, 13106 Rousset, France*
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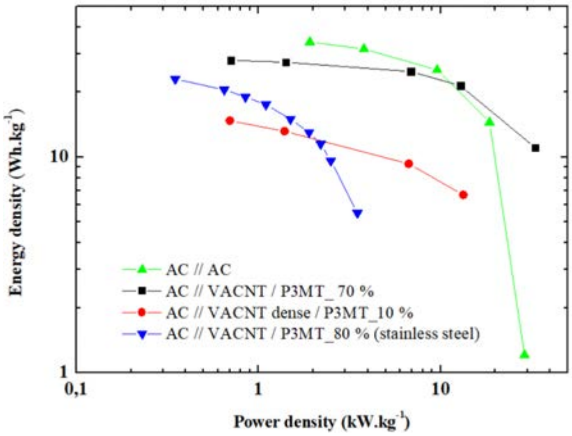
Vertically aligned carbon nanotubes (VACNT) based materials are efficient candidates to build supercapacitor electrodes. Our approach enables to get versatile materials able to tune the supercapacitor performances, which is very promising as compared to activated carbon. VACNT with different thickness and density, while possibly incorporating disordered carbon, are successfully obtained through a one-step CCVD thermal process operated on aluminum collector and up-scaled for commercial applications. The specific capacitance is increasing when the VACNT density and/or thickness increases. Electrode performances reach 20 to 450 mF/cm^2, and the supercapacitor volumetric energy is more than 10 times higher when disordered carbon is incorporated between VACNT. It is also possible to homogeneously incorporate electronically conducting polymer (ECP) inside VACNT, enabling to increase even further the specific capacitance (more than 700 mF/cm^2). Supercapacitors made of VACNT/ECP electrodes can reach 28 Wh/kg and 40 kW/kg (weight of active materials in the 2 electrodes), which is promising as compared to activated carbon (see fig.). Prototype devices prepared from VACNT synthesized at laboratory scale or on an industrial production line (Roll to Roll process) exhibit similar performances.



P061 **Tu 17:00 - 18:30**

Thorn-Shaped Pt-Ni Hierarchical Electrodes for High Performance Hydrogen Evolution Reaction

Adeela Nairan[1], Cheng Yang[1]

[1]*Division of Energy and Environment, Graduate School at Shenzhen, Tsinghua University.*

Designing inexpensive and efficient heterogeneous electrocatalysts for hydrogen evolution reaction (HER), while optimizing utilization of noble metals is crucial for renewable energy. However, selective distribution of noble metals on active sites is required for understanding the reaction mechanism and catalyst design. Here we report a novel three dimensional Pt-Ni nanowire arrays (Pt-Ni NWAs), through magnetic field growth process that consists of abundant nanocones on nanowire surface, like the appearance of thorns, as cathode for HER. These nanothorns serve as catalytic active sites and significantly improve the catalytic performance in alkaline medium. In addition, the tips of nanothorns provide numerous locally concentrated electric field, enhancing the free electron density, and thus significantly improve the HER activity on these sites. Benefiting from these features of NWAs, the electrode exhibits superior catalytic activity with an overpotential of 15 mV and 67 mV at current densities of 10 mA cm^{-2} and 200 mA cm^{-2} respectively. Selective distribution of Pt atoms and synergistic effects between Pt and Ni atoms enhances the catalytic activity. The present work provides a new horizon for designing advanced electrode materials in catalysis and energy conversion.

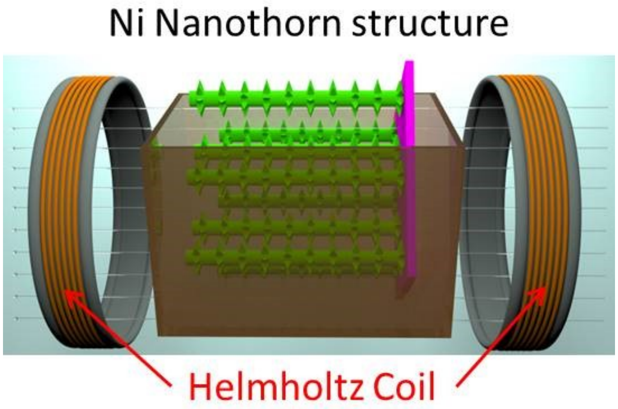


Figure 1. Fabrication mechanism of Ni nanowire arrays through magnetic field growth process.

P063 **Tu 17:00 - 18:30**

Thermoelectric materials and devices based on molecularly doped carbon nanotube films

Yoshiyuki Nonoguchi[1,2], Tsuyoshi Kawai[1]

[1] *Nara Institute of Science and Technology*
[2] *JST PRESTO*

The upcoming IoT society requires portable energy harvesters including thermoelectric generators around room temperature. Here we present a prototype, lightweight thermoelectric generator based on doped single-walled carbon nanotubes. The thermoelectric module is composed of both p- and n-type legs. To achieve this, we demonstrate a rational concept for stabilizing doped carbon nanotubes on the basis of counter-balancing, which affords air-stable p- and n-doped carbon nanotubes [1]. The generator is fabricated by the standard printing and cut-and-paste techniques. The 12 cm-scale generator with a commercial DC-DC converter exhibits thermoelectric outputs high enough to drive small devices such as a light-emitting diode (LED) [2]. We believe such demonstration facilitates the studies not only of further improvements in the thermoelectric properties of carbon nanotube materials but also of the novel design for thermoelectric generators on the basis of thermal engineering.

[1] Y. Nonoguchi et al., Adv. Funct. Mater. 26, 3021-3028 (2016).
[2] M. Ishimaru et al., MRS Adv. doi: 10.1557/adv.2019.3 (2019).

P065 **Tu 17:00 - 18:30**

Ultra-lightweight, Robust and Amphiphobic Carbon Nanotube Foams with Excellent Buoyancy

Pei Cao[1], Zhao Liming[1], Zhang Yongyi[1], Li Qingwen[1]

[1]*Advanced Materials Division, Suzhou Institute of Nano-Tech and Nano-Bionics, Chinese Academy of Sciences, Suzhou 215123, China*

In this report, we demonstrate carbon nanotube foams, which can be massively synthesized with ultra-low density, high compressibility, excellent mechanical robustness and amphiphobicity, may serve as a type of promising marine material for corrosion resistance and buoyant management. The CNT networked precursors are firstly formed with a desired size by winding a continuous CNT aerogel, sock layer by layer on a roller which is generated and blown out from an alcohol floating CVD process. Then alcohol vapor treatment under high temperature (typically at 1100°C), the exterior and interior of the CNT networked structures can be uniformly coated with amorphous carbon, leading to the foam with greatly enhanced compressive strength, structure stability even under severe deformation and excellent water repellence as well. Further vapor deposition of FDTS (1H, 1H, 2H, 2H-perfluorodecyltrichlorosilane) enable the CNT foam to be both hydrophobic and eleophobic, which is applicable to a variety of environmental conditions. More importantly, such robust and amphiphobic foams also exhibit superbuoyancy in water and oil, nearly 10 times higher than conventional polymer based buoyant materials, which ensure the great promise for applications in various marine transportation.

P067 **Tu 17:00 - 18:30**

Spinning-Disc Confocal Microscopy in the Second Near-Infrared Window (NIR-II)

Alessandra Antonucci[1], Alessandra Antonucci[1], Nils Schuergers[1], Benjamin Lambert[1], Andrea Latini[2], Raino Ceccarelli[2], Andrea Santinelli[2], Andrii Rogov[3], Daniel Ciepielewski[3], Ardemis Boghossian[1]

[1]*École Polytechnique Fédérale de Lausanne (EPFL), Lausanne, CH-1015, Switzerland*
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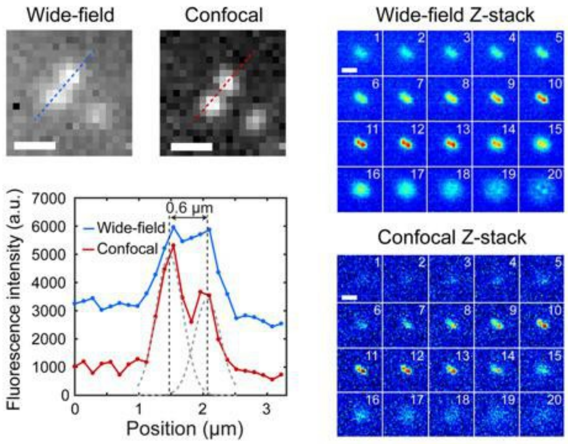
Fluorescence microscopy in the second near-infrared optical window (NIR-II, 1000-1350 nm) has become a technique of choice for non-invasive in vivo imaging. The deep penetration of NIR light in living tissue, as well as minimal or complete absence of tissue autofluorescence within this range, offers increased resolution and contrast with even greater penetration depths. Here, we present a custom-built spinning-disc confocal laser microscope (SDCLM) that is specific to imaging in the NIR-II. The SDCLM achieves a lateral resolution of 0.5±0.1 μm and an axial resolution of 0.6±0.1 μm, showing a ~17% and ~45% enhancement in lateral and axial resolutions, respectively, compared to the corresponding wide-field configuration. We furthermore showcase several applications that demonstrate the use of the SDCLM for in situ, spatiotemporal tracking of NIR particles and bioanalytes within both synthetic and biological systems.



P069 **Tu 17:00 - 18:30**

Doping-Dependent Energy Transfer from Conjugated Polyelectrolytes to (6,5) Single-Walled Carbon Nanotubes

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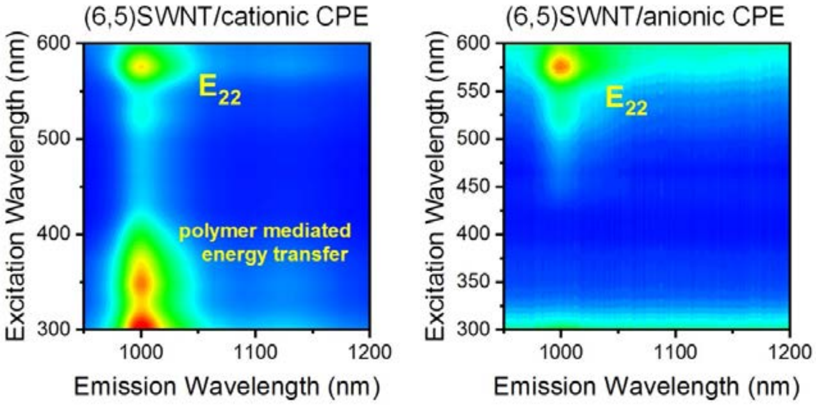
Efficient sorting of semiconducting or even monochiral single-walled carbon nanotubes (SWCNTs) can be achieved by polymer-wrapping on a large scale. After removal of the excess polymer, the energy transfer and hence the emission properties of the polymer/nanotube hybrids can be investigated, e.g., via photoluminescence excitation-emission (PLE) maps. Furthermore, the exchange of the sorting polymer with other conjugated polymers for a given type of SWCNT is possible and thus the formation of a range of new hybrids. Here, we employ polymers with ionic pendant side chains, so called conjugated polyelectrolytes (CPE) to redisperse (6,5) SWCNTs in methanol. Nanotube dispersion with either anionic or cationic polyfluorene-based CPEs show good photoluminescence when the nanotubes are excited directly via E_{22}. Moreover, for the cationic CPE, energy transfer from the polymer to the (6,5) nanotube is observed, but not for the anionic CPE (see PLE maps). As CPEs are known for their self-doping properties, we investigate the origin of the energy transfer and emission differences by tailored chemical doping of the dispersions and electrochemical doping of networks.



P071 **Tu 17:00 - 18:30**

Optical Response of Finite-Thickness Plasmonic Films with Periodic Cylindrical Anisotropy

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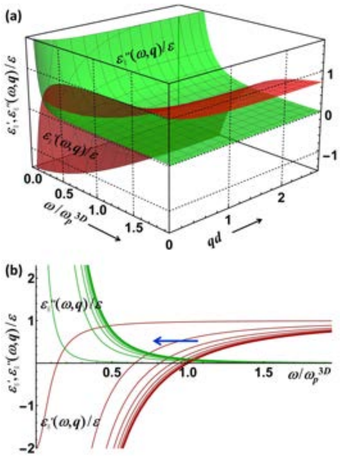
Periodically aligned carbon nanotube (CN) films are currently in the process of intensive experimental development in the hope of creating a new generation of ultrathin metasurfaces and nonlinear optical devices with characteristics adjustable on demand by means of CN diameter, chirality and periodicity variation[1-4]. Here, the plasma frequency and the dielectric response tensor are derived and analyzed for the finite-thickness plasmonic film formed by periodic parallel arrays of metallic cylinders embedded in a host dielectric matrix[5]. The plasma frequency is shown to exhibit the unidirectional spatial dispersion for the thick and ultrathin films, respectively. The associated unidirectional dielectric response can be tuned by the film material composition and thickness, the cylinder length and cylinder-radius-to-film-thickness ratio. The theory developed is discussed in application to the finite-thickness periodically aligned CN films for which the importance of the nondispersive interband plasmon modes of individual CNs is stressed in the ultrathin film regime.

[1]X.He, et al., Nat.Nano11,633(2016); [2]K.-C.Chiu, et al., NL17,5641 (2017); [3]A.L.Falk, et al., PRL118,257401(2017); [4]A.Graf, et al., Nat.Comm.7,13078 (2016); [5]I.V.Bondarev, Opt.Mater.Exp.9,285(2019)



Real (red) and imaginary (green) parts of the unidirectional dielectric response (a) and their respective contour plots (b) calculated as functions of the dimensionless frequency, wave vector and film thickness

P073 **Tu 17:00 - 18:30**

Using Alkaline Oxidation to Prepare Commercial Carbon Materials for Elemental Analysis

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Routine chemical analysis of Nanocarbons is dependent on analytical tools that are fast, easy to operate/maintain and accessible, such as inductively coupled plasma optical emission spectroscopy or ICP-OES.

Last year, we communicated the use of alkaline oxidation (a.k.a. fusion) to digest a certified sample of carbon nanotubes produced by the National Research Council Canada (SWCNT-1). That work validated fusion as an alternative approach to ashing and wet digestion for the preparation of Nanocarbons to be analyzed by ICP-OES [1]. Now, we would like to show how the method can be extended to commercial Carbon Materials (Figure 1). Accordingly, we studied samples of single-walled CNTs, expandable graphite and carbon black. For all these, reference mass fractions of targeted elements were provided by a primary method, Neutron Activation Analysis (NAA) [2]. In addition to the chemical analysis, we also looked into the way that the alkaline salt interacts with the different Carbon Materials.

[1] Simoes, F. R. F.; Abdul-Hamid, E.; Smajic, J.; Batra, N. M.; Costa, P. M. F. J. Analytical Methods (2019), doi: 10.1039/c8ay02213e.

[2] Kameník, J.; Simões, F. R. F.; Costa, P. M. F. J.; Kucera, J.; Havránek, V. Journal of Radioanalytical and Nuclear Chemistry (2018), 318, 2463.

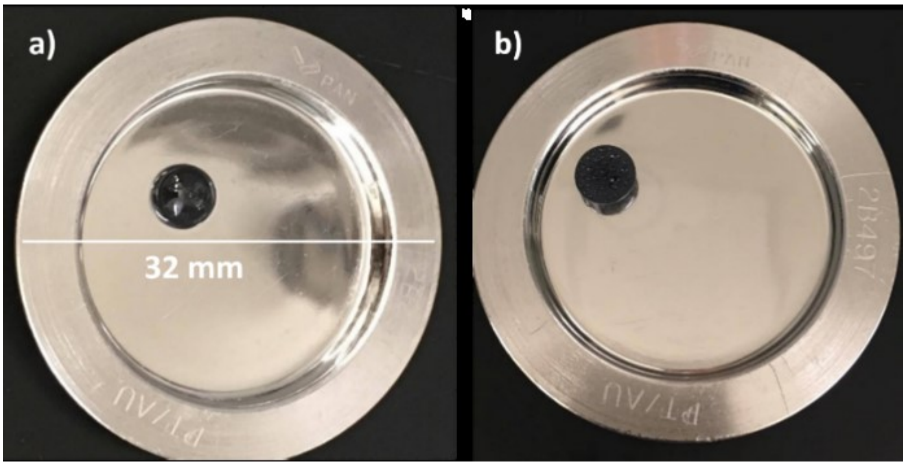

Figure 1: A glass-like bead of the fused product standing on a Pt plate (from a sample of SWCNT-1 and a lithium carbonate flux), a) top-side of the bead, b) bottom side-of the bead.

P075 **Tu 17:00 - 18:30**

Charge carrier localization in doped carbon nanotubes revealed by linear and nonlinear spectroscopy

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Doping of semiconductor nanostructures with mobile and delocalized charges is essential for their application in electronic devices.

Here, we report on spectroscopic investigations of redox doped semiconducting carbon nanotubes with focus on the localization and delocalization of surplus charges (see Fig. 1a). For moderate doping, the induced modifications of exciton- and trion-photophysics in VIS-NIR absorption, photoluminescence and femtosecond pump-probe spectroscopy suggest that surplus charge carriers become spatially localized. Further evidence of carrier localization is obtained from FTIR spectroscopy with strongly non-Drude type behavior (see Fig. 1b top). For heavily doped carbon nanotubes with completely bleached excitonic absorption bands the non-Drude absorption is replaced by a Drude-like free carrier response (Fig. 1b bottom). This is interpreted as evidence for the transition from carrier localization at moderate charge densities to carrier delocalization for heavily doped nanotubes in the degenerate regime.

Our findings show that the integration of doped semiconductor nanostructures into electronic devices might be affected by charge localization due to strongly enhanced Coulomb interaction in low-dimensional systems.

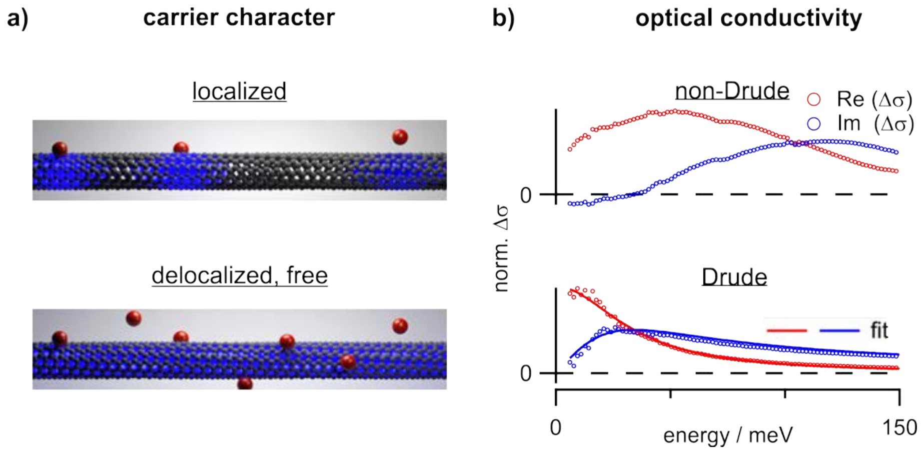

Fig. 1: a) Limiting cases of localized and delocalized carriers and b) experimental optical conductivity data.

P077 **Tu 17:00 - 18:30**

Characterisation of the inner shell extraction from double-wall carbon nanotubes by in situ Raman PLE spectroscopy after ultracentrifugation.

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[1]*Experimental Condensed Matter Physics, University of Antwerp, Antwerp, 2610, Belgium*
[2]*CIRIMAT, Paul-Sabatier University, Toulouse, 31062, France*

The optical properties of double-wall carbon nanotubes (DWCNT), consisting of two coaxial single-wall CNTs, are modulated by the inter-wall van der Waals interaction and the relative chiral angles of the individual CNTs [1]. A debatable topic regarding DWCNTs concerns whether inner tubes fluoresce (PL) or not, although single-DWCNT experiments show drastic PL-quenching for the inner CNT [2]. However, to characterise the PL from DWCNTs, they are typically solubilised using sonication. Here, we demonstrate that sonication extracts the inner tubes from the DWCNTs, leading to fluorescing SWCNTs. First, the DWCNTs were purified from SWCNTs and bundles using density gradient ultracentrifugation (DGU). Then, sonication is applied, after which the extracted inner tubes were separated from the DWCNTs by DGU and characterised by in situ resonant Raman and PL-spectroscopy as a function of height in the centrifuge tube [3]. These subsequent in situ DGU experiments unambiguously prove the extraction of inner SWCNTs from DWCNTs, even by very brief sonication. In addition, this extraction process is sonication time dependent and quickly saturates.

[1] A Ghedjatti et al Nano Lett 11, 4840 (2017)
[2] D Levshov et al Phys Rev B 96, 195410 (2017)
[3] S Cambré et al Nanoscale 7, 20015 (2015)

P079 **Tu 17:00 - 18:30**

Charge Transfer Process at the Interface of Carbon Nanotube/WS_2 Mixed Dimensional Heterostructures

Rui Feng[1]

Mixed dimensional van der Waals (vdW) heterostructures constructed by one dimensional(1D) and two dimensional(2D) materials can combine their dimensional properties to behave as anisotropic and non-planar mixed-dimensional vdW heterojunctions which are promising in the development of optoelectronics devices. In this case, the interaction between electron and photon at the interface of 1D and 2D materials plays a crucial role in the behavior of devices. We construct carbon nanotubes (CNT)/monolayer WS_2 mixed dimensional vdW heterostructure to investigate excitonic behavior of WS_2 which reflects the charge transfer process at the interface of CNT and WS_2. Photoluminescence spectra (PL) of both metallic-CNT/WS_2(M-CNT/WS_2) and semi conductive CNT/WS_2(S-CNT/WS_2) heterostructures are investigated. The total PL is enhanced in the former on while weaken in the latter one. Besides, the peak positions of both exciton and trion get redshift in M-CNT/WS_2 which get blueshift in S-CNT/WS_2. It is inferred that the charge is transferred from WS_2 to M-CNT while the contrary process happens in S-CNT/WS_2. Later excitation power dependent PL also confirmed this conclusion. This research reveals the charge transfer process at the interface of 1D/2D mixed dimensional vdW heterostructures.

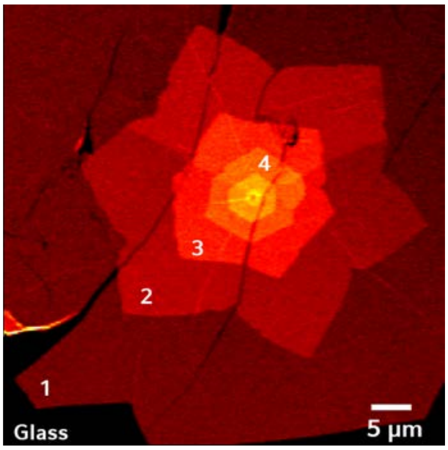
P081 **Tu 17:00 - 18:30**

Ultrafast Microscopy and Spectroscopy of Graphene

Achim Hartschuh[1], Veit Giegold[1], Lucas Lange[1], Richard Ciesielski[1]

[1] *Department of Chemistry and CeNS, LMU Munich, 81377 Munich, Germany*

We studied the ultrafast response of graphene using transient scattering microscopy and spectroscopy. In the experiment, the intensity of the elastically scattered light from a tightly focused spot is detected for variable time delay and energy detuning between excitation and probe pulse. The transient signal of graphene features pronounced G and 2D band phonon resonances, which scale linearly with both pump and probe pulse fluence and decay on the picosecond timescale. We discuss the characteristics of these phonon resonances based on complementary Raman spectra of graphene obtained for pulsed excitation.



Transient scattering microscopy image of graphene and few layer graphene taken at zero delay between fs pump and probe pulses.

P083 **Tu 17:00 - 18:30**

Highly Sensitive Surface-Enhanced Raman Spectroscopy Substrate with Nanometer-Scale Quasi-Periodic Nanostructures

Yuanhao Jin[1], Qunqing Li[2], Shoushan Fan[3]

We introduce a simple and cost-effective approach for fabrication of effective surface-enhanced Raman spectroscopy (SERS) substrates. It is shown that the as-fabricated substrates show excellent SERS effects in various probe molecules with high sensitivity, i.e., picomolar level detection, and also good reliability. With a SERS enhancement factor beyond 108 and excellent reproducibility (less than 5%) of signal intensity, the fabrication of the SERS substrate is realized on a four-inch wafer and proven to be effective in pesticide residue detection. The SERS substrate is realized firstly through the fabrication of quasi-periodic nanostructured silicon with dimension features in tens of nanometers using super-aligned carbon nanotubes networks as an etching mask, after which a large amount of hot-spots with nanometer gaps are formed through deposition of a gold film. With rigorous nanostructure design, the enhanced performance of electromagnetic field distribution for nanostructures is optimized. With the advantage of cost-effective large-area preparation, it is believed that the as-fabricated SERS substrate could be used in a wide variety of actual applications where detection of trace amounts is necessary.

P085 **Tu 17:00 - 18:30**

Near-Infrared Confocal Imaging of Single-Walled Carbon Nanotube Uptake in Bacterial Cells

Alessandra Antonucci[1], Nils Schuergers[1], Vitalijs Zubkovs[1], Ardemis Boghossian[1]

[1]*École Polytechnique Fédérale de Lausanne (EPFL), Lausanne, CH-1015, Switzerland*

The distinctive properties of single-walled carbon nanotubes (SWCNTs) have inspired many innovative applications in the field of cell nanobiotechnology. Most studies to date have focused on eukaryotic cells capable of internalizing functionalized SWCNTs, however, the effect of SWCNT functionalization on transport across the thick cell wall of prokaryotes remains unexplored. Herein, we explore SWCNT uptake in Gram-negative cyanobacteria and demonstrate selective internalization of SWCNTs decorated with charged protein wrappings. These functionalized SWCNTs are shown to traverse the outer cell wall of filamentous and unicellular strains of cyanobacteria, independent natural competency for DNA uptake, with adsorption and internalization rate constants of kads = (9.08 ± 0.16)x10^{-8} s^{-1} and kin = (1.466 ± 0.011)x10^{-4} s^{-1}, respectively. A custom-built, spinning disc confocal microscope enabled direct imaging of the near-infrared (NIR) SWCNT fluorescence within cells, revealing a highly inhomogeneous distribution of SWCNTs, that is overlooked using conventional NIR widefield imaging. The nanobionic cells show sustained photosynthetic activity and growth, offering a powerful avenue for engineering photosynthetic organisms with augmented and even inherited nanobionic capabilities.

P087 **Tu 17:00 - 18:30**

A Nanobioengineering Frontier for Next-Generation Optical Devices

Ardemis Boghossian[1]

[1]*École Polytechnique Fédérale de Lausanne (EPFL), Lausanne, CH-1015, Switzerland*

The vast expansion of available synthetic biology tools has led to explosive developments in the field of materials science. No longer confined to engineering just synthetic materials, the increased accessibility of these tools has pushed the frontier of materials science into the field of engineering biological and even living materials. By coupling the tunability of nanomaterials with the prospect of re-programming living devices, one can re-purpose biology to fulfill needs that are otherwise intractable using traditional engineering approaches. Optical technologies in particular could benefit from capitalizing on untapped potential in coupling the optical properties of nanomaterials with the specificity and scalability of biological materials. This presentation highlights specific applications in optical sensing and light-harvesting energy technologies that exploit the synergistic coupling of nanobio-hybrid materials. We discuss the development of bio-conjugated single-walled carbon nanotubes (SWCNTs) for near-infrared fluorescence sensing and the application of these nanobioptic sensors for continuous measurements in living cells and organisms. We further explore the development living photovoltaics based on bioengineered, photosynthetic organisms with augmented capabilities.

P089 **Tu 17:00 - 18:30**

Application of carbon nanotubes based drug carriers in biomedical field

Cheng-hua Ding[1], Yue Sun[1], Hua-ping Pan[1]

[1]*School of chinese medicine, Jiangxi University of Traditional Chinese Medicine, Nanchang, 330004, China*

As a low-dimensional new nanomaterial, carbon nanotubes(CNTs) can be used for drug delivery. Compared with the traditional drug carriers, the modified CNTs based drug carriers have advantages such as strong cell penetrating ability, large specific surface area, high drug loading, strong stability and targeting. It has become one of the hotspots in the research of drug delivery systems. At present, there are many reports about using CNTs to carry different anti-tumor drugs, such as doxorubicin, epirubicin, carboplatin, cisplatin, paclitaxel, methotrexate, hexamethylene amide, gemcitabine, etc., for investigation of anti-human breast cancer, ovarian cancer, liver cancer and so on. It was reported that these CNTs based drug delivery systems exhibit highly utilization of anticancer drugs and enhance anticancer effects. Also, CNTs can be applied to carry antifungal drugs, folic acid, epidermal growth factor, etc. for the treatment of related diseases. However, how to improve the safety and effectiveness of CNTs based drug carriers and how to prepare it in large quantities has yet to be resolved. We believe that these obstacles are constantly being eliminated with the development of scientific technology.

P091 **Tu 17:00 - 18:30**

A highly selective array of sensors based on NPs-decorated CNT for medical applications

Sonia Freddi[1], Stefania Pagliara[1], Giovanni Drera[1], Andrea Goldoni[2], Luigi Sangaletti[1]

[1]*I-Lamp and Università Cattolica del Sacro Cuore, 25121 Brescia (Italy)*
[2]*Elettra – Sincrotrone Trieste, 34128 Trieste (Italy)*

We developed a platform of 5 gas sensors, based on carbon nanotubes (CNT) functionalized with nanoparticles of Au, TiO_2, ITO, and Si. The array has been exposed to a selected series of target gas molecules (ammonia, nitrogen dioxide, hydrogen sulfide, water, benzene, ethanol, acetone, 2-propanol, sodium hypochlorite, and several combinations of two gases) related to some specific diseases, and the data has been analyzed with the principal component analysis (PCA). The results show that this sensors array is able to detect different target gas and to discriminate each molecule in the 2D PCA space. In particular, the possibility to include in the array a humidity sensor significantly increases the capability to discriminate the response to volatile organic compounds (VOCs). This leads to an improvement in selectivity that could meet the requirements for gas detection applications in the field of breath analysis, where sensors are exposed to a variety of different molecules and where the humidity can severely affect the overall response of the sensor.

P093 **Tu 17:00 - 18:30**

The Impact of Exposed Surface Area on the Response of SWCNT Optical Sensors

Shang-Jung Wu[1], Alics Judith Gillen[1], Daniel Jerome Siefman[1], Claire Bourmaud[1], Benjamin Lambert[1], Ardemis Boghossian[1]

[1]*École Polytechnique Fédérale de Lausanne (EPFL), Lausanne, CH-1015, Switzerland*

Due to their distinct and advantageous fluorescence properties, semiconducting single-walled carbon nanotubes (SWCNTs) are being applied to a variety of optical sensing applications. Limitations in solubility and biocompatibility have been overcome by non-covalently functionalizing the surface of the SWCNT with wrappings using techniques that retain its inherent fluorescence. Though wrappings based on surfactants and single-stranded DNA (ssDNA) have been extensively studied for this purpose, they are limited by factors such as lack of selectivity and lower fluorescence quantum yield, respectively.In this study, we take advantage of the higher fluorescence emission of surfactant-coated SWCNTs and focus on new approaches that can tune their selectivity as sensors. Through the concomitant monitoring of both the fluorescence intensity and wavelength position of emission peaks, we demonstrate the ability to increase the selectivity of sensors based on surfactant-suspended SWCNTs while retaining their higher fluorescence intensity. These results provide not only a promising avenue for rationally designing SWCNT sensors, but also insight on the mechanisms governing the selectivity of existing SWCNT-based optical sensors.

P095 **Tu 17:00 - 18:30**

Salt micro/nanolenses formed by ionic transport for optical visualization of carbon nanotubes and enhanced Raman spectroscopy

Yun-Tae Kim[1], Hyegi Min[2], Michael Strano[3], Jae-Hee Han[4], Chang Young Lee[2]

[1] *UNIST/School of Life Sciences, Ulsan, 44919, Republic of Korea*
[2] *UNIST/School of Energy and Chemical Engineering, Ulsan, 44919, Republic of Korea*
[3] *MIT/Department of Chemical Engineering, Cambridge, Massachusetts 02139, USA*
[4] *Gachon University/Department of Energy and IT, Seongnam 13120, Republic of Korea*

Optical visualization of 1-dimensional (1D) nanomaterials, such as single-walled carbon nanotubes (SWNTs), greatly eases the study of their properties and applications, but current approaches tend to be temporary and/or destructive. Here we report salt crystals formed by ionic transport along the exterior of SWNTs not only addresses the challenges in visualization, but also enhance Raman scattering of various molecular species. Applying an electrical bias to an aqueous solution of alkali metal halides placed at the end of a SWNT array causes ionic transport along the exterior of SWNTs and subsequent formation of salt crystals. Due to the hygroscopicity, the salt crystals transition to liquid droplets above deliquescence relative humidity, enabling optical visualization under various ambient conditions indefinitely. When necessary, the salts can be removed completely without damaging the nanotubes by rinsing with water. The salt crystals also serve as micro/nanolenses that amplify Raman scattering of SWNTs by orders of magnitude, as well as various molecular species captured within the lens by the transport. Our approach can have broad implications for optical visualization of various 1D nanostructures and molecular spectroscopy in salty environment.

P097 **Tu 17:00 - 18:30**

Macrophage behavior on the titanium electrodeposited carbon nanohorn

Sadahito Kimura[1], Eri Hirata[1], Sari Takada[1], Masatoshi Sakairi[2], Masako Yudasaka[3], Atsuro Yokoyama[1]

[1]*Graduate School of Dental Medicine, Hokkaido University, Sapporo 060-8586, Japan*
[2]*Faculty of Engineering, Hokkaido University, Sapporo 060-8628, Japan.*
[3]*Nanomaterials Research Institute (NMRI), AIST, Tsukuba 305-8565 Japan*

A carbon nanohorn is a graphene-lie tubule with a cone-shaped tip, thousands of which assemble to form a robust spherical aggregate. Recently, we reported that CNHs promote bone formation in the early stage of bone healing. CNHs coated on AnTi by simple electrophoretic deposition (CNH/AnTi) may be regulators of a variety of immune reactions without triggering any cytotoxicity.

In this study, the activation profile of the macrophages was evaluated on CNH /AnTi in vitro. Mouse-derived monocyte-macrophage-like cells (J774A.1) were cultured on AnTi and CNH/AnTi. After cell culturing, J774.A1 adhered and extended more on CNH/AnTi than those on AnTi. The titers of the pro-inframmatory cytokines (i.e. TNFα, IL1β and IL6) in the culture supernatants at 24 hours were measured by ELISA. IL1β production of the cells on CNH/AnTi was higher than that of on AnTi, and TNFα and IL6 production were the same as on AnTi. On the other hands, there were few genes upregulated or downregulated with CNHs and GO analysis suggests that there is no significant difference of the macrophages between on the CNH/AnTi and AnTi.

The effect of CNHs on macrophage and bone formation needed further research but these results suggested that the CNH coating slightly caused inflammatory reactions of macrophages.

Plenary Venue Poster

P002 **Tu 19:00 - 21:00**

Wavelength-dependent Resonant Raman Spectroscopy of Graphene Nanoribbons Synthesized inside Carbon Nanotubes

Miles Martinati[1], Sofie Cambré[1], Wim Wenseleers[1], Hans Kuzmany[2], Lei Shi[2], Thomas Pichler[2], Jeno Kürti [3], János Koltai[3], Gergo Kukucska[3], Kecheng Cao[4], Ute Kaiser Kaiser[4], Takeshi Saito[5]

[1]ECM Physics Laboratory, University of Antwerp, B - 2610 Antwerp, Belgium
[2]Faculty of Physics, University of Vienna, 1090 Wien, Austria
[3]Department of Biological Physics, ELTE Eötvös Loránt University, 1117 Budapest, HU
[4]Electron Microscopy Group of Materials Science, Ulm University, Ulm 89081, Germany
[5]Nanomaterials Research Institute, 305 - 8565 Tsukuba, Japan

Graphene nanoribbons (GNR) are strips of sp^2-hybridized carbon atoms with optical and electronic properties critically dependent on their width and structure. Heat treatment of single-walled carbon nanotubes (CNTs) exposed to ferrocene represents an efficient way to synthesize well-defined GNRs inside the hollow core of the CNTs. In this study, an extensive optical characterization of GNRs encapsulated inside CNTs was performed by means of wavelength-dependent resonant Raman spectroscopy (RRS) in a broad laser excitation wavelength range (400-800nm). RRS allowed us to directly measure the vibrational frequencies as well as the electronic transition spectra of the GNRs. The results were compared with DFT calculations showing a very good agreement and resulting in the assignment of the structure of the encapsulated ribbons. In particular, 6- and 7-armchair GNR were observed, demonstrating that the method holds promise towards the selective synthesis of homogeneous GNRs.

P004 **Tu 19:00 - 21:00**

Field-induced carrier injection in TMDC heterostructures

Mina Maruyama[1], Susumu Okada[1]

[1]*University of Tsukuba, Tsukuba, 305-8571, Japan*

Transition metal dichalcogenides (TMDCs) are representative semiconducting two-dimensional materials which consist of transition metal atomic layer sandwiched by chalcogen atomic layers in prismatic manner. Thus, they are regarded as constituent layered materials for designing van der Waals (vdW) heterostructures with TMDCs or other two dimensional materials, such as graphene and h-BN, by layer-by-layer stacking. In this work, we investigated carrier accumulation in vdW heterostuctures of TMDCs under an external electric field for providing a guiding principle to design the field-effect transistor (FET) of TMDC vdW heterostructure using the density functional theory combined with the effective screening medium methods. Our calculations showed that the distribution of the accumulated electrons by the field depends on the mutual arrangement of constituent TMDC with respect to the electrode and the carrier species, because of the alignment of the band edges of the TMDCs. For the heterosheet of MoS_2/WS_2 where the MoS_2 is situated at the electrode side, the injected electron is mostly injected into a MoS_2 layer, whilethe injected electron is penetrated into the second layers for the opposite TMDC arrangement.

P006 **Tu 19:00 - 21:00**

Synthesis of vertically-aligned single-walled carbon nanotubes having small diameters by ACCVD using Ir catalysts

Takahiro Maruyama[1], Takuya Okada[1], Kamal Sharma[1], Tomoko Suzuki[1], Takahiro Saida[1], Shigeya Naritsuka[1]

[1]*Meijo University, Nagoya 468-8502, Japan*

To fabricate SWCNT devices in conventional LSI process, it is important to grow high-density semiconducting SWCNTs having small diameters below ~1 nm, since the band gap of a SWCNT is in inverse proportion to its diameter. So far, several groups reported vertically aligned (VA) SWCNT growth, but in most cases, the average diameters were larger than 1 nm [1]. In this study, we performed SWCNT growth by alcohol catalytic chemical vapor deposition (ACCVD) using Ir catalysts to attain high-yield growth of small-diameter SWCNTs.
Using Ir catalysts, SWCNTs were grown on SiO_2/Si substrates by ACCVD. The grown SWCNTs were characterized by FE-SEM, Raman spectroscopy and photoluminescence (PL).
SEM observation showed that VA-SWCNTs were grown from Ir catalysts. The SWCNT length became longer, as the growth time increased, and it reached 2 micro-meter at the growth time of 60 min. The SWCNT diameter depends on the catalyst thickness. When Ir thickness was 0.2 nm, SWCNT diameters were distributed between 0.83 and 1.1 nm. We will also discuss the electronic type of grown SWCNTs based on Raman and PL results.

[1] T. Maruyama et al. Mater. Express 1 (2011) 267.

P008 **Tu 19:00 - 21:00**

Analysis of Reaction Products in CNT growth process by CVD

Hideki Masuda[1], Yu Kikuchi[1], Kanade Matsuo[1], Toshihiko Fujimori[2], Takeshi Hikata[2], Soichiro Okubo[2], Yoshikazu Ito[1], Jun-ichi Fujita[1]

[1] *Univ. of Tsukuba, Ibaraki, 305-8573, Japan*
[2] *Sumitomo Electric Industries, Ltd., Osaka, 554-0024, Japan*

Demand for ultra-long CNTs has been increasing to apply CNT to bulk assemblies while maintaining the high strength of individual CNTs. We focused on incorporating plastic deformation of CNTs into the CVD synthesis process, using the shear stress of gas laminar flow. Here we investigated the (intermediate) reaction products in CVD for tracking the CNT growth.
We introduced ethanol and ferrocene (as carbon sources and catalyst precursors) into the heated furnace tube (~1000 °C) with Ar (carrier gas) (Fig. 1(a)). We sampled the reaction products at various positions in the furnace tube. From the upstream side, we observed Fe-based fine particles with a diameter of ~20 nm derived from ferrocene and hollow carbon structures formed by carbon precipitation of carburized Fe-based particles (Fig. 1(b)). At other positions, we observed the deformed structures of the Fe-based fine particles (Fig. 1(c)). Also, we observed the CNT and the fine particles with a width of 5 nm or less (Fig. 1(d)). These products were distributed depending on the position in the furnace tube. In our CVD process using gas laminar flow, we have identified that finally elongated CNTs can be formed through the division of the fine particles and the deformation of the hollow carbon structures.

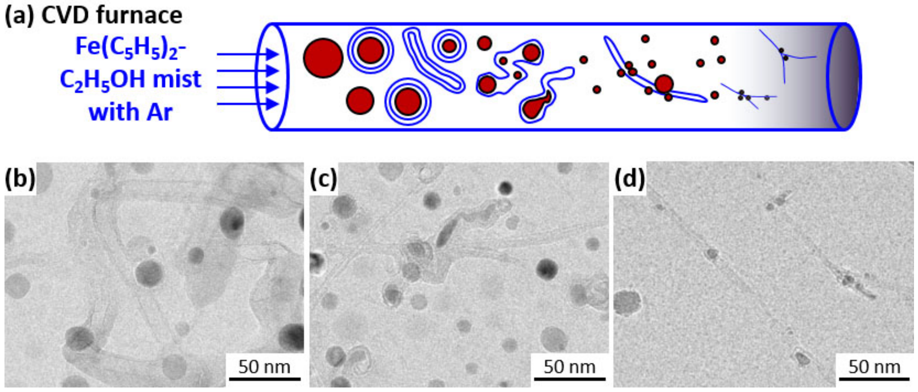


Fig. 1. (a) Schematic illustration of the CVD furnace. (b-d) TEM images of observed reaction products in the CVD.

Plenary Venue Poster

P010 **Tu 19:00 - 21:00**

Flexible free-standing-mode triboelectric generator realized by surface modification

Masahiro Matsunaga[1], Jun Hirotani[2], Shigeru Kishimoto[2], Yutaka Ohno[2,3]

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[2] *Department of Electronics, Nagoya University, Nagoya, 464-8603, Japan*
[3] *IMaSS, Nagoya University., Nagoya, 464-8601, Japan*

Triboelectric generator (TEG), which converts mechanical energy into the electricity by triboelectric electrification and electrostatic induction, is a promising candidate of power sources for wearable electronics [1]. Previously, we reported wearable TEG using a carbon nanotube (CNT) thin film as a stretchable and transparent electrode [2]. The TEG worked at single-electrode mode, which required an external ground electrode. The structure restricted to the degree of freedom for the application. Here, to remove the issue, we fabricated the TEG which was consisted of two electrodes with different surface modification of triboelectric layers.

The TEG was composed of the CNT thin film sandwiched with PDMS layers. After spin-coating PDMS onto a plastic substrate, the CNT transparent electrodes were patterned on the PDMS by the spray coating of CNT ink. The top PDMS was spin-coated to cover the CNT electrode. To form the different triboelectric surface, we then applied different treatments (CF_4 plasma and APTES treatment) to modify the PDMS surface on the respective electrodes. We obtained the simultaneous peak power density of 3.5 W/m2.

This work was supported by JST/CREST (JPMJCR16Q2).

[1] Z. L. Wang, Mater. Today 20, 74 (2017)
[2] M. Matsunaga et al., NT18, PA069 (2018)

P012 **Tu 19:00 - 21:00**

Over 40 GPa of breaking limit stress with long and highly crystalline CNTs

Kanade Matsuo[1], Yu Kikuchi[1], Kentaro Watanabe[1], Hideki Masuda[1], Toshihiko Fujimori[2], Takeshi Hikata[2], Soichiro Okubo[2], Yoshikazu Ito[1], Jun-ichi Fujita[1]

[1] *University of Tsukuba, Tsukuba 305-8573, Japan*
[2] *Sumitomo Electric Industries, Ltd., Osaka 554-0024, Japan*

The extremely high breaking stress exceeds 80 GPa of a single CNT would be the most attractive behavior for the constructional application. However, the bundling of the CNTs soonly deteriorated the breaking limit stress due to the misalignment.
We demonstrated the CNTs bundles constructing with over 100 long and highly aligned CNTs, still maintained the strength up to 40 GPa. We synthesize the long and high crystallinity CNTs using iron-oxide nanoparticles dispersed on the Si/SiO$_2$ substrate as the growth catalyst, and pure methane laminar-flow at 920-980 °C. The Gas analysis suggested the existence of an iron block in the specimen support effectively suppressed the pyrolysis reaction during CNT growth. The Raman spectrum Map suggested the free-standing CNTs bridged over a 1mm width slit engraved in the Si/SiO$_2$ substrate, and the D/G rate of the CNT is negligibly small. Fig. 1(a) suggested the fiber has three CNTs with a diameter of 1.5-2.5 nm. We also measure the tensile stress of the CNT bundle using Gas-flow and nano-mechanical methods making up with TiO$_2$ decoration for visualizing CNT. The single CNT showed 80-100 GPa of the strength. While the strength decreased with the bundle width, but the bundle consisted with about 100 of CNTs still keep 40 GPa, as shown in Fig. 1(b).

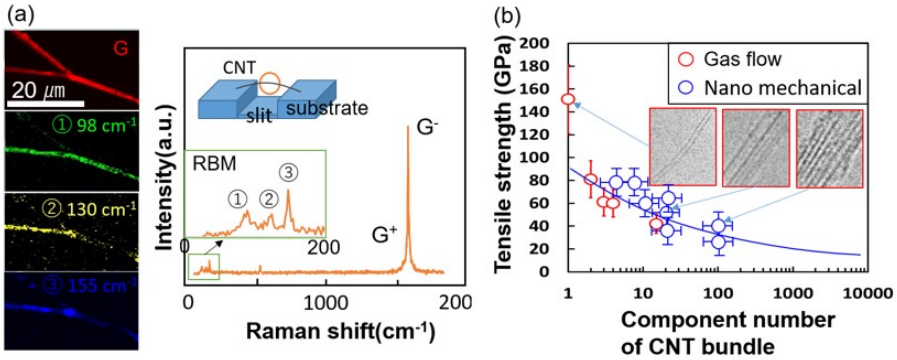

Fig. 1. (a) Raman spectral-Maps of free-standing CNTs. (b) The relationship between the tensile strength and the component number of CNT bundle.

Plenary Venue Poster

P014 **Tu 19:00 - 21:00**

The Effects of Hydrogen chemical potential on the graphene precursors during transition metal graphene CVD.

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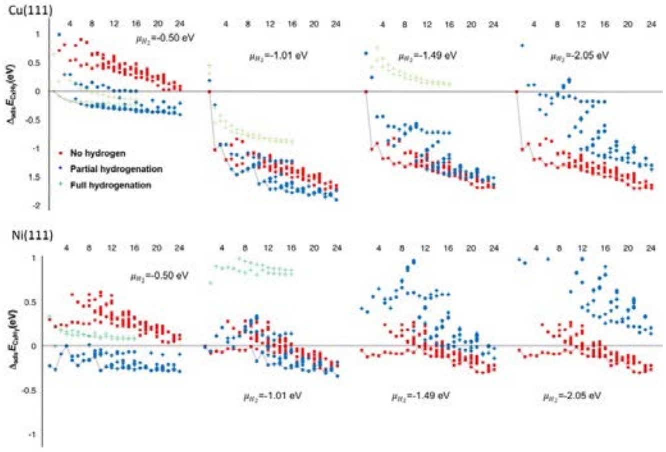
[2]*Institute for Basic Chemistry, Center for Multidimensional Carbon Materials, Ulsan, 44919, South Korea*

The technological potential of graphene is extensive and far reaching and one of the main methods of producing graphene in a usable amount is via chemical vapor deposition on transition metal catalytic substrates. This method involves exposing metal catalyst surfaces to a feedstock of hydrocarbons, hydrogen, argon and sometimes other gasses at high temperature, allowing for their decomposition and reformation into graphene at the surface. Understanding the fundamentals of this growth is often limited to computational investigations due to the small size and time scales however, these investigations often neglect on of the more important components of the feedstock gas, hydrogen. To this end we have investigated the effects of hydrogen chemical potential on the thermochemistry of a set of small potential graphene precursors on Cu(111) and Ni(111) substrates. We find that hydrogen helps facilitate the early formation of ring structures due to its ability to passivate edge structures effectively. Further, with decreasing hydrogen chemical potential the lowest energy pathway becomes more dominated by completely dehydrogenated precursors.



precursor energies as a function of fragment size and hydrogen chemical potential.

P016 **Tu 19:00 - 21:00**

Nanotube functionalisation for improved nanocomposite fibers

Joseph Moore[1]

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Nanocomposites are critically influenced by interfacial interactions between the reinforcement and matrix. Polyvinyl alcohol (PVOH) of varying molecular weights were grafted-to single- walled carbon nanotubes (SWCNTs), to improve the interfacial interaction with a homopolymer PVOH matrix. An intermediate grafted-PVOH molecular weight (10 kDa) maximized grafting ratio, and the final composite mechanical performance; the positive effects were attributed to the increased degree of dispersion of the SWCNTs in the dope, as well as the favorable interface. The PVOH grafting increased the stability of the SWCNT loading fractions (up to 45 wt.%), offering increased strength (up to 1100 MPa) and stiffness (up to 38.5 GPa) alongside high strain-to-failure (up to 23.3%).
Functionalisation strategies may also be used for pure SWCNT fibers, leading to a more easily dispersed spinning dopes and increased interactions between SWCNTs in the fiber.

P018 **Tu 19:00 - 21:00**

Mechanical and electrical structures of nano-carbon materials imaged by lock-in thermography

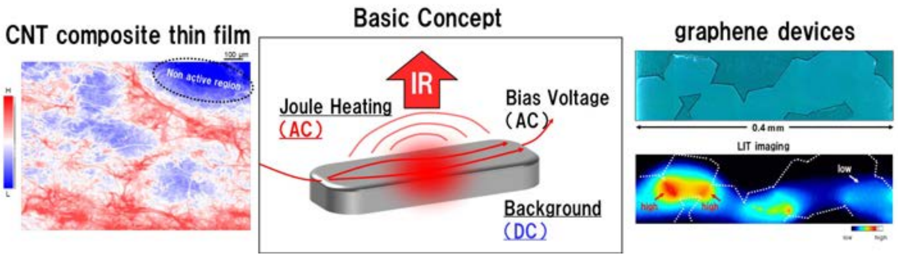
Takahiro Morimoto[1], Hideaki Nakajima[1], Toshiya Okazaki[1]

[1] *National Institute of Advanced Industrial Science and Technology (AIST)*

In nano-material science, for realization the new functional materials and devices, it is important to control the mechanical and electrical structures. It is difficult, however, to expect the bulk properties only from the nanometer-scale information by conventional method due to the large scale-gap between a nanometer-scale to a real scale. Therefore, the multi-scale and rapid methods are desired for optimization and maximization of various properties both functional materials and devices.

Recently, we have developed new method based on the lock-in thermography (LIT) technique [1,2] for the current density imaging with non-destructive, multi-scale and rapidly measurements. The intensity image of LIT method corresponds to Joule heating from the only nano-material current density distributions by signal separation process in a frequency space. Figure shows the current density distribution image in the CNT composite materials and current dissipation image in graphene devices. They are directly corresponding to the resistance and current distributions. Therefore, we can discuss the bulk electric and mechanical bulk properties based on these LIT images.

[1] T. Morimoto et al., submitted. (arXiv:1811.10910.). [2] H. Nakajima et al., Science Advances, eaau3407, 2019



The basic concept of the LIT method (center), and the results of the CNT composite thin film (left) and the graphene device (right).

P020 **Tu 19:00 - 21:00**

Analysis of the resistance switching properties in the multi-stacking composed of Pt/graphene oxide/Ag2S/Ag

Ryota Negishi[1]

[1] *Graduate School of Engineering, Osaka University*

Ag_2S-based switches have attracted attention due to its neuromorphic switching operation, in which voltage inputs cause the formation and annihilation of conducting Ag filaments. Since the switching behavior mainly depends on Ag_2S bulk material, enhancing controllable parameters is essential. In this work, we propose a modification method in the design of the previously known Ag/Ag_2S neuron-inspired devices by the addition of a modulating layer of graphene oxide (GO). Figure 1(a) shows the current-voltage curves observed from the Ag/Ag_2S devices with and without GO layer. The clear hysteretic behavior of the connection between the Pt and $Ag/Ag_2S/GO$ wires reveals the compatibility between GO thin films and the filamentary switching of Ag_2S. In addition, GO-modulated samples exhibited the lower OFF state currents (from 10^{-7}A in Ag/Ag_2S to 10^{-8} in $Ag/Ag_2S/GO$) due to the insulating nature of GO. As shown in Fig. 1(b), the time evolution analysis of the conducting states revealed that the volatility of the filaments increases by introducing GO layers when the same input was applied to the system. Therefore, we conclude that the additional GO layers have a modulation effect on the neuromorphic properties on Ag_2S-based switches.

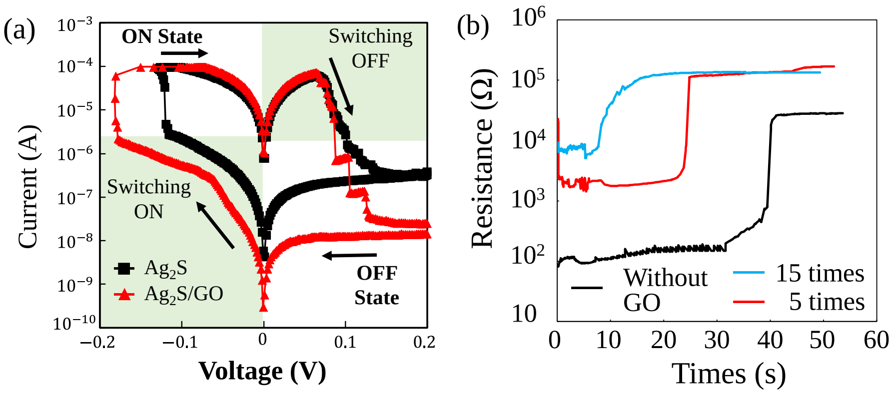


Fig. 1 (a) I-V curves observed using the sweeping voltage mode of the characterization system and (b) volatility observed by monitoring the time evaluation of the conducting states.

P022 **Tu 19:00 - 21:00**

Synthesis of highly crystalline multilayer graphene from defective graphene oxide materials

Ryota Negishi[1], Yuriko Tadano[1], Yuta Nishina[2], Masashi Akabori[3], Yoshihiro Kobayashi[1]

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[2]*Okayama University, Kita-ku, Okayama, 700-8530, Japan*
[3]*Center for Nano Materials and Technology, JAIST, Nomi 923-1292, Japan*

Multilayer graphene with a weak interlayer coupling is one of promising candidates for the channel material as a high performance electrical device due to the both high conductivity and carrier mobility. In this study, the highly crystalline multilayer graphene was synthesized from a defective graphene oxide (GO) material. Thermal treatment in a reactive ethanol environment at high temperature of 1300ºC was utilized for the restoration of graphitic structures in the GO thin film. Figure 1 shows the carrier transport properties of the multilayer graphene evaluated by hall measurements with van der Pauw method. The conductivity improves with increasing the number of graphene layers. This means that the current efficiently flows in each graphene layer. On the other hand, the carrier mobility is independent to the number of layers. In general, the carrier mobility of multilayer graphene with order stacking degrades with increasing the number of layers because the electrical band structure approaches a parabolic dispersion due to a strong electrical coupling between layers. This result indicates that the electrical band structure in the multilayer graphene is similar to that of the monolayer graphene due to the weak interlayer coupling between layers.

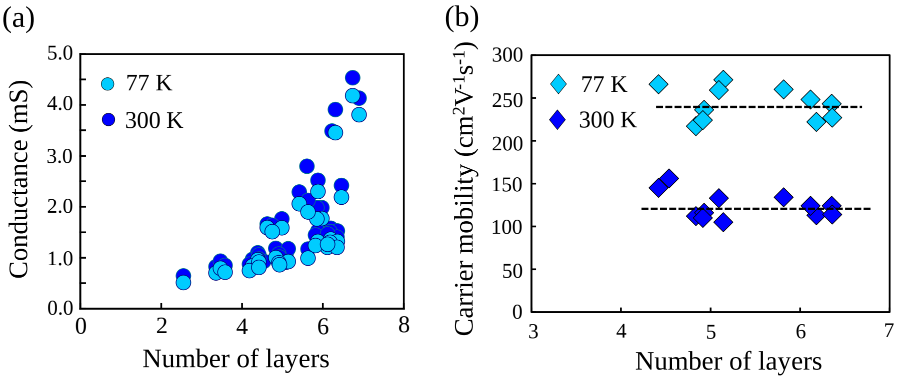

Fig. 1 (a) Conductance and (b) carrier mobilities in the multilayer graphene devices as a function of the number of layers.

P024 **Tu 19:00 - 21:00**

Local strain suppression layer for low-voltage operable, robust, and stretchable carbon nanotube integrated circuits

Yuya Nishio[1], Taiga Kashima[1], Jun Hirotani[1], Shigeru Kishimoto[1], Yutaka Ohno[1, 2]

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[2] *Inst. of Materials and Systems for Sustainability, Nagoya University, Japan*

The stretchable devices, which can intimately contact with dynamic free-form surfaces, are key components to realize wearable healthcare systems. Carbon nanotube (CNT) is considered to be a promising material for stretchable devices. However, there still exists a difficult challenge to realize a transistor having low-voltage operation, robust property against external strain, and high stretchability, simultaneously. In this work, we introduce the local strain suppression layer on the channel region to minimize the effect of externally applied strain.

Stretchable CNT thin-film transistors (TFTs) were fabricated on polydimethylsiloxane. The channel and electrodes consisted of CNT thin films. A 50-nm Al_2O_3layer was used for a gate dielectric layer. A parylene-C layer was formed on top of the channel region as a local strain suppression layer.

Due to the strain suppression layer, the drain current showed no degradation against the external strain up to 35 %. Furthermore, the TFTs operated at low voltage of -2 V. We also fabricated CNT integrated circuits. The fabricated inverters operated at low voltage of -1.5 V. The 3-stage ring oscillators operated at 6 kHz. These results verify that the local strain suppression layer is effective to realize low-power stretchable devices.

Plenary Venue Poster

P026 **Tu 19:00 - 21:00**

Ab Initio Study of Surfactant and Water Molecules on Defective Single-Wall Carbon Nanotubes

Mari Ohfuchi[1,2]

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[2] *Nagoya University, Nagoya 464-8603, Japan*

We investigated the adsorption of sodium dodecyl sulfate (SDS) surfactants onto single-wall CNTs (SWCNTs) using ab initio methods, and reported that the adsorption energy of dodecyl sulfate (DS) ions for metallic CNTs is much stronger than those for semiconducting CNTs [1]. This can cause a larger aggregation number of DS ions on metallic SWCNTs and a separation of SWCNTs by electronic type. In this study, we examine the adsorption of surfactant and water molecules onto defective SWCNTs. We show that the defects can make as much difference in the adsorption energy of DS ions as that between metallic and semiconducting SWCNTs. We also show that the difference between pristine and defective SWCNTs in the adsorption aspects of water clusters based on the adsorption energy of water molecules.

[1] M. Ohfuchi, J. Phys. Chem. C 122, 4691 (2018).

P028 **Tu 19:00 - 21:00**

Carrier accumulation in graphene/hBN heterostructures under an external electric field

Susumu Okada[1]

[1] *University of Tsukuba, Tsukuba, 305-8571, Japan*

A single sheet or thin films of h-BN are regarded as the supporting substrate or the insulating layer for other two-dimensional materials, such as graphene and transitionmetal dichalcogenides, owing to their atomically flat surfaces and insulating electronic property. Indeed, graphene adsorbed on h-BN exhibits remarkable transport properties compared with that on surfaces of bulk insulating materials. In this work, we aim to explore the field screening ability of h-BN thin films for graphene in the field effect transistor (FET) structure to give the guiding principle for designing the FET using h-BN as an insulating layer for the gate electric field. Using the density functional theory combined with the effective screening medium method, we found that h-BN thin films act as insulating layers for carrier accumulation in graphene under the low carrier concentrations. In contrast, under high carrier concentrations, hole is spilled over the outermost h-BN layer while the most of the electron is still accommodated in graphene, indicating their asymmetric field screening ability for carrier injection in graphene.

P030 **Tu 19:00 - 21:00**

Defective carbon nanotubes: conductance loss and enhanced piezoresistivity

Jörg Schuster[1,2,3], Fabian Teichert[3,4]

[1]Fraunhofer Institute for Electronic Nanosystems – ENAS, 09126 Chemnitz, Germany
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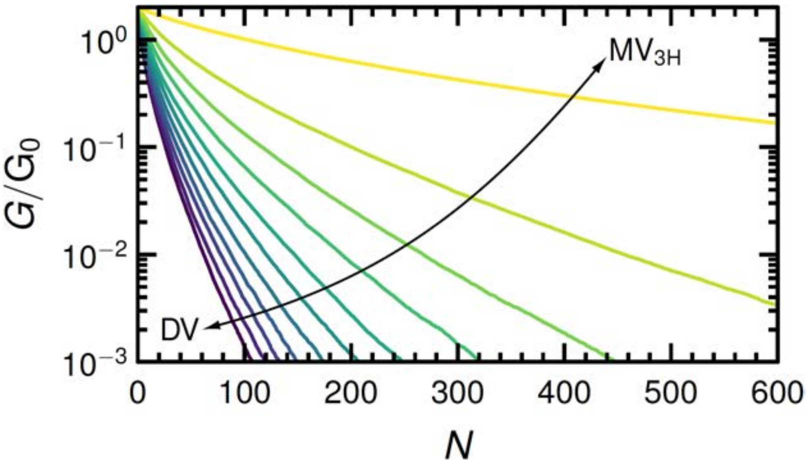
[4]Institute of Physics, Technische Universität Chemnitz, 09107 Chemnitz, Germany

Defects are present in any material. For low-dimensional materials such as CNTs, even individual defects modify the conductance drastically. We use quantum transport theory based on an efficient implementation of the recursive Green's function approach to calculate the conductance of defective CNTs.
Based on statistical simulation studies of large ensembles of CNTs with randomly positioned defects we calculate the conductance loss due to defects of various types. We investigate electron transport in the regime of strong localization. Hence, the conductance depends exponentially on the number of defects and is characterized by the localization length, which is shown to be a function of defect type, CNT diameter and chirality. Based on our findings we provide a set of simple formulas to predict defect induced conductance losses.
Surprisingly, defective CNTs can show an enhanced response to external strain compared to the ideal ones. As axial strain is applied to defective CNTs, piezoresistive gauge factors above 500 are observed in our quantum transport simulations. The enhancement of the gauge factor, which depends on strain, reaches up to 100%. Degradation of the gauge-factor is observed as well. Both aspects must be considered when designing CNT-based strain sensors.



Normalized Conductance of CNTs as a function of defect number and defect type.

P032 **Tu 19:00 - 21:00**

Li-Endohedral Fullerenes on Top of Laminated Carbon Nanotube Electrode-based Perovskite solar Cells Induce Exceptional Stability

Ahmed Shawky[1], Il Jeon[1], Esko Kauppinen[2], Shigeo Maruyama[1,3], Yutaka Matsuo[1,4]

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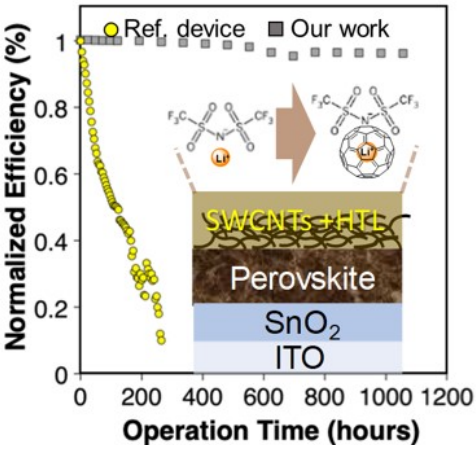
[2]*School of Science, Aalto Univ. Aalto, FI-00076, Finland*
[3]*Energy Nano Engineering Lab., AIST, Ibaraki 305-8564, Japan*
[4]*School of Chemistry and Materials Science, USTC, Anhui 230026, China*

Replacing the metal electrode by carbon nanotubes (CNTs) is one of the most effective ways in emerging solar cell technology. This aims to enhance the device stability of PSCs due to no ion migration and outstanding encapsulation effect. In perovskite solar cells (PSCs), the use of Spiro-MeOTAD with hygroscopic Li salt limits the full potential of the CNT-PSCs in terms of long-term stability.

Therefore, we incorporated the mixture of spiro-MeOTAD and Li@C_60 salt into the CNT top electrodes in PSCs (as shown in the figure). The solution is drop-casted onto the laminated CNT film in PSCs. This led to more effective hole extraction by avoiding [Li+@C_60]TFSI− in the pathway and more effective anti-oxidation activity by placing Li@C_60 next to air. From various investigations, we found that 2 h stirring for the HTL solution gave the highest Photo-conversion efficiency (PCE) of 17% and the longest stability of unencapsulated devices. The obtained PCE is close to the reference devices while the device stability is about 100 times greater. Such excellent stability is attributed to no ion-migration and antioxidant activity of Li@C_60 that uniformly covering the CNT electrode. We also discovered a new reaction within the spiro-MeOTAD and Li@C_60 salt.



Normalized PCE of our structured PSC (inset) vs. light soaking time compared with reference device.

P034 **Tu 19:00 - 21:00**

DFT-1/2 approximate quasiparticle corrections on band gap calculation of 2D materials

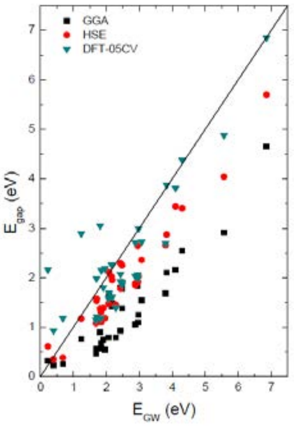
Lara Kühl Teles[1], Ivan Guilhon[1], Daniel Schwalbe Koda[1], Marcelo Marques[1], Luiz Guimarães Ferreira[2]

[1] *Instituto Tecnológico de Aeronáutica, DCTA, São José dos Campos, 12228-900 Brazil*
[2] *Instituto de Física, Universidade de São Paulo, São Paulo, SP, CP 66318, 05315-970, Brazil*

While 2D systems open possibilities for new physics and applications, they present a greater challenge for electronic structure calculations, especially concerning excitations. The achievement of a fast and accurate practical model that incorporates approximate quasiparticle corrections can further open an avenue for a more reliable band structure calculations of complex systems as e. g. interactions of 2D materials with substrates or molecules, as well as the formation of van der Waals heterostructures.

In this work, we demonstrate that the performance of the fast-free parameter DFT-½ method is comparable with state of art GW and superior of the HSE06 hybrid functional in the majority set of the 34 different 2D materials studied, with the same computational cost as standard DFT calculations. We provide criteria to predict the small number of cases in which the method is not adequate. The success of the DFT-½ method is associated to the atomic orbital character of the states at the top of the valence band and bottom of conduction band. Finally, we show that this result can be improved to 0.53 eV with the inclusion of conduction self-energy correction for binary materials with Pauling electronegativity difference above 0.15.

[1] I Guilhon et al., PRB 97, 045426 (2018).



Comparison of energy bandgaps calculated using GW and GGA, HSE, and DFT-1/2, represented by black squares, red circles, and green triangles, respectively. The solid black line illustrates the perfect agreement with the considered GW results.

P036 **Tu 19:00 - 21:00**

Ethanol sensing with surface-mounted metal-organic-framework functionalized graphene transistors

Sandeep Kumar[1,2], Kai Müller[3], Simone Dehm[1], Manuel Rommel[1], Tobias Schlöder[1], Artem Fediai[1], Qiang Zhang[1], Wolfgang Wenzel[1], Christof Wöll[3], Lars Heinke[3], Ralph Krupke[1,2]

[1]*Institute of Nanotechnology, Karlsruhe Institute of Technology, Germany*
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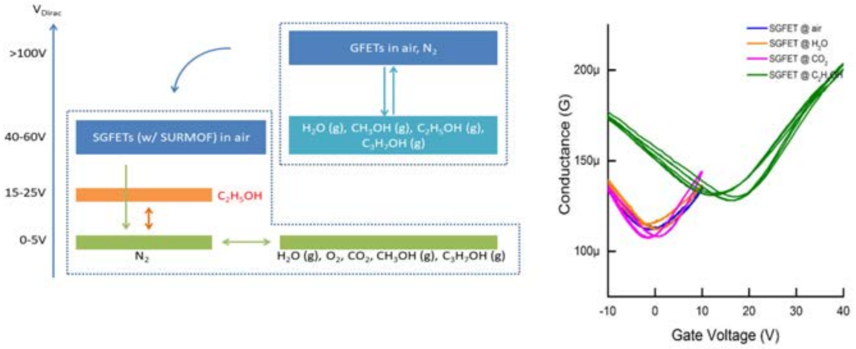
Surface-mounted metal-organic frameworks (SURMOFs) are crystalline nanoporous layers constituting of metal cation nodes and organic linker molecules, providing precisely controlled nano-environments for various applications [1,2]. The affinity of the host framework towards specific guest molecules can be tailored by selecting the appropriate SURMOF building blocks. In this work we followed the idea of combining a graphene field effect transistor (GFET) sensitive to environmental changes, with a SURMOF which provides the required selectivity for sensing applications. We have grown Cu(BDC) SURMOF-2 (BDC = benzene-1,4-dicarboxylate) on top of CVD-graphene on Si/SiO_2 (300nm) based on liquid-phase epitaxy. The SGFET devices show shifts in the Dirac voltage under exposure to ethanol molecules but remain insensitive against other gases (H_2O, CO_2 etc.) and alcohols (IPA, methanol). The response times of the SGFETs are on the order of tens of seconds and resetting occurs at similar timescales by current annealing. Simulations are undergoing to reproduce the experimental observations.

[1] Kreno et al. Chem. Rev. 112 , 1105–1125 (2012)
[2] Heinke, Wöll Adv. Mater. (2019) 10.1002/adma.201806324



Left: Schematic showing shifts in the Dirac voltage for graphene-FETs with SURMOF (SGFET) and without (GFET) under exposure to various gases. Selectivity and sensitivity to ethanol is only observed for SGFET. Right: Selected transconductance curves.

P038 **Tu 19:00 - 21:00**

Large intravalley scattering due to pseudo-magnetic fields in crumpled graphene

Péter Kun[1], Gergo Kukucska[2], Gergely Dobrik[1], János Koltai[2], Jeno Kürti[2], László Péter Biró[1], Levente Tapasztó[1], Péter Nemes-Incze[1]

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Lattice defects in graphene can be observed via Raman spectroscopy, making possible the detection and classification of grain boundaries, vacancies, adatoms etc. Nevertheless, direct Raman spectroscopic evidence of scattering on lattice imperfections that are smooth on the atomic scale is still lacking. Such smooth scatterers include strain fluctuations, that may be a key factor in reducing the charge carrier mobility in state of the art graphene devices, especially if wrinkles are introduced during the sample preparation processes.
Here we show a first example of resonant Raman scattering on smooth potentials, such as pseudo-magnetic fields generated by corrugations in graphene [1]. The strain induced vector potential shifts the phase of the charge carriers, in addition to the Berry phase. This lifts the restriction on backscattering, enabling a drastic increase in the intravalley backscattering rate by orders of magnitude, evidenced by the enhancement of the D' peak in the Raman spectrum. We observe an increase of the D'/D peak intensity ratio by up to a factor of 300 on sharp graphene folds. We also reproduce our experimental observations by numerical calculations of the double resonant Raman spectra.

References

[1] P. Kun et al., npj 2D Mater. Appl., 3, 11 (2019).

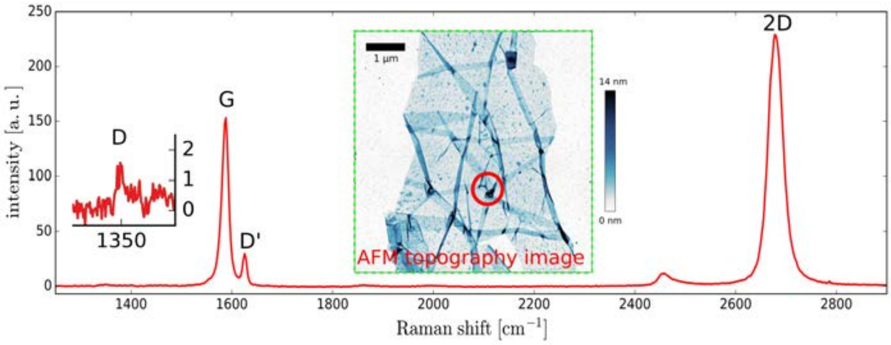

Figure 1. Raman spectrum of graphene (532 nm excitation) showing a large D' peak measured at the crumpled area (circled on the inset). Inset: zoom of the D peak region of the spectrum. Inset: AFM image of the crumpled area.

P040 **Tu 19:00 - 21:00**

Chemical interaction of sapphire substrate with $HfCl_4$ during chemical vapor deposition of HfS_2

Mirine Leem[1], Hyangsook Lee[2], Wonsik Ahn[1], Taejin Park[3], Hoijoon Kim[1], Hyoungsub Kim[1,4]

[1]*School of Advanced Materials of Science and Engineering, Sungkyunkwan University*
[2]*Samsung Advanced Institute of Technology*
[3]*Semiconductor Research and Development Center, Samsung Electronics*
[4]*SKKU Advanced Institute of Nanotechnology, Sungkyunkwan University*

With its high carrier mobility, HfS_2 has been regarded as a promising semiconducting 2-dimensional (2D) material, and the need for the development of an appropriate synthesis method keeps increasing. Among various synthetic methods, chemical vapor deposition (CVD) technique has been commonly used for growing large-area 2D films. Particularly, for the CVD of HfS_2, sapphire (crystalline Al_2O_3 and $HfCl_4$ have been commonly used as a substrate and a Hf precursor, respectively [1-2]. While developing the HfS_2 CVD process, we observed an interesting chemical interaction of the Al_2O_3 substrate with $HfCl_4$ under a $HfCl_4$-rich process condition: substrate etching and Hf-oxide formation. We will report the resulting surface morphology and microstructure of the CVD-processed samples. In addition, the expected chemical reaction paths will be discussed based on the thermodynamic calculation. We believe that understanding of the underlying mechanism for the observed morphological and microstructural evolution will be helpful in optimizing the CVD process for the HfS_2 growth.

[1] Wang et al., 2D Materials, 4, 3, 031012
[2] Zheng et al., Applied Surface Science, 2018, 435, 563-567

P042 **Tu 19:00 - 21:00**

Impact of temperature and excitation laser power on the Raman spectra of chemically functionalized MoS_2

Narine Moses Badlyan[1], Wanzheng Zhang[2], Kathrin Knirsch[2], Andreas Hirsch[2], Janina Maultzsch[1]

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In the past few years, transition metal dichalcogenides (TMDCs), such as molybdenum disulfide (MoS_2), have attracted particular attention due to their unique physical and electrical properties, which make them promising for applications in optoelectronics, photonics, and biotechnology.

Due to their large surface, they offer the opportunity to tune their electronic and optical properties as well as the nature of their interaction with the environment by covalent or non-covalent functionalization.

Here we present a spectroscopic study of MoS_2, functionalized with organic molecules and compare it with a chemically exfoliated and reference sample. We discuss the effect of excitation laser power as well as of temperature on the Raman spectra. Our results suggest that the covalent functionalization is removed under certain conditions. In addition, we analyze the differences between mechanically exfoliated MoS_2 and MoS_2 powder used as starting material.

P044 **Tu 19:00 - 21:00**

Anomalous electrical transport properties of multilayer graphene with turbostratic stacking

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Multilayer graphene was synthesized by overlayer growth of graphene on a monolayer graphene template using a chemical vapor deposition method under a high process temperature of 1300°C. Structural analysis using Raman spectra revealed that the synthesized multilayer graphene forms highly crystalline graphene layers with a turbostratic stacking structure. Figure 1 shows the transfer characteristics and hole mobilities of the field effect transistors with the multilayer graphene channel. The carrier mobility of the multilayer graphene showed higher value than those of the monolayer graphene template. The improvement of the electrical transport properties is caused by the turbostratic stacking structure that has the electronic band dispersion similar to that of monolayer graphene. This result means that the synthesis of graphene layers grown on the graphene template is effective to improve the carrier transport properties in multilayer graphene sheets.

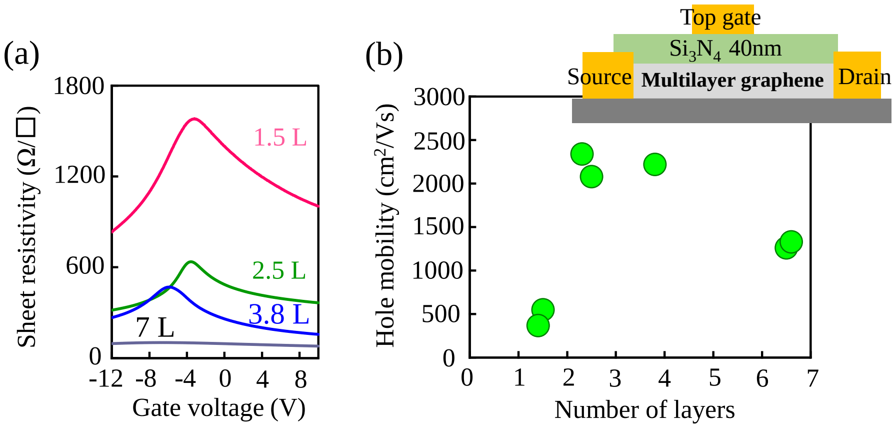

Fig. 1 (a) transfer characteristics and (b) hole mobilities of the field effect transistor with the multilayer graphene channel.

P046 **Tu 19:00 - 21:00**

Structural Characterization of Defects in Hexagonal Boron Nitride Using Scanning Probe Spectroscopy

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Lattice defects formed in 2D hexagonal boron nitride (hBN) have emerged as unique nanopores. Their most useful property is photoluminescence (PL) from the defects in the form of single-photon emission even at room temperature. Even though the defects exhibit PL at multiple wavelengths in a visible range, which vary from defect to defect, the statistic characterization and analysis have been limited attention. To systematically characterize individual defects of hBN, we develop scanning probe spectroscopy system combined with an atomic force microscope and a time-correlated single photon counting module. This system allows us to automatically measure thousands of PL spectra at each point, and correlate with PL lifetime, PL excitation, and thickness from individual defects. The statistical analysis of these collected data provides us insight into physical and chemical properties of nanoscale defects in hBN and potential for ultrasensitive sensing and quantum photonics.

P048 **Tu 19:00 - 21:00**

Intertube energy transfer in dilute SWNT-polymer matrices

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Energy transfer (ET) and exciton dynamics play a crucial role for the performance of nanotubes in devices and applications based on semiconducting single-wall carbon nanotubes (s-SWNTs). Here, We studied ET by transient two-color pump-probe spectroscopy of drop-cast, (6,5)-SWNT-polymer matrix films. We adjusted the average intertube distance from about 7 nm to about 50 nm by varying the polymer content in the films.
Wavelength-resolved transient absorption spectra were obtained for parallel and orthogonal pump-probe polarizations. These spectra were used to determine population dynamics at magic angle conditions (fig. 1a) as well as the anisotropy decay for a three-dimensional polarization model (fig. 1b).
The dynamics of population decay is seen to slow down with increasing polymer content, resulting from larger average distances between SWNTs in the sample.
The acceleration of exciton population decay in samples with lower polymer content can be explained by diffusive exciton transport to nanotube ends or to structural, as well as chemical, impurities on neighbouring nanotubes.

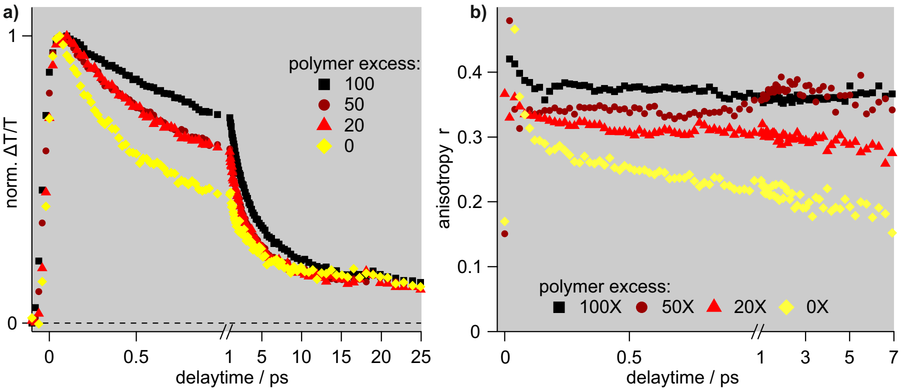

Fig 1: Results for transient absorption measurements of (6,5) s-SWNT polymer matrices: a) Population decay at magic angle configuration, b) Polarization anisotropy decay.

P050 **Tu 19:00 - 21:00**

Controlling Photon Antibunching from 1D Emitters using Optical Antennas

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Single-photon emission is a hallmark of atom-like 0D quantum emitters and a key technology for quantum information [1]. In higher dimensional nanostructures, multiple spatially separated electronic excitations may exist giving rise to more than one emitted photon at a time. Therefore, efficient localization of the excited state energy at local minima in the energy landscape is required for antibunching [2]. In numerical calculations we show that optical nanoantennas can be used to control the photon emission statistics of 1D nanostructures and to convert them into single-photon sources at room temperature. We performed photon correlation experiments on single (6,5) SWCNTs, wrapped in SDS/DOC [3] or DNA [4], with and without the presence of a sharp gold tip. Our results indicate that, in addition to improving the performance of single photon sources, optical antennas have the potential to open up a broad range of materials for quantum information technology.

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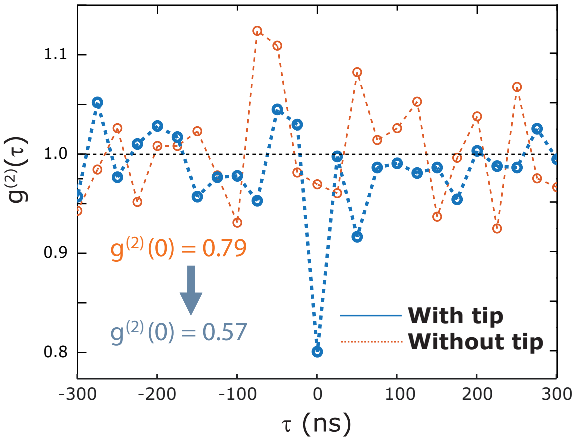

P052 **Tu 19:00 - 21:00**

2D Raman bands in chirality-defined individual double-walled carbon nanotubes

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Second-order Raman scattering processes, involving electron/hole scattering by two TO phonons with opposite momenta (so-called 2D band) has been explored in many different ways for both graphene and single-walled carbon nanotubes. These studies were critical to gain a comprehensive insight into the electronic and vibrational behaviors of such nanostructures, providing a rich knowledge of structural parameters (like number of layers in Bernal stacked few layers graphene) and environment impact as pressure or tension effects. In this work, we report the first systematic study of the 2D band in 17 individual, spatially isolated and suspended double-walled carbon nanotubes (DWCNTs). The atomic structure of DWCNTs was unambiguously identified by combination of Electron Diffraction, High-Resolution Transmission Electron Microscopy, Rayleigh and Raman spectroscopies. Raman spectra of the 2D band of DWCNTs were measured using more than 30 laser excitation lines from the IR to the visible range (1.46 - 2.71 eV). Our results provide new insights into the effects of inter-tube coupling on second-order Raman scattering processes at the single nanotube level and will allow for the correct interpretation of the 2D spectra in samples containing a distribution of different DWCNT species.

P054 **Tu 19:00 - 21:00**

Reabsorption effect observed in Raman spectra of single-chirality single-wall carbon nanotubes

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In the Raman spectra of single wall carbon nanotubes (SWCNTs), the radial breath mode (RBM) signal can be used to evaluate relative concentration of various (n,m) SWCNTs in mixture samples. However, reabsorption effect in Raman spectra of SWCNTs has not been clearly reported, which should seriously affect Raman spectral analysis. Here, we systematically analyzed the Raman intensity change by modifying SWCNT concentrations and the focal depth in the confocal micro-Raman measurement. A significant decrease in both RBM and G+ intensity of (8,3) and (10,3) solutions were observed with the focus deeply into the solutions. This decrease can be explained by the reabsorption of Raman scattering. In addition, both RBM and G+ intensities have a nonlinear variation with the SWCNT concentration when the focus was localized into the solutions. Interestingly, the rate of intensity variation was different for RBM and G+ band, which is originated from that the reabsorption influence is different between RBM and G+ band. This work was supported by the National Key R&D Program of China (Grant 2018YFA0208402), the National Natural Science Foundation of China (Grants 51472264, 11634014, 51820105002, 51872320, 51561022), and the Key Research Program of Frontier Sciences, CAS (Grant QYZDBSSW-SYS028).

P056 **Tu 19:00 - 21:00**

Detecting Energy Transfer among Highly Suspended Carbon Nanotubes in Aqueous Solution by Photoluminescence

Shilong Li[1,2], Dehua Dehua [1,2], Jiaming Cui[1], Xiaojun Wei[1,3], Weiya Zhou[1,2,3], Sishen Xie[1,2,3], Hiromichi Kataura[4], Huaping Liu[1,2,3]

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Exciton energy transfer (EET) often occurs among different single-wall carbon nanotubes (SWCNTs) when they are present in the form of bundles. However, it is unclear that whether EET occurs between different nanotubes highly suspended in aqueous solution.

Here, we employed photoluminescence (PL) spectra to probe the EET between different (n, m) SWCNTs highly dispersed in the aqueous surfactant solution. A significant decrease in PL intensity of (6, 5) SWCNTs was observed after mixing with (9, 4) SWCNTs. Through the detailed analysis on PL spectra change, the decreased PL intensity can be attributed to the attenuation of the incident and emission light, and the EET from the (6, 5) nanotubes to (9, 4) with larger diameters. In addition, the EET rate exponentially increased with an increase in SWCNT concentration. We supposed that the EET was probably originated from momentary contact of random nanotubes in surfactant solution, which results from the thermal motion and collision of SWCNTs.

This work was supported by the National Key R&D Program of China (Grant 2018YFA0208402), the National Natural Science Foundation of China (Grants 51472264, 11634014, 51820105002, 51872320, 51561022), and the Key Research Program of Frontier Sciences, CAS (Grant QYZDBSSW-SYS028).

P058 **Tu 19:00 - 21:00**

EXCITON-POLARITON RELAXATION IN SINGLE-WALLED CARBON NANOTUBE NETWORKS

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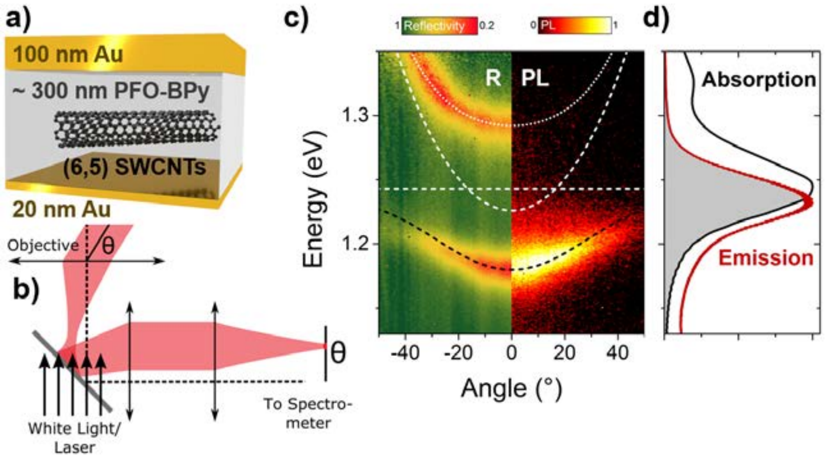
Exciton-polaritons are hybrid light-matter quasiparticles that form upon strong coupling of an excitonic transition and a photon mode, e.g. in a Fabry-Pérot cavity. They show intriguing properties such as small effective mass but also strong non-linearities that can lead to inversionless polariton lasing. Owing to their unique optical and electronic properties semiconducting single-walled carbon nanotubes (SWCNTs) have emerged as an excellent material to create optically and electrically pumped exciton-polaritons at room temperature (Nat. Mater. 2017, 16, 911). For their practical application and to possibly achieve polariton lasing, efficient relaxation is important. Here we investigate the impact of various parameters, such as nanotube density, detuning of the cavity and excitation wavelength, on the relaxation of polaritons in metal-clad microcavities with purified and polymer-wrapped (6,5) SWCNTs by angle-resolved reflectivity and photoluminescence spectroscopy. We find that intrinsic phonons, e.g. the D-mode (165 meV), seem to play an important role in the relaxation dynamics of SWCNT exciton-polaritons. We also find that high packing-densities of nanotubes enhance polariton relaxation compared to cavities with equal coupling but with well-separated SWCNTs in a matrix.



a) Gold-clad microcavity with (6,5) SWCNTs embedded in polymer matrix. b) Schematic of angle-dependent optical measurement. c) Characteristic polariton modes (reflectivity and photoluminescence). d) Absorption and emission of SWCNT reference.

P060 **Tu 19:00 - 21:00**

Emission enhancement of carbon nanotubes using nanobeam cavities

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We observe enhanced emission from air-suspended carbon nanotubes by coupling to air-mode photonic crystal nanobeam cavities. Using finite-difference time-domain simulations, cavities are designed to have large evanescent fields in air that enable efficient coupling to the nanotubes [1]. We fabricate devices from silicon-on-insulator wafers, and carbon nanotubes are grown over the cavities by chemical vapor deposition.

The devices are characterized by photoluminescence spectroscopy. We observe optical coupling when the nanotube emission is close to the cavity resonance [Fig. 1(a)]. Taking advantage of laser-heating-induced blueshifts of the nanotube emission, the detunings from the cavity peak can be reduced [2]. The cavity emission can be increased by bringing into resonance [Fig. 1(b)], and we find that the enhancement can be explained by a simple cavity quantum electrodynamical model using the spectral overlap between the nanotube and cavity peaks. We also perform time-resolved photoluminescence measurements and analyze the emission lifetime.

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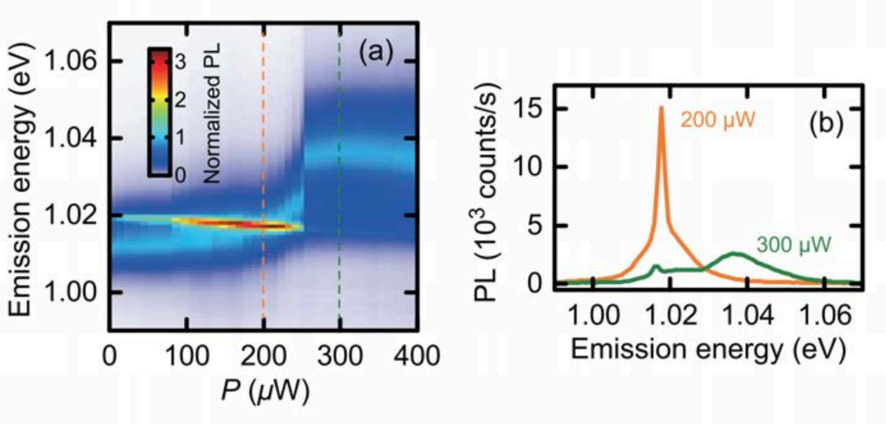

(a) Excitation power dependence of PL. PL is normalized with respect to the nanotube peak height. Dashed lines indicate the powers where spectra in (b) are taken. (b) Comparison of PL spectra at $P = 200$ μW (orange) and 300 μW (green).

P062 **Tu 19:00 - 21:00**

Thermal exciton radiation of single-walled carbon nanotubes

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The optical properties of single-walled carbon nanotubes (SWNTs) have attracted much attentions for a long time, because they arise from many-body quantum correlations. In contrast to photoluminescence phenomena, thermal radiation, which is one of the fundamental light emission process, remains unclear because of technical difficulties in heating nanotubes without disturbing intrinsic properties of SWNTs. Here, we report the fundamental thermal radiative properties of intrinsic semiconducting and metallic SWNTs suspended in a vacuum [1]. We employed continuous-wave laser irradiation for heating SWNTs, which provided non-contact local heating while retaining the neutral charge balance of the nanotubes throughout the measurements. At 1,000–2,000 K, an intrinsic semiconducting SWNT emitted linearly polarized, narrow-band near-infrared radiation, in contrast to its broadband metallic counterpart. We confirmed that the narrow-band radiation originated from radiative recombination of thermally generated excitons. The fundamental high-temperature photophysics of semiconducting SWNTs are dominated by robust quantum correlations even at 2,000 K. [1] T. Nishihara, A. Takakura, Y. Miyauchi, and K. Itami, Nat. Commun. 9, 3144 (2018).

P064 **Tu 19:00 - 21:00**

Identification of CNT species populations in TGA peaks

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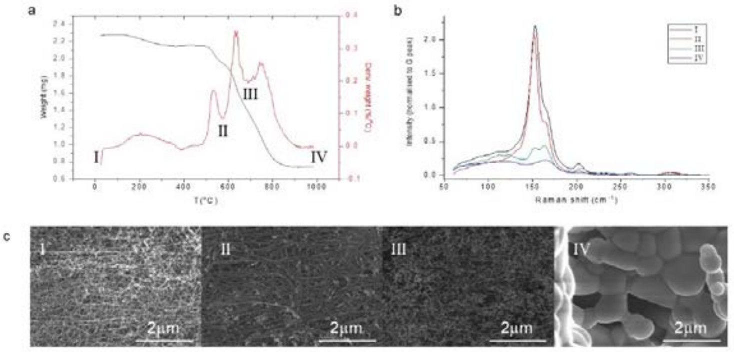
Direct spinning of CNT fibres by floating catalyst CVD is a multi-parameter process and generally produces fibres with varied compositions in terms of CNT type, residual catalyst, and amorphous carbon, depending on synthesis conditions. To close the loop between measured fibre properties and synthesis optimisation, the identification of a fibre's composition is crucial. In light of recent findings, we use thermogravimetric analysis (TGA), paired with Raman spectroscopy and SEM, to investigate the various nanotube populations produced in the process. The samples were burned in several stages, each time beyond one of the successive transitions. The changes associated with different TGA peaks were visualised by SEM and tracked by Raman, in particular by the radial breathing mode (RBM) and intensity and symmetry of the G peak, (indicative of CNT diameter and metallicity respectively). The common assumption is that, due to bond curvature, single wall nanotubes burn at lower temperatures, while populations at higher burn-temperatures are usually assumed to be multi-walled. However, here we suggest that the largest population of SWCNTs with an RBM at 152 cm^{-1} (population III) burns at surprisingly high temperatures.



(a) TGA weight loss showing the different populations as peaks in its derivative (b) corresponding RBM regions of the Raman spectra and (c) SEM images of the populations.

P066 **Tu 19:00 - 21:00**

Fermi-level dependence of THz high-harmonic generation in single-wall carbon nanotubes

Hiroyuki Nishidome[1], Kohei Nagai[2], Kento Uchida[1], Yota Ichinose[1], Kengo Fukuhara[1], Junji Nozaki[1], Junko Eda[1], Yohei Yomogida[3], Junichiro Kono[2,4], Koichiro Tanaka[1], Kazuhiro Yanagi

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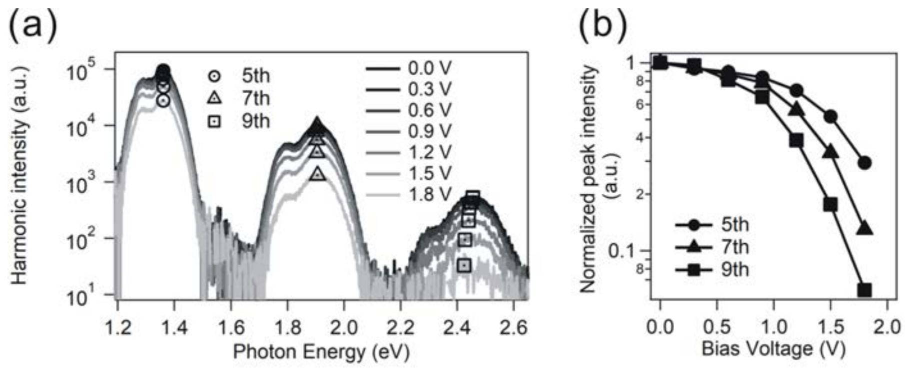
High-harmonic generation (HHG) is one of the unique phenomena in the extreme nonlinear optics, where the ground state becomes unstable due to strong light-matter interactions. In solid, there are two mechanisms in HHG, i.e. interband and intraband mechanisms, but their contributions to HHG are still elusive because various physical parameters, such as crystal structure, band structures, conduction electrons and so on, affect the HHG.

In this study, we investigated the relationship between HHG intensity and Fermi-level in single-wall carbon nanotubes by electrolyte gating method.

We prepared a high-purity (6,5) thin film, transferred it to a sapphire substrate, fabricated side-gating devices, and injected carrier by the shift of gate voltage through electric double layer formation using ionic liquid. The results are shown in Fig.(a). We observed decrease of HHG intensities as the shift of gate voltage. This suggests that the interband mechanism plays more dominant role for 5th, 7th and 9th HHG than the intraband mechanism. Moreover Fermi-level dependences of different order intensities normalized at 0 V are plotted in Fig.(b). This shows that higher-order harmonics decrease more rapidly. To understand the background, we calculated HHG spectra based on quantum Liouville equation.



(a) HHG spectra as a function of gate voltage (b) Fermi-level dependence of 5th, 7th and 9th order harmonic generation. Each intensity is normalized at 0 V

P068 **Tu 19:00 - 21:00**

Ultrafast non-linear 2D microspectroscopy reveals coherent phonon-mediated intra- and intervalley exciton interaction in an individual SWCNT

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Further developments in molecular electronics, adressing SWCNTs, would benefit strongly from insights in the spatio-temporal evolution of molecular processes. Ultrafast non-linear techniques provide tracking of energy transfer pathways e.g., mediated via electron-phonon coupling [1]. A comprehensive way to observe these dynamics is coherent 2D fluorescence microspectroscopy [2]. This method is a generalization of transient absorption spectroscopy with frequency-resolved pump and probe steps, combined with spatially-resolved optical microscopy. This provides, e.g., to observe the phonon-mediated formation and annihilation dynamics of initially bright and dark-state excitons due to the strong exciton-phonon coupling on the femtosecond timescale. Here, we utilize the third-order 2D signal for monitoring the trapped intra- and intervalley exciton interaction in a SWCNT [3,4]. To this end, an transform-limitted LCD-shaped four-pulse sequence is focused on an (6,4) SWCNT and the fluorescence is detected as a function of inter-pulse time delays and phases.

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P070 **Tu 19:00 - 21:00**

Photon correlation spectroscopy of alky defect states in carbon nanotubes

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Photoactive defect states in semiconducting single-walled carbon nanotubes (CNTs) have the potential to enable novel applications in quantum photonic technologies. While early experiments have established cryogenic CNTs as quantum light emitters [1], more recent work has identified luminescent defect states as sources of single photons up to room temperature [2,3]. For chemically-engineered CNTs, sp^3 functionalization offers means to deterministically influence the corresponding trap state properties via the characteristics of the covalent side chains. Recent findings show that the incorporation of sp^3 alkyl defects into the sp^2 lattice of narrow-diameter CNTs promotes the formation of both neutral and charged localized excitons [4] with remarkably high luminescent quantum yields. Here, we report the results of cryogenic photoluminescence correlation spectroscopy carried out on individual nanotubes functionalized with sp^3 side-wall chemistry.

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P072 **Tu 19:00 - 21:00**

Super-resolution imaging of air-suspended carbon nanotubes by extracting nonlinear excitonic processes

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When excitons in carbon nanotubes spontaneously recombine, emission occurs at diameter-dependent wavelengths including the near-infrared window, which allows for deep-tissue imaging [1]. As another decay pathway, excitons efficiently go through annihilation process upon collision with one another due to one-dimensional diffusion, which has a nontrivial influence on the fluorescence efficiency [2]. Focusing on this efficient annihilation process, we demonstrate super-resolution imaging of air-suspended nanotubes. Through the comparison of fluorescence signals in sublinear and linear regimes [Figs. 1(a) and (b)], we extract the efficiency of the annihilation process. Spatial images of the extracted annihilation efficiency [Fig. 1(c)] of the nanotubes have resolution beyond the diffraction limit, as shown in Fig. 1(d). We investigate excitation power dependence of the annihilation process by experiment and Monte Carlo simulation, and the resolution improvement of the annihilation images can be quantitatively explained by the superlinearity of the annihilation process.

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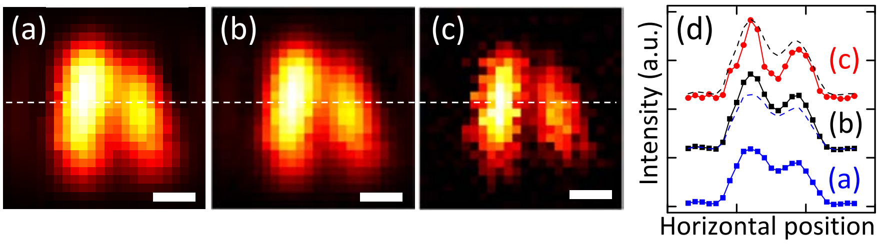

(a,b) Confocal fluorescence images measured with excitation powers of 0.8 and 0.1 μW, respectively. (c) Visualized annihilation efficiency extracted from (a) and (b). (d) Cross-section profiles of (a-c). Scale bars are 500 nm.

P074 **Tu 19:00 - 21:00**

Electroluminescence from aryl-functionalized monochiral carbon nanotubes with deep exciton traps

Adnan Riaz[1,2], Marco Gaulke[1,2], Felix Pyatkov[1,2], Avishek Saha[3], Simone Dhem[1,2], Han Htoon[3], Stephen Doorn[3], Ralph Krupke[1,2]

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Single walled carbon nanotubes are promising quantum emitters in the telecom wavelengths, and electrically-driven non-classical light emission has been demonstrated at low temperature [1,2]. Yet, for obtaining single-photon emission from nanotubes at room temperature, exciton localization is required at deep exciton traps as can be formed by low-level covalent functionalization chemistry. Here we report the first observation of electroluminescence from aryl-functionalized monochiral (6,5) nanotubes. Deep exitonic traps are created by functionalization with 3,5-Dichlorobenzene diazonium, which lead to defect (D) state emission at telecom wavelengths (figure 1a). The electrically-driven emission is highly stable and has been measured from cryogenic temperature to room temperature and Trion (T) emission of the defect states can be observed as well. At 4K we observe new peaks in the electroluminescence spectra which we assign to RBM phonon replica (PR) (figure 1b), in analogy to replicas from low-energy squashing modes reported in low temperature photoluminescence spectra [3].

[1] X. He et al., Nature Materials 17 (2018) 663.
[2] S. Khasminskaya et al., Nature Photonics 10 (2016) 727.
[3] J. Lefebvre et al., Physical Review B 70 (2004) 045419.

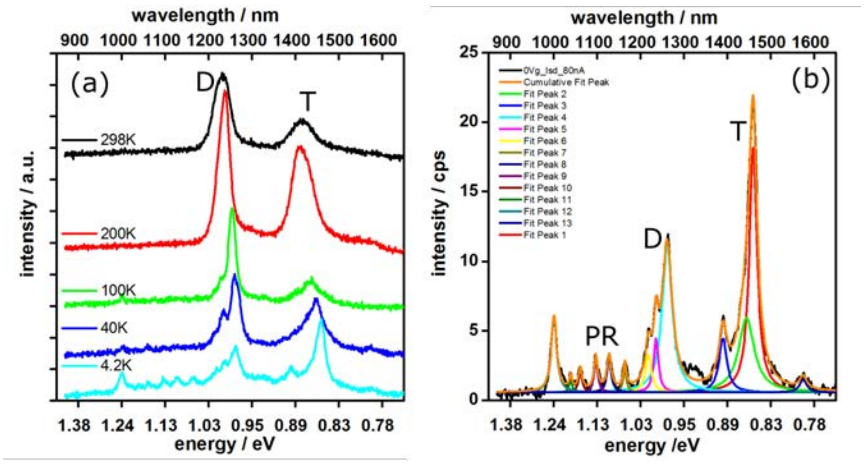

Figure 1: (a) Temperature dependent electroluminescence spectra from aryl functionalized (6,5) tubes showing defect states emission (D) and trion emission (T). (b) Spectrum at 4K showing phonon replica (PR), intrinsic E_{11}, defect and trion emission.

P076 **Tu 19:00 - 21:00**

Quantification of Atmospheric and Chemically Induced p-Doping in Carbon Nanotubes by Electron Paramagnetic Resonance

Andreas Sperlich[1], Michael Auth[1], Florian Oberndorfer[2], Klaus Eckstein[2], Bernd Sturdza[1], Vladimir Dyakonov[1], Tobias Hertel[2]

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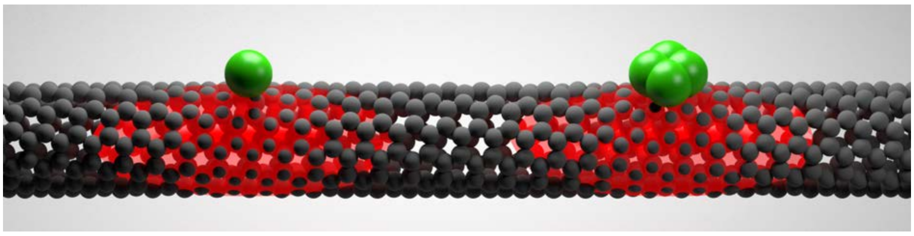
[2] *Institute of Physical and Theoretical Chemistry, Julius Maximilian University of Würzburg, 97074 Würzburg, Germany*

Control over doping of semiconducting single-wall carbon nanotubes (SWNTs) by (electro-) chemical methods is a challenge for future applications of SWNTs in carbon-based electronics and photonics. We investigate doping quantitatively by means of electron paramagnetic resonance (EPR) for the first time. We identify spin signals from atmospheric p-doping by the water-oxygen redox couple and SWNT defects. The concentration of these radical-like signals is on the order of only a few spins per (6,5)-SWNT. Upon addition of the doping agent $AuCl_3$ the EPR signal intensity increases linearly, which we ascribe to p-doping of the nanotube. We compare the spin with the charge density derived from the shift of the nanotubes' S1 absorption. At low doping levels both - spin and charge density - do actually coincide, suggesting all charge carriers are localized in Coulomb traps. However, at moderate doping levels, the EPR signal saturates and subsequently decreases for higher doping. We attribute this finding to the interaction between spins in neighboring sites that results in the formation of EPR silent diamagnetic biradicals. For excessive doping the EPR signal vanishes, indicating that the Fermi level is shifted into the valence band and carriers become delocalized.



6,5-SWNT with surface adsorbed dopants (green) that induce p-doping (red) in the carbon nanotube.

P078 **Tu 19:00 - 21:00**

Defects Enable Dark Exciton Photoluminescence with Increased Lifetimes

Trevor Tumiel[1], Amanda Amori[1], Zhentao Hou[1], Todd Krauss[1,2]

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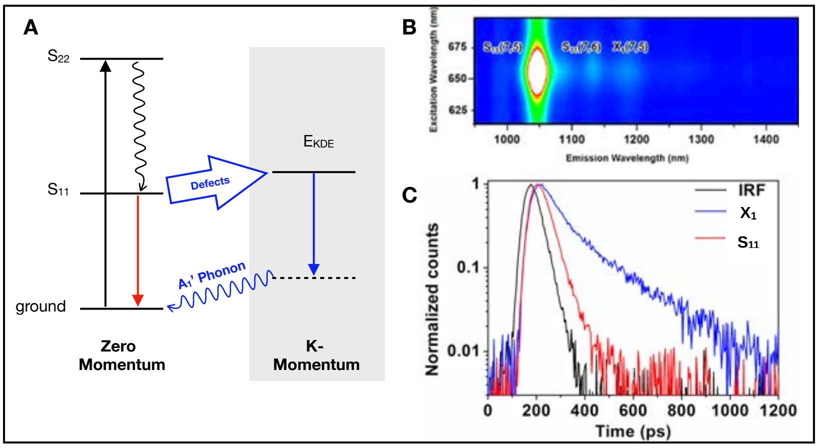
[2] *University of Rochester/The Institute of Optics, Rochester, NY, 14627, United States*

For three (n,m) species of single-walled carbon nanotubes (SWCNTs) we found that the K-momentum dark exciton (KDE) state exhibited a 5-fold decrease in intensity (relative to the bright S_{11} state) as samples were cooled to 77 K. Since the KDE state is optically forbidden, an open question is how the KDE state is populated and why it is so prominent in the photoluminescence spectrum. We will discuss data strongly suggesting that populating the KDE state involves elastic scattering of S_{11} excitons from defects. Time-correlated single photon counting measurements of multiple (n,m) species of SWCNTs also revealed that the photoluminescence decay of the KDE state has a significant component with a lifetime exhibiting nearly a 10-fold increase compared to S_{11} state lifetimes. The longer lifetime for the KDE state is consistent with a forbidden transition that requires optical phonon emission to mediate exciton recombination. Engineering defects to promote a longer-lived KDE state can be utilized to circumvent fundamental obstacles in developing efficient nanotube-based photochemical processes.



(A) Basic scheme for defect scattering to the KDE state. (B) Photoluminescence excitation (PLE) map displaying PL from the S_{11} state and KDE (X_1) state. (C) Representative PL decay curves from S_{11} (red), KDE (blue), and instrument response (black).

P080 **Tu 19:00 - 21:00**

Environmental effects probed by cryogenic photoluminescence of individual carbon nanotubes

Shen Zhao[1], Manuel Nutz[1], Jonathan Noé[1], Ming Zheng[2], Jeffrey Fagan[2], Alexander Högele[1]

[1] *Ludwig-Maximilians-Universität München, München, Germany*
[2] *National Institute of Standards and Technology, Gaithersburg, Maryland, United States*

The photoluminescence of semiconducting single-walled carbon nanotubes (SWNTs) is sensitive to both the exterior and interior environmental factors. Room-temperature studies have established surfactant-related changes in the photoluminescence energy [1] as well as pronounced differences between empty SWNTs and nanotubes filled with alkane [2] or water [3,4] molecules. For the latter, the nanotube photoluminescence allows monitoring quasi-phase transitions of the interior water filling upon cool-down to cryogenic temperatures [5]. Here, we present extensive studies of (9,1)-purified SWNTs with different surfactants and interior fillings at the temperature of liquid helium. With cryogenic photoluminescence carried out at the level of individual nanotubes, we reveal various effects of both environmental factors on the nanotube photoluminescence properties such as changes in emission energy, line shape or line multiplicity.

[1] J. Lefebvre er al., Appl. Phys. A 78, 1107 (2004).
[2] J. Campo et al., Nanoscale Horiz. 1, 317 (2016).
[3] W. Wenseleers et al., Adv. Mater. 19, 2274 (2007).
[4] J. A. Fagan, ACS Nano 5, 3943 (2011).
[5] X. Ma et al., Phys. Rev. Lett. 118, 027402 (2017).

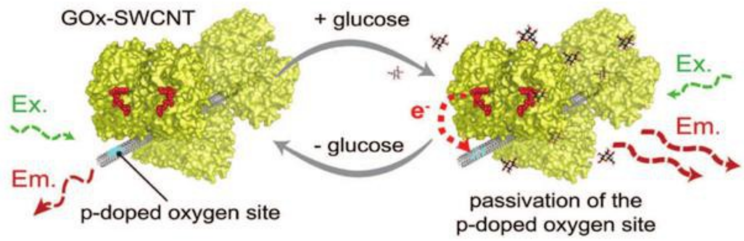
P082 **Tu 19:00 - 21:00**

Mediatorless, Reversible Optical Nanosensor Enabled through Enzymatic Pocket Doping

Alessandra Antonucci[1], Vitalijs Zubkovs[1], Nils Schuergers[1], Benjamin Lambert[1], Esra Ahunbay[1], Ardemis Boghossian

[1]*École Polytechnique Fédérale de Lausanne (EPFL), Lausanne, CH-1015, Switzerland*

The existing single-walled carbon nanotube (SWCNT) optical sensors that rely on charge transfer for signal transduction often require exogenous mediators that compromise the stability and biocompatibility of the sensors. This study presents a reversible, mediatorless, near-infrared glucose sensor based on glucose oxidase-wrapped SWCNTs (GOx-SWCNTs). GOx-SWCNTs undergo a selective fluorescence increase in the presence of aldohexoses, with the strongest response toward glucose. When incorporated into a custom-built membrane device, the sensor demonstrates a monotonic increase in initial response rates with increasing glucose concentrations between 3×10^{-3} and $30\text{x}10^{-3}$M and an apparent Michaelis–Menten constant of $\text{K}_{M}(app)\approx$ $13.9\text{x}10^{-3}$ M. A combination of fluorescence, absorption, and Raman spectroscopy measurements suggests a fluorescence enhancement mechanism based on localized enzymatic doping of SWCNT defect sites that does not rely on added mediators. Removal of glucose reverses the doping effects, resulting in full recovery of the fluorescence intensity. The cyclic addition and removal of glucose is shown to successively enhance and recover fluorescence, demonstrating reversibility that serves as a prerequisite for continuous glucose monitoring.



P084 **Tu 19:00 - 21:00**

Chirality-Sorted Single-Walled Carbon Nanotubes for Multidrug/Gene Delivery and Imaging.

Anton Naumov[1], Md. Tanvir Hasan[1], Elizabeth Campbell[1], Giridhar Akkaraju[1]

Single-Wall Carbon Nanotubes (SWCNT) have been previously utilized for a single drug delivery/imaging, however their chirality-dependent band gap provides a promise of multiwavelength imaging in near-infrared allowing multi-drug tracking. Such combination therapy targeting several factors at once is needed for complex conditions like nonalcoholic steatohepatitis (NASH) involving both fibrosis and inflammation. We utilize (6,5) and (7,5) SWCNTs chirality-sorted by aqueous two-phase extraction for the delivery and drug-specific in-vitro imaging of drug and gene therapeutics targeting inflammation and fibrosis respectively. These active agents, each bound non-covalently to SWCNTs of a specific chirality purified from the sorting surfactants are delivered to HepG2 cells and imaged via hyperspectral microscopy imaging at resonant transitions of (6,5) and (7,5) SWCNTs. This allows to deliver and track each therapeutic separately. The therapeutic efficacy of each formulation is further demonstrated by dose-dependent cytoxocity of SWCNT-bound PX-866 in HepG2 cancer cells and the > 90% knockdown of CCR5 expression with SWCNT/siRNA transfection. This study verifies the feasibility of utilizing chirality-sorted SWCNTs for the delivery and component-specific imaging of combination therapies.

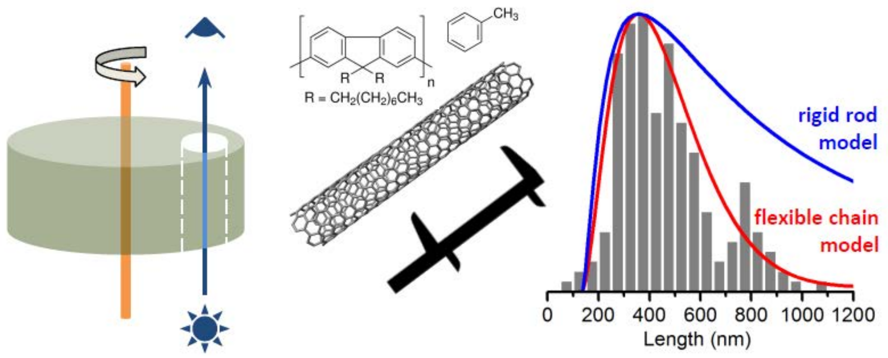
P086 **Tu 19:00 - 21:00**

Quantification of the Number of Adsorbed DNA Molecules on Single-Walled Carbon Nanotubes

Robert Nißler[1], Florian A. Mann[1], Parth Chaturvedi[2], Jan Horlebein[1], Daniel Meyer[1], Lela Vukovic[2], Sebastian Kruss[1,3]

[1] *Institute of Physical Chemistry, Göttingen University, Germany*
[2] *Department of Chemistry and Biochemistry, University of Texas at El Paso, El Paso*
[3] *Center for Nanoscale Microscopy and Molecular Physiology of the Brain, Göttingen, Germany*

Single-walled carbon nanotubes (SWCNTs) have unique photophysical properties and promise many novel applications. Noncovalent functionalization with single-stranded DNA (ssDNA) is one of the most used approaches and variation of ssDNA sequences lead to major advances in separation of SWCNT chiralities and SWCNT-based sensors. However, the exact number of adsorbed ssDNA molecules on ssDNA/SWCNT complexes are not precisely known. Here, we determine the number of adsorbed ssDNA molecules per SWCNT for different ssDNA sequences. For this purpose, we directly quantified free and adsorbed ssDNA and the concentration of SWCNTs using an approach based on filtration, absorption spectroscopy, and atomic force microscopy. The number of adsorbed ssDNA molecules on 600 nm long (6,5)-SWCNTs varied between $\approx$860 for (GT)5 and $\approx$130 for (A)30. The sequence (GT)$_{15}$ occupied an average SWCNT segment of $\approx$2.3 nm, while the SWCNT segment length of (GT)$_x$ repeats increased linear with sequence length x. Molecular dynamics simulations with experimentally determined values as parameters showed that (GT)$_{15}$ ssDNA stacked on top of each other on the SWCNTs in contrast to simulations with an excess SWCNT surface. This result highlights the importance of knowing the number of adsorbed ssDNA molecules per SWCNT.



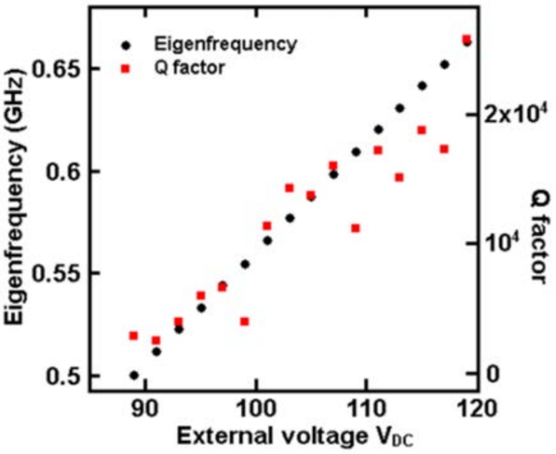
P088 **Tu 19:00 - 21:00**

Nanoscale imaging of the extracellular space near synapses in live brain tissue by single carbon nanotube tracking

Chiara Paviolo[1], Joana S. Ferreira[2], Antony Lee[1], Laurent Groc[2], Laurent Cognet[1]

[1]*Université de Bordeaux, Institut d'Optique & Centre National de la Recherche Scientifique, UMR 5298, 33400 Talence, France*
[2]*Université de Bordeaux, Interdisciplinary Institute for Neuroscience, UMR 5297, 33076 Bordeaux, France*

Molecular mobility through the brain extracellular space (ECS) is essential to many physiological events, such as signal transmission or ion homeostasis. Hence, understanding local ECS diffusive environment and morphology represents a key step to understand chemical-based neural communication and synaptic connectivity. We have recently used single-walled carbon nanotubes (SWCNTs) to characterize the local ECS nanoscale organization and diffusivity in young and adult rodent brain by near infrared (NIR) microscopy. Here, we extend this work further by showing local morphology and dynamics of the ECS around synapses. To correctly identify presynaptic regions, a structured illumination technique (named HiLo microscopy) was implemented in parallel to NIR imaging. This technique relies on the acquisition of one structured and one uniform image to obtain pictures with good optical sectioning. Single-molecule tracking of individual SWNCTs at different distances from the synaptic centre (from 300 to 1200 nm) provided nanoscale maps of the ECS and quantitative information on the local diffusivity. After treatment of the tissues with tetrodotoxin or bicuculline, SWCNT tracking revealed a local modification of the synaptic diffusive environment compared to basal conditions.



Spatial map of the instantaneous relative diffusivity coefficient obtained from an individual SWCNT freely diffusing in the ECS of a rat organotypic slice. Scale bar = 2 µm.

P090 **Tu 19:00 - 21:00**

Bio-sensing at the edge of graphene and h-BN

Ralph Scheicher[1]

[1] *Division of Materials Theory, Uppsala University, SE-751 20 Uppsala, Sweden*

Designing the next generation of solid-state biosensors requires developing detectors which can operate with high precision at the single-molecule level. Nano-scaled architectures created in two-dimensional hybrid materials offer unprecedented advantages in this regard. We have theoretically explored a novel system consisting of a nanopore formed within a hybrid sheet composed of a graphene nanoroad embedded in a sheet of hexagonal boron nitride (h-BN). The sensitive element of this setup is comprised of an electrically conducting carbon chain forming one edge of the nanopore. This design allows detection of DNA nucleotides translocating through the nanopore based on the current modulation signatures induced in the carbon chain. Our findings show that the current localized in the carbon chain running between the nanopore and h-BN is characteristically modulated by the unique dipole moment of each molecule upon insertion into the pore, demonstrating that dipole-induced conduction modulation is a promising approach to detect and distinguish biomolecules, not necessarily limited to applications for DNA sequencing.

References:

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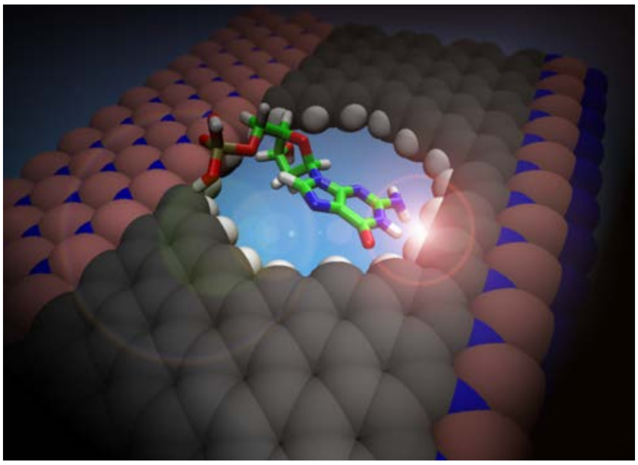


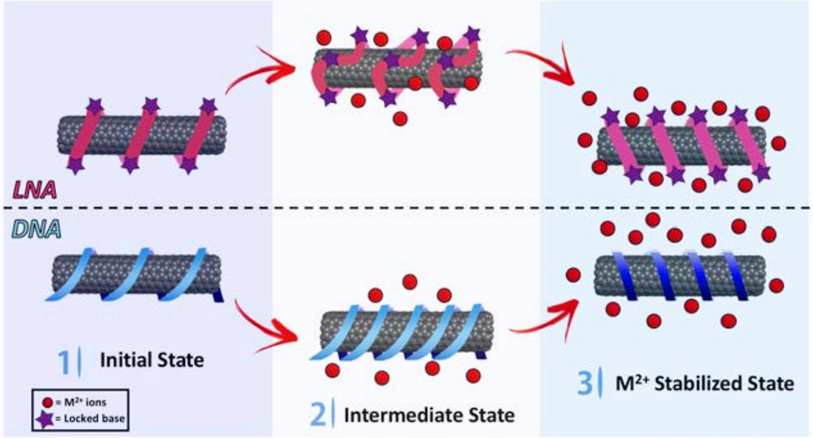
P092 **Tu 19:00 - 21:00**

Xeno Nucleic Acid Nanosensors for Enhanced Stability

Shang-Jung Wu[1], Alice Judith Gillen[1], Justyna Kupis-Rozmysłowicz[1], Carlo Gigli[2,3], Nils Schuergers[1], Ardemis Boghossian[1]

[1]*École Polytechnique Fédérale de Lausanne (EPFL), Lausanne, CH-1015, Switzerland*
[2]*Politecnico di Torino, Turin 10129, Italy*
[3]*Université Denis Diderot (Paris VII), Paris 75013, France*

The omnipresence of salts in biofluids creates a pervasive challenge in designing sensors suitable for in vivo applications. Fluctuations in ion concentrations have been shown to affect the sensitivity and selectivity of optical sensors based on single-walled carbon nanotubes wrapped with single-stranded DNA (ssDNA-SWCNTs). We herein observe fluorescence wavelength shifting for ssDNA-SWCNT-based optical sensors in the presence of divalent cations at concentrations above 3.5 mM. In contrast, no shifting was observed for concentrations up to 350 mM for sensors bioengineered with increased rigidity using xeno nucleic acids (XNAs). Transient fluorescence measurements reveal distinct optical transitions for ssDNA- and XNA-based wrappings during ion-induced conformation changes, with XNA-based sensors showing increased permanence in conformational and signal stability. This demonstration introduces synthetic biology as a complementary means for enhancing nanotube optoelectronic behaviour, unlocking previously unexplored possibilities for developing nano-bioengineered sensors with augmented capabilities.



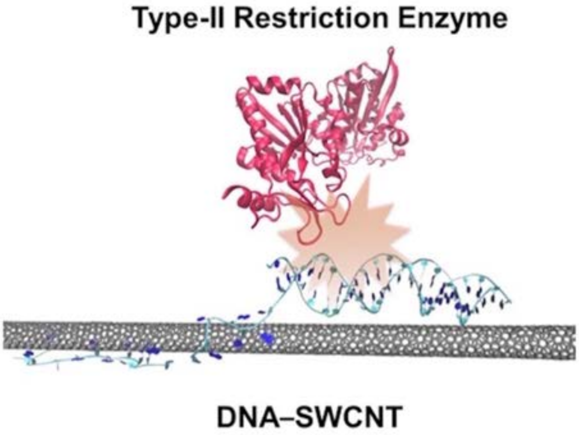
P094 **Tu 19:00 - 21:00**

Characterization of Double-Stranded DNA on Single-Walled Carbon Nanotubes (SWCNTs)

Shang-Jung Wu[1], Nils Schuergers[1], Kun-Han Lin[1], Alice Judith Gillen[1], Clémence Corminboeuf[1], Ardemis Boghossian[1]

[1]*École Polytechnique Fédérale de Lausanne (EPFL), Lausanne, CH-1015, Switzerland*

DNA has been extensively studied due to its versatility as a dispersant of SWCNTs. Its specificity and binding affinity to various analytes has exhibited a strong sequence dependence. As a result, through modifications of the nucleotide sequence, the DNA conformation on the SWCNT surface can be tailored to suit specific needs for techniques such as single-molecule detection, in vivo imaging, and chirality separation. To date, most research has focused on the interaction between single-stranded DNA and SWCNT surface, with less focus on the nature of the interaction of double-stranded DNA (dsDNA) and SWCNTs. As a result, the exact interaction mechanism governing this type of complex remains strongly debated and largely unknown. In this study, we employ various biochemical methods to infer the conformation of dsDNA on the surface of SWCNTs. Our methods are based on imaging techniques for identifying DNA-modifying enzyme activity in the presence of dsDNA-SWCNT complexes. Our findings suggest that dsDNA can partially retain its native conformation on the SWCNT surface, and the degree of dsDNA accessibility is strongly sequence dependent. These findings offer new possibilities for SWCNT sensing applications that employ dsDNA, such as the optical detection of DNA-protein interactions.



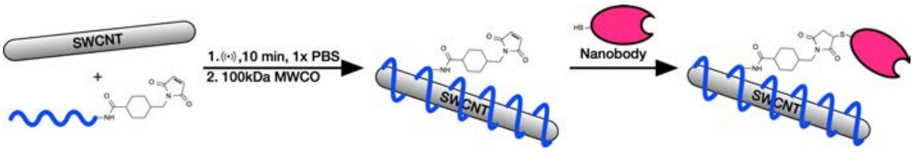
P096 **Tu 19:00 - 21:00**

Nano^2 - Nanotube-nanobody conjugates for near-infrared immunolabeling in vitro and in vivo

Florian A. Mann[1], Zhiyi Lv[2], Niklas Herrmann[1], Jörg Großhans[2], Felipe Opazo[3], Sebastian Kruss[1]

[1]*Institute for Physical Chemistry, Göttingen University, 37077, Germany*
[2]*Institute for Developmental Biochemistry, Göttingen University, 37077, Germany*
[3]*Center for Biostructural Imaging of Neurodegeneration, Göttingen, 37075, Germany*

Single-walled carbon nanotubes (SWCNT) are a highly interesting material for biomedical applications as their non-bleaching fluorescence in the near-infrared window leads to enhanced tissue penetration.
Here, we present a strategy that combines these outstanding properties of SWCNTs with the highly specific molecular recognition of nanobodies. Nanobodies are the smallest recombinant antibody fragments that are still functional and are only about 20% of the size of an original antibody. In this work, we make use of a hybrid functionalization strategy for the oriented attachment of green fluorescent protein (GFP)-binding nanobodies to the nanotube's surrounding organic phase. The use of GFP-targeting nanobodies opens up a large space of possible applications as there are thousands of GFP-modified model organisms available. First, we characterize the nanobody/SWCNT conjugates and show that they are functional and bind GFP. Furthermore, we label single GFP-tagged kinesin motors in living drosophila embryos and track their directional movement during embryogenesis.
In summary, we show that nanobody conjugated SWCNTs show great potential for targeted nIR imaging and labeling.



Program Wednesday

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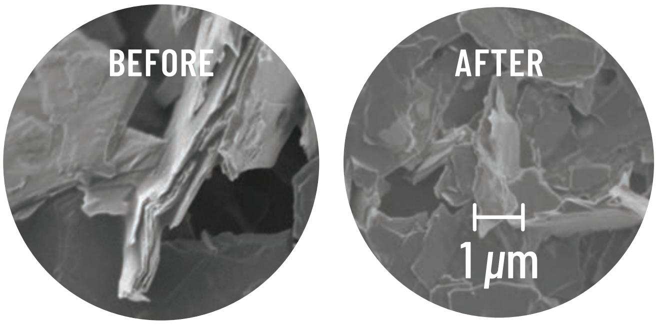

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Plenary program Franconia Hall

Session PI5 Chair: Janina Maultzsch

08:30 - 09:15	K3	**Tony F. Heinz** (Stanford University) *Probing and Controlling Excitons in 2D Semiconductors*
09:15 - 09:40	I10	**Young Hee Lee** (Sungkyunkwan University) *Towards in-Situ Single-Crystal Growth for Van Der Waals Heterostructure Thin Film*
09:40 - 10:05	C4	**Shigeo Maruyama** (University of Tokyo) *Application of One-Dimensional Van Der Waals Heterostructures Coaxially Wrapped Around Single-Walled Carbon Nanotubes*

Coffee break CCW Lobby

Session PI6 Chair: Michael S. Arnold

10:35 - 11:00	I11	**Richard Martel** (Université de Montréal) *Interfacial Phenomena and Second Order Resonances in Nanocarbons and Exfoliated Black-Phosphorus*
11:00 - 11:25	C5	**Michael Engel** (IBM) *Graphene-Enabled, Directed Nanomaterial Placement From Solution for Large-Scale Device Integration*
11:25 - 11:50	C6	**Kimmo Mustonen** (University of Vienna) *Atomic Scale Imaging and Covalent Modification of a Graphene-Carbon Nanotube Heterostructures*
11:50 - 12:15	C7	**Ado Jorio** (UFMG) *Micro Versus Nano-Raman Spectroscopy in Two-Dimensional Systems*

Lunch break

Electronics Symposium (CNTFA19) Panorama 11

Chair: Esko I. Kauppinen

14:00 - 14:20	SEI13	**Mark Hersam** (Northwestern University) *Self-Aligned Short-Channel Van Der Waals Heterojunction Devices*
14:20 - 14:40	SEI14	**Youfan Hu** (Peking University) *Wafer-Scale Fabrication of Ultrathin Flexible Electronic Based on Carbon Nanotubes With High Performance*
14:40 - 15:00	SEI15	**Lijun Liu** (Peking University) *Carbon Nanotube Complementary Gigahertz Integrated Circuits and Their Applications on Wireless Sensor Interface Systems*
15:00 - 15:20	SEI16	**Er-Xiong Ding** (Aalto University) *Scalable Production of Semiconducting SWCNTs by Floating Catalyst Chemical Vapor Deposition for Ultrahigh-Performance Electronics*

15:45 meet for guided tours

Energy Symposium (NMES19) Franconia Hall

Chair: Suguru Noda

14:00 - 14:20	SEn13	**Robin Nicholas** (Oxford University) *Solubilization of Single and Multi-Walled CNT With Ethylene-Vinyl Acetate for Conductive Films and Charge Extraction in Perovskite Solar Cells*
14:20 - 14:40	SEn16	**Volodymyr Koman** (MIT) *Ultra-High Thermal Effusivity Materials Based on Graphene for Resonant, Ambient Thermal Energy Harvesting*
14:40 - 15:00	SEn15	**Bingqing Wei** (University of Delaware) *Tailoring Carbon Nanostructures for Energy Storage Applications*
15:00 - 15:20	SEn14	**Il Jeon** (University of Tokyo) *Carbon Nanotubes to Outperform Metal in Perovskite Solar Cells via Dopant Engineering and Hole-Selectivity Control*

15:45 meet for guided tours

Chair: Annick Loiseau

14:00 - 14:20	S2D14	**Bruno Dlubak** (Unité Mixte de Physique CNRS-Thales) *Introducing 2D Materials for Magnetic Tunnel Junctions*
14:20 - 14:40	S2D15	**Lara Kühl Teles** (Instituto Tecnologico de Aeronautica) *Towards the Survival of Quantum Spin Hall Phase of Group-IV Overlayers on Substrates*
14:40 - 15:00	S2D16	**Ilka Kriegel** (Italian Institute of Technology) *Light Driven Capacitive Charging of 0D-2D Hybrids*
15:00 - 15:20	S2D17	**Patrick Zeller** (Elettra - Sincrotrone Trieste) *Chemical Analysis of Suspended Graphene by Spatially Resolved X-Ray Photo-Electron Spectroscopy*

15:45 meet for guided tours

Spectroscopy Symposium (NSAP19) Panorama 12

Chair: Stephen Doorn

14:00 - 14:20	SSp2	**Annick Loiseau** (LEM, CNRS-ONERA) *Comparing Resonant Raman Spectroscopy and Atomic Resolution Transmission Electron Microscopy for SWCNT Sample Characterization*
14:20 - 14:40	SSp3	**Adnan Riaz** (KIT) *Electroluminescence Excitation Mapping of Excitons and Trions in Monochiral Carbon Nanotube Devices*
14:40 - 15:00	SSp4	**Georgy Gordeev** (Freie Universität Berlin) *Electronic Coupling Between the Walls of Double-Walled Carbon Nanotubes*
15:00 - 15:20	SSp5	**Leandro Malard** (Universidade Federal de Minas Gerais) *Nonlinear Optical Spectroscopy and Imaging in 2D Materials*

15:45 meet for guided tours

NanoBio Symposium (CNBMT19) Panorama 10

Chair: Ming Zheng

14:00 - 14:20	SNB2	**Charlotte Allard** (Ecole Polytechnique de Montreal) *Encapsulated Dyes in Nanotubes: a Biological Perspective*
14:20 - 14:40	SNB3	**Sebastian Kruss** (Georg-August-Universität Göttingen) *Targeted Near Infrared Sensing and Imaging With Carbon Nanotubes*
14:40 - 15:00	SNB4	**YuHuang Wang** (University of Maryland) *Electrical Sensing With a Tube-in-a-Tube Semiconductor*
15:00 - 15:20	SNB5	**Alessandra Antonucci** (Ecole Polytecnique Federale de Lausanne) *Real-Time Near-Infrared Confocal Imaging of Bacterial Cell Division in the Presence of Single-Walled Carbon Nanotubes*

15:45 meet for guided tours

Abstracts Wednesday (Oral)

Franconia Hall **We 08:30 - 09:15**

Probing and controlling excitons in 2D semiconductors

Tony F. Heinz[1]

[1] *Dept. of Applied Physics, Stanford University, Stanford, CA 94305, USA and SLAC National Accelerator Laboratory, Menlo Park, CA 94025, USA*

In 2D semiconductors, the reduced dimensionality and reduced dielectric screening causes many-body interactions to play a central role in the materials' electronic and optical properties. As a consequence, excitons dominate the optical excitations, just as in semiconducting carbon nanotubes. Here, we discuss advances in understanding the excitonic properties of 2D semiconductors consisting of monolayers of and heterostructures formed from transition metal dichalcogenide (TMDC) within the MX_2 (M = Mo, W; X = S, Se, Te) family.

By preparing semiconductor monolayers encapsulated in h-BN, we have gained a comprehensive picture of the various excitonic states supported in these materials. In addition to 2-body neutral exciton states, we can produce 3-body charged excitons (trions), 4-body biexcitons, and 5-body charged biexcitons. We observe moreover strong sensitivity to the surrounding dielectric media. This can be used to alter deliberately the electrical and optical gaps of the 2D semiconductor through Coulomb engineering.

Stacking two monolayers with distinct band-gaps gives rise to the possibility of charge separation and the formation of interlayer excitons after optical excitation. We describe the nature of these interlayer states and their strong tunability through the Stark effect in an electrostatically gated structure. In addition to providing fundamental understanding of these interlayer excitons, our results demonstrate the availability of broadly tunable light sources based on 2D semiconductor heterostructures.

Plenary Venue I10 (invited)

Franconia Hall **We 09:15 - 09:40**

Towards in-situ single-crystal growth for van der Waals heterostructure thin film

Young Hee Lee[1]

[1]IBS CINAP, Sungkyunkwan University

Recent development of van der Waals layered materials such as graphene, hexagonal BN, and transition metal dichalcogenides have drawn much attention due to their fascinating uniquely defined physical and chemical properties. What is missing is the synthesis of singlecrystallinity and wafer-scale scalability in van der Waals layered materials and more importantly, heterostructures. In this talk, we will introduce several examples of synthesizing the graphene in monolayer and multilayers and furthermore heterostructures of other van der Waals layered materials.

Plenary Venue C4 (contributed)

Franconia Hall **We 09:40 - 10:05**

Application of one-dimensional van der Waals heterostructures coaxially wrapped around single-walled carbon nanotubes

Shigeo Maruyama[1,2], Rong Xiang[1], Taiki Inoue[1], Yongjia Zheng[1], Ming Liu[1], Yuta Sato[3], Akihito Kumamoto[4], Yan Li[5], Shohei Chiashi[1], Esko Kauppinen[6], Kazu Suenaga[3], Yuichi Ikuhara[4]

[1] *Department of Mechanical Engineering, The University of Tokyo, Tokyo 113-8656, Japan*
[2] *Energy NanoEngineering, AIST, Tsukuba 305-8564, Japan*
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[4] *Institute of Engineering Innovation, The University of Tokyo, Tokyo 113-8656, Japan*
[5] *College of Chemistry and Molecular Engineering, Peking University, Beijing 100871, China*
[6] *Department of Applied Physics, Aalto University School of Science, FI-00076 Aalto, Finland*

We have synthesized a new coaxial nanotube structure, in which mono- or few-layer hexagonal boron nitride nanotube (BNNT) seamlessly wrap around a single-walled carbon nanotube (SWCNT), and result in an atomically smooth coaxial tube consisting of two different materials, as shown in Fig. 1(a) [1]. TEM-EELS clearly demonstrated the BNNT-SWCNT coaxial structure. We have tried various morphologies of SWCNTs as starting material, e.g. vertically aligned array, horizontally aligned array, suspended SWCNTs, and dry-deposited random network films. We can clearly observe the coaxial structure from originally isolated SWCNTs. We found no correlation between chiral angle of inner SWCNT and outer BNNT for 'double-walled' SWCNT-BNNT shown in Fig. 1(b). We concluded that these are one-dimensional van der Waals heterostructure. We have further developed the 1D coating CVD for transition metal dichalcogenide nanotubes, such as MoS_2 nanotube as shown in Fig. 1 (c). We can grow MoS_2 nanotubes around relatively large diameter SWCNT or SWCNT@BNNT. We will discuss properties and applications of the 1D heterostructures though optical absorption, Raman scattering, photoluminescence, FT-IR, and photo-voltaic effect.

Reference: [1] Rong Xiang et al., arXiv:1807.06154 (2018).

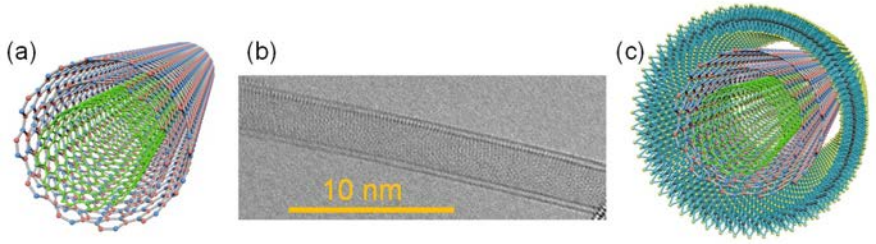


Figure 1 (a) Schematics of SWCNT@BNNT, (b) High resolution TEM image of SWCNT@BNNT, (c) Schematics of SWCNT@BNNT@MoS_2NT

Figure 1 (a) Schematics of SWCNT@BNNT, (b) High resolution TEM image of SWCNT@BNNT, (c) Schematics of SWCNT@BNNT@MoS_2NT

Plenary Venue I11 (invited)

Franconia Hall **We 10:35 - 11:00**

Interfacial phenomena and second order resonances in nanocarbons and exfoliated black-phosphorus

Richard Martel[1]

[1] *Département de chimie, Université de Montréal, Montréal, Canada, Email: r.martel@umontreal.ca*

Carbon nanotubes, graphene and exfoliated black-phosphorus (bP) exhibit optical properties that can be tuned through chemical and physical processes taking place at their surfaces. About 20 years of studies on such interfacial phenomena in my group with nanocarbons on oxide surfaces can be summarized with simple redox phenomena related to water/oxygen reaction pathways in ambient conditions giving unintentional doping, Fermi level pinning and irreversible device degradations. A better understanding of this interfacial chemistry helped us, however, identifying surprising second order resonances in the optical responses of nanocarbons [1] and more recently in bP materials. [2] Here, we will focus the discussion on the mid-infrared spectra of nanocarbon materials, where intriguing optical signatures are identified after chemical (covalent) grafts. The observed dependence on defect density, doping and wavelength provides clear assignments to second order resonances involving the scattering of photons by localized defects and high momentum phonons. Negative amplitudes assigned to optically forbidden phonons are key elements considered in a mechanism involving Fano anti-resonance. [1] These features appear general and can be used as tools to gain a quantitative assessment of defect density. Through the application of covalent bonding and patterning, it appears now possible to gain specific assignments to every features in the mid-IR spectra and to explore new ways to amplify optical signals at the nanometer scale.

Work in collaboration with F. Lapointe, B. Rousseau, V. Aymong, P. Gagnon, E. Gaufrès, P. Desjardins and M. Côté.

[1] J. Phys. Chem. C 121, 9053–9062 (2017); Phys. Rev. Lett. 109, 097402 (2012)
[2] Nano Letters, 18 (2), 1018-1027 (2018); Nature Materials, 14, 826-832 (2015)

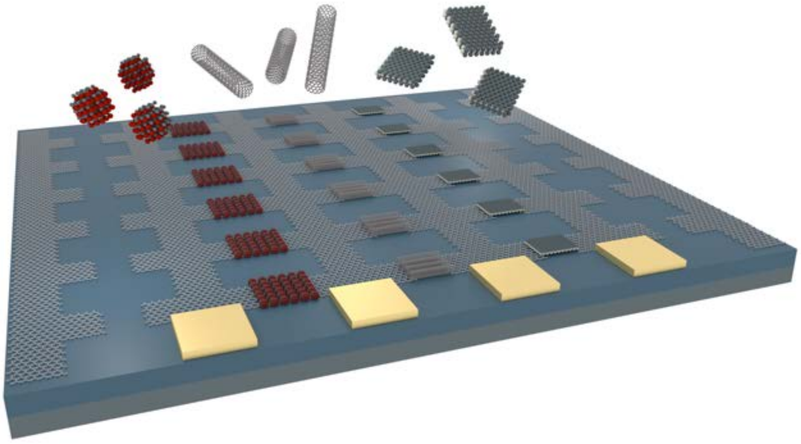
Franconia Hall **We 11:00 - 11:25**

Graphene-enabled, directed nanomaterial placement from solution for large-scale device integration

Michael Engel[1], Damon Farmer[2], Jaione Tirapu Azpiroz[1], Jung-Woo T. Seo[3], Joohoon Kang[3], Phaedon Avouris[2], Mark C. Hersam[3], Ralph Krupke[4], Mathias Steiner[1]

[1]*IBM Research, Rio de Janeiro, RJ 22290-240, Brazil*
[2]*IBM Research, Yorktown Heights, NY 10598, USA*
[3]*Northwestern University, Evanston, IL 60208, USA*
[4]*Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany*

Placing of nanomaterials at predefined locations with nanoscale precision is still one of the unsolved problems that inhibit their large-scale integration in the domain of semiconductor industry. The application of electric-field assisted placement techniques eliminates the need for chemical treatment; however, it requires the use of conductive placement electrodes that limit the performance, scaling, and integration density of electronic devices. Here, we report a method for directed, electric-field assisted placement of solution-based nanomaterials by using large-scale graphene layers featuring patterned nanoscale deposition sites. The structured graphene layers are fabricated by transfer or synthesis on standard substrates, then are removed without residue once nanomaterial deposition is completed by a plasma-based process. We demonstrate the broad applicability by assembling representative zero-, one-, and two-dimensional semiconductors at predefined substrate locations and integrate them into nanoelectronic devices. This graphene-based placement technique affords nanoscale resolution at wafer scale and could enable mass manufacturing of nanoelectronics and optoelectronics involving a wide range of nanomaterials prepared via solution-based approaches.



3D illustration of electric field assisted, directed placement of quantum dots (0D), single-walled carbon nanotubes (1D), and layers of molybdenum disulfide (2D) at large scale using sacrificial graphene electrodes

Plenary Venue C6 (contributed)

Franconia Hall **We 11:25 - 11:50**

Atomic scale imaging and covalent modification of a graphene-carbon nanotube heterostructures

Kimmo Mustonen[1], Alexander Markevich[1], Christof Hofer[1,3], Mukesh Tripathi[1], Heena Inani[1], Aqeel Hussain[2], Esko I. Kauppinen[2], Toma Susi[1], Jannik C. Meyer[1,3], Jani Kotakoski[1]

[1]University of Vienna, Faculty of Physics, Boltzmanngasse 5, 1090 Vienna, Austria
[2]Aalto University School of Science, P.O. Box 15100, FI-00076 Aalto, Finland
[3]Institute for Applied Physics, Eberhard Karls University of Tuebingen, D-72076, Germany

Graphene and single-walled carbon nanotubes (SWCNTs) are among the most interesting new materials of the last decades. Due to the confinement in either one or two dimensions and that they consist only of surface atoms, their electronic properties are sensitive to any structural perturbations. Nevertheless, while several substitutional impurities in graphene have been reported, only nitrogen has been unquestionably identified in SWCNTs. Here, by using a scanning transmission electron microscope (STEM) we present atomically resolved investigations of a SWCNT-graphene van der Waals (vdW) heterostructure [1] with plasma substituted silicon (Si) impurities [2]. We study the vdW interface in detail and show that the molecules seek preferential stacking, leading into 1D corrugations in graphene. This interaction stabilises the structure and thus allows each atom to be resolved in the STEM experiments. Similar to earlier experiments with graphene [3], we proceed to demonstrate that trivalent Si atoms in the SWCNT walls can be manipulated in a precisely controlled manner by using the STEM probe [4].

1. Mustonen, K. et al. ACS Nano, 12 (8) (2018)
2. Inani, H. et al. arXiv:1902.02611 (2019)
3. Susi T. et al. Phys. Rev. Lett. 113 (2014)
4. Mustonen, K. et al. arXiv:1902.03972 (2019)

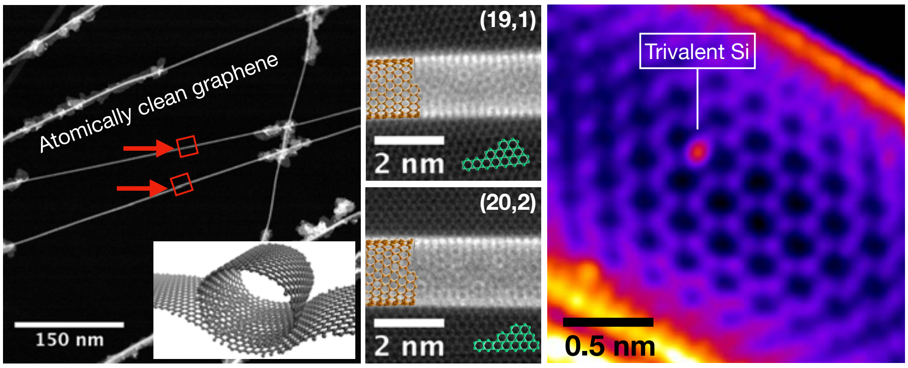


Fig 1. LEFT and CENTER: An overview and atomically resolved STEM closeups of SWCNTs suspended on atomically clean graphene [1]. RIGHT: A trivalent Si substitution in SWCNT lattice [4].

Plenary Venue C7 (contributed)

Franconia Hall **We 11:50 - 12:15**

Micro versus nano-Raman spectroscopy in two-dimensional systems

Ado Jorio[1]

[1] *UFMG/Physics Department, Belo Horizonte, 31270-901, Brazil*

Raman spectroscopy is known to be a valuable tool to the study and characterization of carbon nanostructures. Although the technique provides rich physical and chemical information, it has the drawback of being bound to light diffraction, which limits spatial resolution to the light wavelength scale (in the order of 0.5 microns). Why TERS in 2D is a challenge will be discussed, as well as how we could overcome the problem based on the development of plasmon tunned-tip pyramids. We present results on graphene, $MoS_2$and GaS, with enhancement factors reaching two orders of magnitude. Novel effects such as near-field interferences and dipole approximation breakdown will be discussed.

Company Presentation LB1 (company)

Franconia Hall **We 13:30 - 13:50**

Supercontinuum white light lasers: a review on technology and applications

Nicolai Granzow[1]

[1]*NKT Photonics, Schanzenstr. 39 Bldg. D9-D13, 51063 Cologne, Germany*

Supercontinuum lasers are a technology that combines some of the properties of conventional broadband light sources (like Halogen lamps, Xenon lamps, laser-driven light sources, superluminescent light emitting diodes etc.) with the unique properties of pulsed single-mode lasers: an extremely broad spectral coverage from ~400 nm to 2400 nm emitted as a continuum with an integrated optical power of up to 10 W, and at the same time a perfect Gaussian single-mode beam which can be focused down to the diffraction limit, giving rise to a brightness that exceeds conventional light sources by more than six orders of magnitude, while staying within the spatial resolution regime of optical microscopy if needed. While often used as quasi-cw light sources for steady-state measurements, supercontinuum lasers are also capable of addressing time-resolved measurement techniques due to their typical pulse durations in the ps regime and repetition rates from single-shot to more than 100 MHz.
This unique combination of optical properties adds value within many applications related to modern science, and today there are several thousand system spread across scientific labs worldwide, with applications including bio medical imaging, nano-photonics (e.g. 2d layered materials, carbon nanotubes), spectroscopy or industrial metrology.

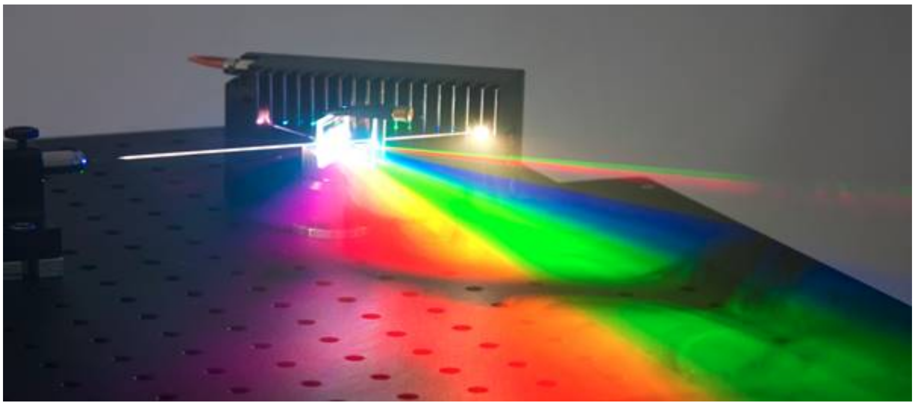


Figure 1. Output of a supercontinuum laser dispersed by a prism in order to visualizing the continuous spectrum in the visible part of the spectrum.

Panorama 11 **We 14:00 - 14:20**

Self-Aligned Short-Channel van der Waals Heterojunction Devices

Mark Hersam[1]

Parallel self-aligned fabrication methods in silicon-based microelectronics have enabled sub-lithographic registration between processing steps, ultimately facilitating substantial advances in circuit complexity. In contrast, while carbon nanotubes and related nanoelectronic materials have shown significant potential for digital and analog electronics due to their high mobilities, ultrathin geometry, and broad range of permutations in van der Waals (vdW) heterojunctions, devices based on vdW nanoelectronic materials have not fully exploited self-aligned fabrication. In this talk, a self-aligned processing method is introduced that enables the realization of field-effect transistors with channel lengths below 150 nm with minimal short-channel effects and improved current saturation using conventional photolithography. In vdW heterojunctions, this self-aligned approach allows dual-gate electrostatic control in both of the constituent semiconductors while concurrently achieving independent gate control of the short-channel series transistors. Since this self-aligned methodology is compatible with a diverse range of nanoelectronic materials and can be implemented in parallel via large-area lithographic processes, it is likely to impact a wide range of vdW heterojunction devices.

Electronics Symposium SEI14 (invited)

Panorama 11 **We 14:20 - 14:40**

Wafer-Scale Fabrication of Ultrathin Flexible Electronic Based on Carbon Nanotubes with High Performance

Youfan Hu[1]

[1] *Department of Electronics, Peking University, Beijing 100871, China*

The challenge associated with an efficient and innocuous delamination operation is one of the major hurdles toward high-performance ultrathin flexible electronics at large scale. Here, a facile, rapid, damage-free approach is reported for detachment of wafer-scale ultrathin electronic foils from Si wafers by capillary-assisted electrochemical delamination (CAED) with a 100% success rate.Such a process incurs neither mechanical damage nor chemical contamination; therefore, the delaminated electronic systems remain intact. Via this approach, carbon nanotube (CNT)-based CMOS technology has been realized on a 2.5 μm-thick plastic foil with high performance. The performances of both the p- and n-type CNT thin film transistors (TFTs) are excellent and symmetric on plastic foil with a low operation voltage of 2 V: width-normalized transconductances (gm/W) as high as 4.69 μS/μm and 5.45 μS/μm, width-normalized on-state currents reaching 5.85 μA/μm and 6.05 μA/μm, and mobilities up to 80.26 cm^2·V^{-1}·s^{-1} and 97.09 cm^2·V^{-1}·s^{-1}, respectively, together with a current on/off ratio of approximately 105. Various high-performance CMOS digital ICs with rail-to-rail output and a ring oscillator on plastics with an oscillation frequency of 5 MHz were demonstrated.

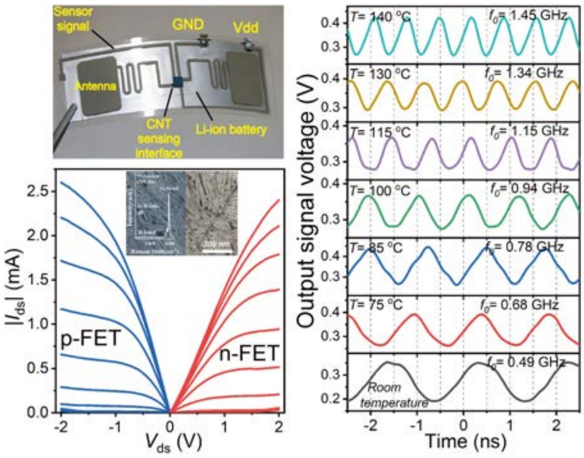
Panorama 11 **We 14:40 - 15:00**

Carbon Nanotube Complementary Gigahertz Integrated Circuits and Their Applications on Wireless Sensor Interface Systems

Lijun Liu[1], Li Ding[1], Lian-Mao Peng[1], Zhiyong Zhang[1]

[1]*Peking University, Key Laboratory for the Physics and Chemistry of Nanodevices and Department of Electronics, Beijing 100871, China*

Along with ultra-low energy-delay products and symmetric complementary polarities, carbon nanotube field-effect transistors (CNT FETs) are expected to be promising building blocks for energy-efficient computing technology. However, the work frequencies of the existing CNT-based complementary metal-oxide-semiconductor (CMOS) integrated circuits (ICs) are far below the requirement (850 MHz) in state-of-art wireless communication applications. In this work, we fabricated deep submicron CMOS FETs with considerably improved performance of n-type CNT FETs and hence significantly promoted the work frequency of CNT CMOS ICs to 1.98 GHz. Based on these high-speed and sensitive voltage-controlled oscillators (VCOs), we then presented a wireless sensor interface circuit with working frequency up to 1.5 GHz spectrum. As a preliminary demonstration, an energy-efficient wireless temperature sensing interface system was realized combining a 150 mAh flexible Li-ion battery and a flexible antenna (centre frequency of 915 MHz). In general, the CMOS-logic high speed CNT ICs showed outstanding energy efficiency and thus may potentially advance the application of CNT-based electronics.



Electronics Symposium SEI16 (contributed)

Panorama 11 **We 15:00 - 15:20**

Scalable production of semiconducting SWCNTs by floating catalyst chemical vapor deposition for ultrahigh-performance electronics

Er-Xiong Ding[1], Abu Taher Khan[1], Qiang Zhang[1], Nan Wei[1], Aqeel Hussain[1], Esko I. Kauppinen[1]

[1] *Department of Applied Physics, Aalto University School of Science, Espoo, Finland*

High-purity semiconducting single-walled carbon nanotubes (s-SWCNTs) are of paramount significance for the fabrication of ultrahigh-performance electronics. Solution separation of s-SWCNTs can achieve the purity higher than 99%, though the separated s-SWCNTs have not exhibited the best performance since their intrinsic electronic properties are degenerative caused by contamination of dispersant and shortening of tubes. Catalyst-supported CVD is limited by low yield and available substrate. Here we report scalable production of high-purity s-SWCNTs by floating catalyst CVD which retains the primitive morphology of tubes with ethanol being adopted as carbon source [1] while methanol as an additive [2]. Optical absorption spectrum demonstrates a high semiconducting ratio of 96%, while electron diffraction presents a purity of 89.3%. Furthermore, the sharp S_{11} indicates a very narrow diameter distribution of SWCNTs (Fig. 1). Electron microscopy images also display isolated, clean and long (~25 µm) tubes. Our study provides a route accessible to bulk synthesis of clean and long s-SWCNTs with high purity as well as narrow band gap distribution.

[1] E.-X. Ding, et al. Nanoscale, 9, 17601 (2017).
[2] E.-X. Ding, et al. In preparation, 2019.

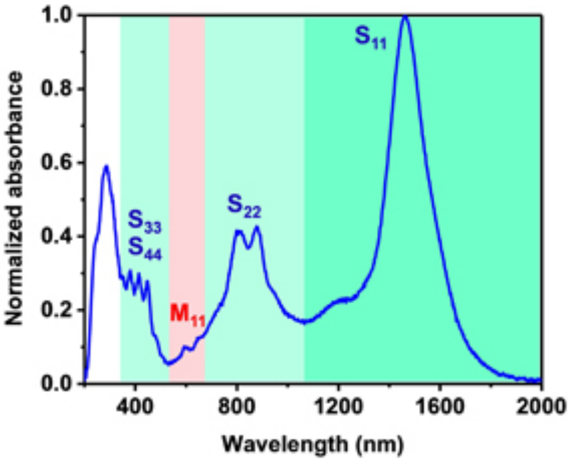


Fig. 1 Optical absorption spectrum of as-synthesized SWCNTs collected from a floating catalyst CVD reactor.

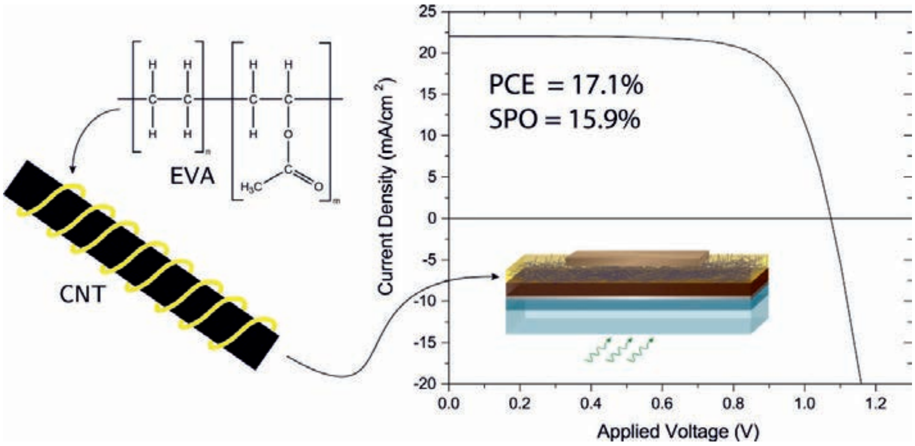
Franconia Hall **We 14:00 - 14:20**

Solubilization of single and multi-walled CNT with ethylene-vinyl acetate for conductive films and charge extraction in perovskite solar cells

Robin Nicholas[1], Giulio Mazzotta[1], Bernd Sturdza[1], Markus Dollman[1], Severin Habisreutinger[2], Greyson Christoforo[1], Zhiping Wang[1], Henry Snaith[1], Moritz Riede[1]

[1] *University of Oxford, Department of Physics, Parks Road, Oxford, OX1 3PU, United Kingdom.*
[2] *Chemistry and Nanoscience Center, NREL, Golden, Colorado 80401, USA*

Carbon nanotube (CNT) solubilization via non-covalent wrapping of conjugated semiconducting polymers is a common technique used to produce stable dispersions for depositing CNTs from solution. Here, we report the use of a non-conjugated insulating polymer, ethylene-vinyl acetate (EVA), to disperse both multi- and single-walled CNTs (MWCNT and SWCNT) in organic solvents. We demonstrate that despite the insulating nature of the EVA, we can produce spray coated semi-transparent films with conductivities of up to 34 S/cm. We show, using photoluminescence spectroscopy, that the EVA strongly binds to individual CNTs thus making them soluble, preventing aggregation, and facilitating the deposition of high quality films. The excellent electronic properties of this composite, are demonstrated by the fabrication of perovskite solar cells using EVA/SWCNT and EVA/MWCNTs as the selective hole contact, obtaining power conversion efficiencies of up to 17.1%, demonstrating that the insulating polymer does not prevent the charge transfer from the active material to the CNTs and allows it to be efficiently collected by the top electrode.



Franconia Hall **We 14:20 - 14:40**

Ultra-High Thermal Effusivity Materials based on Graphene for Resonant, Ambient Thermal Energy Harvesting

Volodymyr Koman[1], Anton Cottrill[1], Albert Liu[1], Michael Strano[1]

[1]*Department of Chemical Engineering, Massachusetts Institute of Technology, USA*

Materials science has made progress in maximizing or minimizing the thermal conductivity of materials, however, the thermal effusivity – related to the product of conductivity and capacity – has received limited attention, despite its importance in the coupling of thermal energy to the environment. We design materials that maximize the thermal effusivity by impregnating high surface area copper (Cu) and nickel (Ni) foams with conformal chemical vapor deposited graphene (G) and octadecane (OD) as a phase change material, achieving the highest value in the literature, to date. These composite materials are ideal for ambient energy harvesting in the form of what we call broadband thermal resonators to generate persistent electrical power from ambient thermal fluctuations over large ranges of frequencies. To illustrate, we experimentally measure persistent energy harvesting from diurnal frequencies at an outdoor location in Cambridge, Massachusetts. Thermal resonance devices of this type may provide renewable and persistent energy sources over extended periods.

Reference:
Nature Communication volume 9, page 664 (2018).

Energy Symposium SEn15 (invited)

Franconia Hall **We 14:40 - 15:00**

Tailoring Carbon Nanostructures for Energy Storage Applications

Bingqing Wei[1,2]

[1]*Department of Mechanical Engineering, University of Delaware, Newark, DE 19716, USA*
[2]*Center for Nano Energy Materials, Northwestern Polytechnical University, Xi'an, China*

As sustainable and renewable energy sources such as solar and wind power are intermittent in nature, reliable electrochemical energy storage systems, mainly including rechargeable batteries and electrochemical capacitors, are purposely explored to promote efficient utilization of these energy sources and are a growing challenge. The development of high energy storage devices has been one of the most important research areas in recent years and relies mostly on the successful engineering of electrode materials. Carbon nanostructures such as carbon nanotubes (CNTs) and graphene have been full of surprises since their emergence and are intensively investigated for use as electrode materials in energy storage devices. Utilizing CNTs, graphene, and their composites for various energy storage applications such as Li-ion and L-S batteries, and supercapacitors are under scrutiny because of their improved electrochemical activity, cost-effectiveness, benign environmental nature, and promising electrochemical performance. In this presentation, I will discuss our research strategies and efforts to employ carbon nanostructures for different energy storage applications including flexible and even stretchable electricity storage devices.

Energy Symposium SEn14 (contributed)

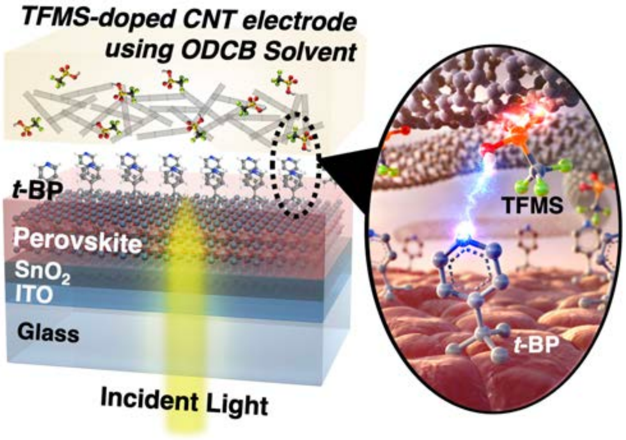
Franconia Hall **We 15:00 - 15:20**

Carbon Nanotubes to Outperform Metal in Perovskite Solar Cells via Dopant Engineering and Hole-Selectivity Control

Il Jeon[1], Ahmed Shawky[1], Yutaka Matsuo[1], Shigeo Maruyama[1], Esko Kauppinen[2]

[1] *Department of Mechanical Engineering, The University of Tokyo, Japan*
[2] *Department of Applied Physics, Aalto University School of Science, Finland*

Lead halide perovskite solar cells (PSCs) have received considerable attention around the world as a promising alternative energy source. Their certified power conversion efficiencies (PCEs) now exceed 20% and only a few challenges remain before commercialisation, which include long-term stability and fabrication-costs. The metal electrodes in PSCs are typically evaporated in vacuum by thermal deposition. This incurs substantially high fabrication costs. Further, using metal electrodes induces an ion-migration, which is detrimental to the long-term stability of the perovskite layer. Thus, it is crucial that we find an alternative to the metal electrodes which can bring down the fabrication cost of PSCs and improve the device stability. We report carbon nanotube (CNT)-laminated PSCs, in which triflic acid (TFMS) in o-dichlorobenzene was found to give the doping effect without reacting with the perovskite and 0.05 v% was the optimal concentration that showed the maximum doping effect with no damage to the device (PCE = 18.1%). We optimised the CNT density and spiro-MeOTAD concentration to obtain a PCE of 19.0% by applying dense CNTs with 1.7 times higher spiro-MeOTAD concentration compared to the reference.



2D Materials Symposium S2D14 (invited)

Panorama 13 **We 14:00 - 14:20**

Introducing 2D Materials for Magnetic Tunnel Junctions

Bruno Dlubak[1]

[1] *Unité Mixte de Physique CNRS-Thales, 91767 Palaiseau, France*

2D materials have opened novel exciting opportunities in terms of functionalities and performances for spintronics devices. Here we present experimental results on 2D materials integration in vertical spin valves. We show that a graphene layer integrated by CVD prevents ferromagnets oxidation [1], enabling the use of novel low-cost processes for spintronics such as ALD [2]. The use of graphene on ferromagnets allows to preserve a highly surface sensitive spin polarizer/analyzer behavior and adds new enhanced spin filtering property [1][2]. In a second part, we will present characterizations of spin valves making use of monolayer h-BN tunnel barriers grown by CVD on Fe or Co[3]. In the case of the h-BN/Co interface, observed inversion of the spin polarization is analyzed, with ab-initio calculations in support, in the light of h-BN hybridization with the ferromagnetic metal in contact [3]. These different experiments unveil promising uses of 2D materials for spintronics [4].

1. Dlubak et al. ACS Nano 6, 10930 (2012) ; Weatherup et al. ACS Nano 6, 9996 (2012)
2. Martin et al. ACS Nano 8, 7890 (2014) ; APL 107, 012408 (2015)
3. Piquemal-Banci et al. APL 108, 102404 (2016) ; ACS Nano 12, 4712 (2018)
4. Review: Piquemal-Banci et al. J. Phys. D : Appl. Phys. 50, 203002 (2017)

2D Materials Symposium S2D15 (contributed)

Panorama 13 **We 14:20 - 14:40**

Towards the survival of quantum spin Hall phase of group-IV overlayers on substrates

Lara Kühl Teles[1], Filipe Matusalém[1], Daniel Schwalbe Koda[1], Marcelo Marques[1], Friedhelm Bechstedt[2]

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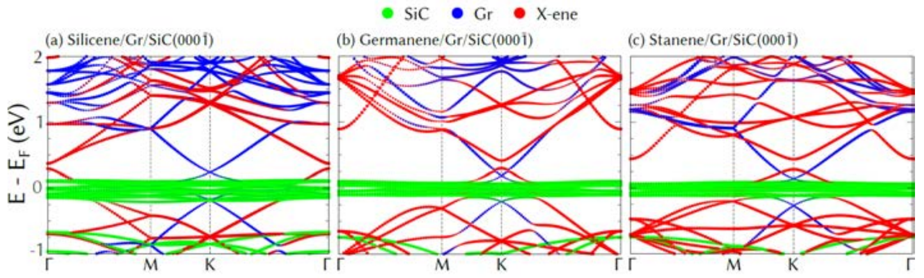
[2]*Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität, Jena, Germany*

Two-dimensional (2D) topological insulator, known as quantum spin Hall (QSH) insulator, is a promising quantum phase for achieving dissipationless transport. The search for 2D realistic materials that can provide the QSH effect considering the feasibility of their experimental preparation is a growing field. Therefore, it is desirable to go beyond the ground-state studies of freestanding materials, especially considering those that cannot be exfoliate and need to be grown on a certain substrate.
By means of first-principles electronic structure calculations, we discuss the possibilities of synthesizing the group-IV X-ene on a substrate. First, the deposition of Sn on top of Si-terminated 4H-SiC(0001) surface is analyzed. The calculation of Z2 invariant shows that passivated substrates are required to ensure the survival of their exotic properties. Second, the deposition of the group-IV on 4H-SiC substrate intercalated by a graphene sheet, was studied in detail. In contrast to the Si-terminated SiC surface, X-ene/graphene on top of the C-terminated SiC substrate are stable. The topological invariants of the peeled-off X-ene/graphene bilayers indicate the presence of topological character and the existence of a quantum spin Hall phase in the case of germanene/graphene bilayer.



Quasiparticle band structures for most stable geometries of (a) silicene, (b) germanene, and (c) stanene stacked on graphene on C-terminated SiC.

Panorama 13 **We 14:40 - 15:00**

Light driven capacitive charging of 0D-2D hybrids

Ilka Kriegel[1,2,3], Nicholas J. Borys[2,4], Kehao Zhang[5,6], Adam W. Jansons[7], Brandon M. Crockett[7], Kristopher M. Koskela[7], Edward S. Barnard[2], Erika Penzo[2], James E. Hutchison[7], Joshua A. Robinson[5,6], Liberato Manna[1], P. James Schuck[3]

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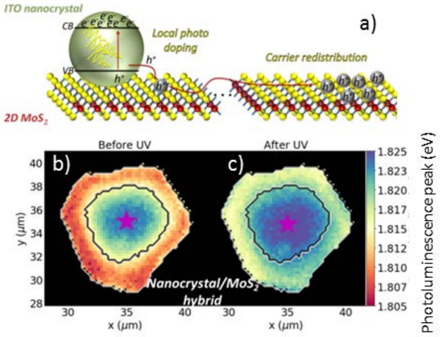
[2] *Lawrence Berkeley National Laboratory, The Molecular Foundry, Berkeley, 94720, USA*
[3] *Columbia University, Department of Mechanical Engineering, New York, 10027, USA*
[4] *Montana State University, Department of Physics, Bozeman, 59717, USA*
[5] *The Pennsylvania State University, Dept. of Mater. Sci. and Eng., Pennsylvania, 16802, USA*
[6] *The Pennsylvania State University, ATOMIC, Pennsylvania, 16802, United States*
[7] *University of Oregon, Department of Chemistry, Eugene, Oregon, 97403, United States*

We report on the cooperative electronic properties of novel 0D 2D hybrids displaying a new nanoscale, light-driven charge-injection scheme. By illuminating this novel hybrid system of indium tin oxide (ITO) nanocrystals and MoS_2 with ultraviolet light, photo-generated holes in the ITO nanocrystals are quasi-permanently injected into MoS_2. P-type photodoping to extents competing with electrostatic gating is observed. The net effect is that the excited carriers are separated over long distances up to 40 µm away from the local (micron sized) optical excitation spot. Carrier accumulation in MoS_2 coincides with regions of initially enhanced n-type doping and preferentially along edges and grain boundaries. This suggests 2D environment control in transition metal dichalcogenides as a tool to introduce a driving force for carrier redistribution. Notably, carrier injection follows a capacitor-like behavior with capacitance values in the atto Farad range, leading to an average optically induced photodoping of each nanocrystal with more than 40 carriers. These studies present a foundational building block for next-generation 2D devices, enabling remote-control of local charge density and opening prospects for novel energy storage schemes. Ref. 1. I. Kriegel, et al. Arxiv 1810.05385 (2018)



a) Illustration of the 0D/2D hybrid (ITO nanocrystal/MoS_2) structure. b) and c) Illustration of photoluminescence variation over an MoS_2 flake before (b) and after (c) exposure to a focused ultraviolet (UV) laser spot (star). Adapted from Ref. 1

2D Materials Symposium S2D17 (contributed)

Panorama 13 **We 15:00 - 15:20**

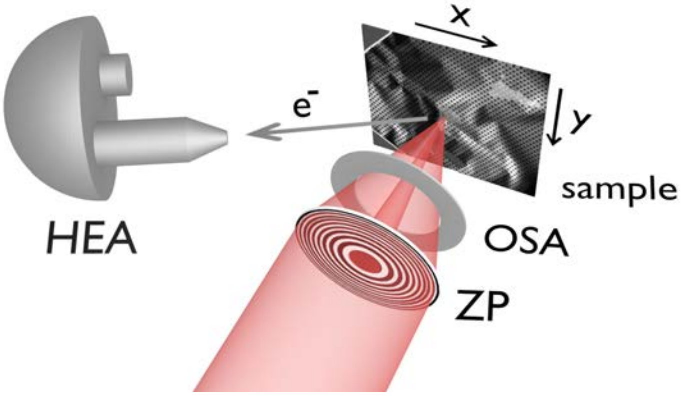
Chemical analysis of suspended graphene by spatially resolved X-ray photoelectron spectroscopy

Patrick Zeller[1], Matteo Amati[1], Luca Gregoratti[1]

[1] *Elettra - Sincrotrone Trieste S.c.P.A., SS14-Km163.5, 34149 Basovizza-Trieste, Italy*

The unique properties of graphene (Gr) are strongly influenced by the supporting substrate which makes it important to perform the investigations at suspended and undisturbed Gr. For instance, Pt nanoparticles nucleate differently on suspended Gr than on supported Gr.[1] Due to the fact that with the available technologies one or few layer Gr can be suspended only over small holes (several µm), spatially resolved measurements are mandatory. Conventional techniques for chemical analysis like XPS typically do not provide the needed spatial resolution. One approach to overcome this limitation is the Scanning Photoemission Microscope hosted at the ESCAmicroscopy beamline at the Elettra synchrotron light source. In this setup the X-ray beam is demagnified to a diameter of ~130 nm which allows a chemical characterization by means of XPS from submicron regions and to map the chemical spatial dispersion. With this setup suspended Gr can be measured without interference of the support. The layer dependency of the C 1s core level of suspended Gr and also the nucleation behavior of Pt nanoparticles on suspended Gr will be demonstrated, showing the capabilities of this microscope.[1,2]

[1] L. Gregoratti et al. Top. Catal. 61 (2018) 1274
[2] T. Susi et al. Phys. Rev. Mater. 2 (2018) 074005



Schema of the experimental setup: The sample (Gr on Quantifoil) is raster scanned with respect to the focused X-ray beam while the emitted photoelectrons are collected by an electron energy analyzer. This allows the chemical analysis of suspended Gr.

Panorama 12 **We 14:00 - 14:20**

Comparing resonant Raman spectroscopy and atomic resolution transmission electron microscopy for SWCNT sample characterization

Annick Loiseau[1], Alice Castan[1], Frédéric Fossard[1], Salomé Forel[2], Guillaume Wang[3], Wim Wenseleers[2], Sofie Cambré[2]

[1] *LEM, ONERA-CNRS, UMR104, U. Paris-Saclay, 92320 Châtillon, France*
[2] *ECMPL, Physics Department, University of Antwerp, Antwerp, Belgium*
[3] *MPQ, U. Paris Diderot –CNRS, Paris, France*

Having access to SWCNTs samples enriched in certain structures is a fundamental goal in order to exploit their properties within the scope of specific applications. One way to produce such samples is to achieve structurally selective growth of SWCNTs. Aside from the obvious scientific challenges related to this very active research field, being able to precisely and accurately assess the composition of a growth sample is a key point for understanding the phenomena underlying growth selectivity.
A widely used characterization methodology for assessing the selectivity of CVD grown SWCNT on flat substrates is based on resonant Raman spectroscopy mappings using a set of discrete laser lines. In this work we thoroughly investigate the reliability of this methodology through cross-characterizations with other techniques on specifically chirality- and/or diameter-sorted samples. By comparing, first, Raman results with atomic resolution transmission electron microscopy statistical analyses, we evidence significant discrepancies between the two techniques. Further comparison with photoluminescence and optical absorption measurements shows that the observed discrepancies clearly stem from the chirality-dependence of SWCNT Raman cross-sections.

Panorama 12 **We 14:20 - 14:40**

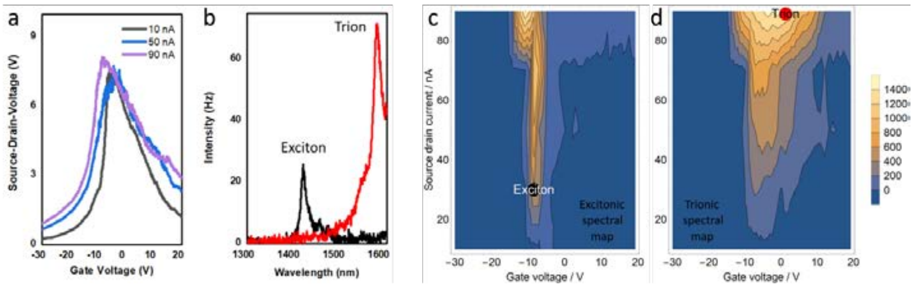
Electroluminescence excitation mapping of excitons and trions in monochiral carbon nanotube devices

Adnan Riaz[1,2], Marco Gaulke[1,2], Felix Pyatkov[1,2], Simone Dehm[1], Han Li[1], Benjamin Flavel[1], Frank Hennrich[1], Manfred Kappes[1], Yuan Chen[3], Ralph Krupke[1,2]

[1]*Institute of Nanotechnology, Karlsruhe Institute of Technology, Germany*
[2]*Institute of Materials Science, Technische Universität Darmstadt, Germany*
[3]*School of Chemical and Biomolecular Engineering, The University of Sydney, Australia*

Single walled carbon nanotubes as emerging quantum-light sources have the potential to fill a technological gap in silicon photonics as on chip, electrically driven, classical or non-classical emitters [1-3]. Unlike in photoluminescence, emission via electrical excitation is heavily influenced by the device architecture and the biasing, and finding optimum operation conditions for a single tube emitter remains challenging. Here, we present an electroluminescence spectroscopy study on individual (9,8) nanotubes in a wide temperature range. At cryogenic conditions excitonic and trionic emissions are exceptional stable and reproducible, appearing at well-defined source-drain and gate voltages. The data was processed into electroluminescence excitation maps for identification of optimum operating conditions, at which emission lines are narrow and device efficiencies high.

[1] F. Pyatkov et al., Nature Photonics 10, 420 (2016)
[2] S. Khasminskaya et al., Nature Photonics 10, 727 (2016)
[3] X. He et al., Nature Materials 17, 663 (2018)



(a) Electrical characterization of (9,8) devices at constant source-drain currents. (b-d) Electroluminescence spectra and integrated intensity maps of excitonic and trionic emissions, controlled by gate voltage and source-drain current.

Panorama 12 **We 14:40 - 15:00**

Electronic coupling between the walls of double-walled carbon nanotubes

Georgy Gordeev[1], Soeren Wasseroth[1], Han Li[2], Ralph Krupke[2,3], Ado Jorio[4], Benjamin Flavel[2,3], Stephanie Reich[1]

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[2]*Institute of Nanotechnology, Karlsruhe Institute of Technology, Karlsruhe 76344, Germany*
[3]*Institute of Materials Science, Technische Universität Darmstadt, Darmstadt 64289, Germany*
[4]*Department of Physics, Federal University of Minas Gerais, Belo Horizonte, Brazil*

Double walled carbon nanotubes (DWCNT) enable direct van der Walls coupling between graphene based lattices with varying crystallographic orientations (twist angles) and electronic interfaces. Despite intense research in the past years, the coupling between the walls is still poorly understood. Here we report a resonant Raman study of double-walled carbon nanotubes sorted by electronic types [1]. The transition energies of nanotubes are deduced from resonant Raman spectroscopy of the radial breathing mode (RBM). The shift of transition energy depends on the metallic and semiconducting type of the other wall. Moreover, the RBMs of the inner wall change in their frequencies as function of the fundamental band gap of the outer wall. This changes manifest a novel mechanism of electronic coupling between the walls. These findings contradict the generally excepted wall-to-wall coupling mechanism of a mechanical nature, responsible for the shifts of the RBM frequencies. An analysis of Raman cross sections yields a peculiar vibrational energy exchange between the walls. The energy flows from the wall with higher optical transition to the wall with lower optical transition.

[1] Li, H. et al. Nat. Nanotechnol. 12, 1176–1182 (2017)

Spectroscopy Symposium SSp5 (invited)

Panorama 12 **We 15:00 - 15:20**

Nonlinear optical spectroscopy and imaging in 2D materials

Leandro Malard[1]

[1]*Dep. de Física, Universidade Federal de Minas Gerais*

In this work we will show our recent developments on the non-linear optical properties of novel 2D materials. We have used both Second Harmonic Generation (SHG) and Coherent Anti Stokes Raman Scattering (CARS) to study mono- and few-layers of semiconducting dichalcogenides and graphene respectively. In the case of the MoS_2 we have observed efficient SHG from odd number of layers due to the absence of inversion symmetry [1]. By using different laser excitation energies, we could probe the resonant effect in the SHG in MoS2, MoSe2 and WS2. By analyzing the resonant profile of SHG we can observe the different types of excitons in this material, which are compared with recent theoretical results in the literature [2]. Because graphene have inversion symmetry, the SHG is almost absent, however third order nonlinearities are greatly enhanced in this material due its peculiar band structure. We will discuss the CARS process in graphene and h-BN [3]. More recently we have also shown that SHG can be a useful tool to identify and characterize grain boundaries and edges in different 2D materials [4].

[1] L. M. Malard et al., Phys. Rev. B 87, 201401 (2013).
[2] A. Corradi, in preparation.
[3] L. Lafetá, Nano Lett. 17, 3447 (2017).
[4] B. R. Carvalho, arXiv:1903.05139 (2019).

Panorama 10 **We 14:00 - 14:20**

Encapsulated Dyes in Nanotubes: a Biological Perspective

Charlotte Allard[1,2], Nathalie Y-Wa Tang[2,3], Etienne Gaufrès[4], Rafaella Oliveira Do Nascimento[2,3], Patrick Desjardins[1,2], Richard Martel[2,3]

[1] *Département de Génie Physique, École Polytechnique de Montréal, Montréal, H3T 1J4, Canada*
[2] *Regroupement Québécois sur les Matériaux de Pointe (RQMP)*
[3] *Département de Chimie, Université de Montréal, Montréal, H3T 1J4, Canada*
[4] *Institut d&#039*
[5] *Optique, Université de Bordeaux, Talence, 33400, France*

Optical imaging has emerged in recent years as a promising alternative for the diagnosis of pathologies at the molecular scale. One imaging approach consists of using contrast agents to mark specific biomarkers with known optical signatures. In this context, we have developed a strategy based on nanoprobes made of dyes encapsulated in nanotubes. The nanoprobes enable the use of different and complementary optical modalities, which are adapted for quantitative analysis and multiplexing.

Dyes in carbon nanotubes (CNTs) are protected from degradation and present a giant Raman signature with narrow emission peaks, free of background fluorescence. The resulting Raman nanoprobe is particularly interesting for multiplexing applications, in which several nanoprobes can be excited at the same wavelength without overlapping in the emission signals. In this work, we will focus on its potential use as a tool for immunotherapy.

Furthermore, preliminary work suggests that dyes in boron nitride nanotubes (BNNTs) are also protected from degradation, while the fluorescence of the dyes is conserved. This allows bimodal imaging, in which Raman and fluorescence are combined for more specificity and sensibility. Examples of imaging experiments with this nanoprobe will be presented.

NanoBio Symposium SNB3 (invited)

Panorama 10 **We 14:20 - 14:40**

Targeted near infrared sensing and imaging with carbon nanotubes

Sebastian Kruss[1]

[1] *Department of Chemistry, Göttingen University, Germany*

Carbon nanomaterials such as semiconducting single-walled carbon nanotubes (SWCNTs) are versatile building blocks for optical biosensors. SWCNTs fluoresce in the near infrared (nIR, 900-1700 nm) and their optoelectronic properties are very sensitive to changes in the chemical environment but a) achieving high selectivity and sensitivity and b) targeting or delivering those sensors to specific locations in cells or organisms is still a great challenge. Therefore, we use novel chemical and physical approaches to better understand SWCNT photophysics and enhance the capabilities of SWCNT-based fluorescent sensors: 1) We tailored the corona phase around SWCNTs to enhance selectivity and photophysics of SWCNT-based sensors for the neurotransmitters dopamine and serotonine. 2) SWCNTs were conjugated to nanobodies that can be targeted in vivo to any Green Fluorescent Protein (GFP) moiety and used for single-particle tracking and microrheology measurements in living drosophila embryos. 3) Peptides were incorporated into the organic corona phase around SWCNTs to target surface receptors on cells (integrins) and label them in the nIR. 4) Immune cells were used for programmed sensor transport and release. They take up SWCNT-based sensors, transport them and release them again.

NanoBio Symposium SNB4 (invited)

Panorama 10 **We 14:40 - 15:00**

Electrical Sensing with a Tube-in-a-Tube Semiconductor

YuHuang Wang[1]

[1] *University of Maryland, College Park, MD 20742 USA*

The fundamental idea of field-effect transistors has fueled the development of innovative electrical sensing technologies for the detection of biological and chemical species. However, it is generally challenging to attain simultaneous ultrahigh sensitivity and selectivity as required for chemical sensing. In this talk, we will discuss progress from our lab toward the demonstration of a tube-in-a-tube (Tube^2) semiconductor for the electrical detection of small molecules and biological molecules. A Tube^2 is equivalent to a single-walled carbon nanotube nested within a chemically tailored, impermeable, and atomically-thick functional shell. We synthetically create this structure from double-walled carbon nanotubes through outer wall-selective covalent chemistry. Compared with single-walled carbon nanotubes and graphene, electrical sensors created using Tube^2 can be readily tailored with robust covalent chemistries to high functional densities for enabling chemical selectivity while maintaining exceptional sensitivity. The implications of these findings to electrical detection of small molecules and biosensing will be discussed.

NanoBio Symposium SNB5 (contributed)

Panorama 10 **We 15:00 - 15:20**

Real-Time Near-Infrared Confocal Imaging of Bacterial Cell Division in the Presence of Single-Walled Carbon Nanotubes

Alessandra Antonucci[1], Nils Schuergers[1], Vitalijs Zubkovs[1], Ardemis Boghossian [1]

[1]*École Polytechnique Fédérale de Lausanne (EPFL), Lausanne, CH-1015, Switzerland*

The chemical and optical properties of single-walled carbon nanotubes (SWCNTs) have inspired a plethora of different applications in the field of cell nanobiotechnology. However, most studies have focused on interfacing SWCNTs with cells of eukaryotic organisms. Herein we present a first comprehensive study focusing on the interaction of SWCNTs with bacterial cells. We identify wrappings that facilitate nanoparticle uptake over the bacterial cell wall, an important first step towards the expansion of nanomaterials' application in the broad field of microbiology. We used a custom-built, spinning disc confocal microscope to image near-infrared (NIR) SWCNT fluorescence within the cells. By performing in situ cell growth and nanoparticle tracking we investigated the fate of internalized SWCNTs upon multiple cell division events. Real-time monitoring revealed that the indefinitely photostable NIR fluorescence is inherited by daughter cells. The imparted NIR fluorescence offers an unprecedented avenue for quantitative and continuous imaging of nanobioengineered cells across multiple generations. Beyond bacterial nanobionics, this technique creates new opportunities for imaging subcellular targeting and trafficking of NIR-fluorescent probes in the field of drug delivery and biosensing.

Program Thursday

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Introduction

For more than 20 years of technological research and development，Professor Xiaogang Sun of Nanchang University founded NanoCarbon Co Ltd successfully and received the investment of 550 million yuan from Zhengzhou DENGCAO Group Co., Ltd. The company consists of JIANGXI NanoCarbon Co Ltd and HENAN NanoCarbon Co Ltd, mainly committed to the industrial production and application of whisker carbon nanotubes. JIANGXI NanoCarbon Co Ltd invested 100 million yuan, with an annual processing of 30 tons of carbon nanotubes powder project. HENAN NanoCarbon Co Ltd as a production base invested 450 million yuan to build an annual processing of 500 tons of carbon nanotubes powder project. Production base construction in two phases, the first stage capacity of 200 tons, the second phase capacity of 300 tons.

The company has completely independent intellectual property rights, accumulative application for 106 patents, of which 2 international PCT patents, and has won the national license of 9 patents for invention. The project technology has reached the international leading level, and has completed the construction of the first domestic production line of carbon nanotubes whisker, At the same time, the whole production process is non-toxic and harmless, green and environmentally friendly.

Whisker carbon nanotubes as a new generation of linear high-end carbon nanotubes, Which can be widely used in lithium ion batteries, electro-thermal conversion devices and nanocomposites， has the characteristics of non-winding, easy to disperse, ultra-high purity, ultra-high crystallinity, electrical conductivity, excellent thermal conductivity and so on. At present, the main products of the company are Whisker CNT powder of various specifications, conductive paste and other carbon-based materials.

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Plenary program Franconia Hall

Session PI7 Chair: Yuichiro Kato

08:30 - 09:15	K4	**H.-S. Philip Wong** (Stanford University) *Progress Towards a Carbon Nanotube Transistor Logic Technology*
09:15 - 09:40	I12	**Matteo Pasquali** (Rice University) *A Better Future for Carbon Nanomaterials?*
09:40 - 10:05	I13	**YuHuang Wang** (University of Maryland) *Dynamic Gating of Infrared Radiation in a Textile*

Coffee break CCW Lobby

Session PI8 Chair: Yuhuang Wang

10:35 - 11:00	C8	**Yoshiyuki Nonoguchi** (Nara Institute of Science and Technology) *Thermoelectric Transport in Polymer-Functionalized Semiconducting Carbon Nanotube Films*
11:00 - 11:25	C9	**Weizhong Qian** (Tsinghua University) *3D Al Foam-Enhanced Graphene-Based High Voltage Supercapacitor*
11:25 - 11:50	C10	**Mattia Scagliotti** (Università degli studi di Roma "Tor Vergata") *Fast Response Graphene/N-Si Photodetector*
11:50 - 12:15	I14	**Ming Xu** (Huazhong U. of Science and Technology) *Advances in Structural Design of Three-Dimensional Nanomaterials for the Extreme Environment Applications*

Lunch break

Electronics Symposium (CNTFA19) Franconia Hall

		Chair: Youfan Hu
14:00 - 14:20	SEI17	**Albert G. Nasibulin** (Skolkovo Institute of Science and Technology) *Holey Single-Walled Carbon Nanotubes for Ultra-Fast Broadband Bolometers*
14:20 - 14:40	SEI18	**Ze Ma** (Peking University) *Improving Performance and Uniformity of Carbon Nanotube Network Based Photodiodes via Yttrium Oxide Coating-and-Decoating*
14:40 - 15:00	SEI19	**Thomas Szkopek** (McGill University) *Large Area Ion Sensitive Graphene Field Effect Transistors*
15:00 - 15:20	SEI20	**Dmitri Lioubtchenko** (Polish Academy of Sciences) *Thin Carbon Nanotube Layers for Terahertz Wave Applications*
		10 minute break
		Chair: Albert G. Nasibulin
15:30 - 15:50	SEI21	**Volodymyr Koman** (MIT) *Colloidal, Nanoelectronic State Machines Based on 2D Materials as Smart Aerosolized Probes and Recorders*
15:50 - 16:10	SEI22	**Alexey Tsapenko** (Skoltech) *Enhancing Optoelectronic Performance of Randomly Oriented Single Walled Carbon Nanotube Films for Transparent and Conducting Applications*
		Coffee break CCW Lobby

Energy Symposium (NMES19) Franconia Hall

Chair: Yanwu Zhu

14:00 - 14:40 SEn17 **Yanwu Zhu** (University of Science and Technology of China)
Construction of Carbon Interface for Electrical Energy Storage

14:40 - 15:00 SEn28 **Juan Vilatela** (IMDEA Materials)
Operando Characterisation of CNT Fibre Fabric-Based Electrodes and Their Application for High-Toughness Batteries

Coffee break CCW Lobby

2D Materials Symposium (GSS19) Panorama 13

Chair: Bruno Dlubak

14:00 - 14:40	S2D18	**Luca Banszerus** (RWTH Aachen) *Electrostatically Defined Quantum Devices in Bilayer Graphene*
14:40 - 15:00	S2D19	**Igor Bondarev** (North Carolina Central University) *Interlayer Exciton Complexes in Planar Stacked Quasi-2D Heterostructures*
15:00 - 15:20	S2D20	**Sabina Caneva** (Kavli Institute of Nanoscience Delft) *Mechanically Controlled Quantum Interference in Graphene Break Junctions*

10 minute break

Chair: Christian Schneider

15:30 - 15:50	S2D21	**Andreas Sperlich** (Julius-Maximilians-Universität Würzburg) *Room Temperature Initialisation and Readout of Intrinsic Spin Defects in a Van Der Waals Crystal*
15:50 - 16:10	S2D22	**Yang Wei** (Tsinghua University) *Mixed-Dimensional Van Der Waals Heterostructures Based on Carbon Nanotubes and 2D Materials*
16:10 - 16:30	S2D23	**Bernard Plaçais** (ENS Paris) *A Dirac Fermion Wave Reflector Based on the Laws of Geometrical Optics*

Coffee break CCW Lobby

Spectroscopy Symposium (NSAP19) Panorama 12

Chair: Achim Hartschuh

14:00 - 14:40	SSp6	**Kaihui Liu** (Peking University) *Optical Spectroscopy of Individual Carbon Nanotubes With Defined Chirality*
14:40 - 15:00	SSp7	**Sofie Cambré** (University of Antwerp) *Controlling the Inner Dielectric Environment of Carbon Nanotubes To Tune Their Optical Properties*
15:00 - 15:20	SSp8	**Yoshikazu Homma** (Tokyo University of Science) *Temperature Change of Water Adsorption Layer on Suspended Single-Walled Carbon Nanotube*

10 minute break

Chair: Ado Jorio

15:30 - 15:50	SSp9	**Yuichiro Kato** (RIKEN) *Exciton Physics in Air-Suspended Carbon Nanotubes*
15:50 - 16:10	SSp10	**Ernesto Joselevich** (Weizmann Institute of Science) *Shaping Nanotubes and Nanowires With Surfaces for Electronics and Optoelectronics*
16:10 - 16:30	SSp11	**Akihiro Ishii** (RIKEN) *Decay Dynamics and Diffusion Properties of Bright and Dark Excitons in Air-Suspended Carbon Nanotubes*

Coffee break CCW Lobby

NanoBio Symposium (CNBMT19) Panorama 10

Chair: Sebastian Kruss

14:00 - 14:20	SNB6	**Eri Hirata** (Hokkaido University) *The Advantages of Carbon Nanomaterials for Bone Tissue Engineering*
14:20 - 14:40	SNB7	**Silvana Fiorito** (National Research Council) *Carbon Nanotubes Impact Microglia Function and Phenotype*
14:40 - 15:00	SNB8	**Minfang Zhang** (AIST) *Quantitative Evaluation of the Biodegradation of Single-Wall Carbon Nanotubes in the Mouse Lung and Liver*
15:00 - 15:20	SNB9	**Daniel Heller** (Memorial Sloan Kettering Cancer Center) *Synthetic Molecular Recognition Optical Nanocarbon Sensors for Diagnostics*

10 minute break

Chair: Dan Heller

15:30 - 15:50	SNB10	**Ming Zheng** (National Institute of Standards and Technology) *Molecular Perceptron: Perception-Based Biosensing Using DNA-Wrapped Carbon Nanotube Arrays*
15:50 - 16:10	SNB11	**Sonia Freddi** (Univerisità Cattolica del Sacro Cuore) *Functionalized CNT-Based Sensors Platform for Breath Analysis Application*
16:10 - 16:30	SNB12	**Gili Bisker** (Tel Aviv University) *Protein Recognition Using Functionalized Fluorescent Single-Walled Carbon Nanotubes*

Coffee break CCW Lobby

Poster Sessions CCW Lobby Level

17:00 - 18:30	Poster Session 5 (odd poster numbers)
19:00 - 21:00	Poster Session 6 (even poster numbers)

Abstracts Thursday
(Oral)

Plenary Venue K4 (keynote)

Franconia Hall **Th 08:30 - 09:15**

Progress towards a carbon nanotube transistor logic technology

H.-S. Philip Wong[1]

[1]*Stanford University, Stanford, CA 94305*

Carbon nanotube (CNT) is a promising channel material for future nanometer-scaled transistors due to its inherently high mobility and injection velocity even at very thin body thickness (1-2 nm). CNT field-effect transistor (CNFET) is projected to enable 9x Energy-Delay-Product (EDP) benefits compared to FinFETs at the 7 nm technology node. Additional benefits come from the low processing temperature, which enable monolithic 3D integration to project 1,000x system-level EDP benefits. This talk will emphasize the recent challenges that have been overcome towards achieving these goals. First, understanding the physics behind hysteresis allowed us to reduce hysteresis to < 0.5% of the VGS sweep range regardless of the CNT-dielectric interface quality. Second, various studies have successfully demonstrated CNT-NFETs with low work-function metal oxides as gate dielectric or low work-function metals as source/drain contacts. Lastly, the measurement of statistical variation of contact resistance down to contact length of 10 nm enables an accurate projection for system-level analysis with the current contact technology. Further advancement will bring CNTs closer to a manufacturing technology and to realizing energy-efficient and high-performance next-generation technology.

Plenary Venue I12 (invited)

Franconia Hall **Th 09:15 - 09:40**

A better future for carbon nanomaterials?

Matteo Pasquali[1]

[1] *Department of Chemical & Biomolecular Engineering*
Department of Chemistry
Department of Materials Science & NanoEngineering
The Smalley-Curl Institute
Rice University, Houston, TX 77005

Carbon nanomaterials (in the sense of graphene and fullerenes) have been around for over three decades. Yet, despite their potential, their adoption continues to be minimal when compared to other carbon materials like carbon fibers, carbon black, and other synthetic carbon-based materials like polymers. Carbon Nanotubes are the poster child for the field. For a long time, their poor adoption was attributed to challenging synthesis, which impaired property control at the nanoscale, coupled with difficult processing, which prevented the translation of properties from the nanoscale to the macroscale. Yet, these hurdles were cleared almost a decade ago: reliable synthesis of high-quality CNTs was attained in the 2000s, and reliable processing and macroscale property demonstration was attained at the beginning of the 2010s. So, why is the field not taking off yet?

In my talk, I will discuss how the slow takeoff may be rooted in our view of CNTs and other carbon nanomaterials as having superior properties that will extend high-end applications and enable new ones. I will discuss how we have an opportunity to look at the field differently and recognize that, perhaps, CNTs and other nanomaterials can make a bigger impact by helping us solve our challenges in energy security and climate change. I will not suggest that we can capture carbon dioxide (CO_2) into CNTs, as this would exacerbate our energy challenge. Rather, I will discuss why carbon nanomaterials could be great candidates to utilize natural gas and other fossil hydrocarbons on a very large scale (GT/yr) to make materials with zero CO_2 footprint and positive hydrogen production. I will outline how such a future requires changing our perspective from that of superior, unique performance to one of high efficiency in synthesis and processing. I will sketch the scientific problems that need to be solved and will present an estimate of the potential benefits of such a transition in how we use fossil hydrocarbons.

Plenary Venue I13 (invited)

Franconia Hall **Th 09:40 - 10:05**

Dynamic Gating of Infrared Radiation in a Textile

YuHuang Wang[1]

[1] *University of Maryland, College Park, MD 20742 USA*

Our human body absorbs and loses heat largely through infrared radiation that peaks at around 10 μm. However, despite thousands of years' development, none of our clothing systems are capable of controlling this major heat exchange channel. The infrared properties of both clothing and our own skin are fixed at a nearly constant level, regardless of whether one feels hot or cold. In contrast, many species in nature have evolved elegant strategies to manipulate light for the purpose of cooling and surviving harsh environments. For instance, Saharan silver ants feature triangular shaped hairs that can reflect near-infrared rays according to the position of the sun to keep themselves cool, while the geckos of Madagascar have photonic skins with changeable colors that can blend in the environment to hide from predators. In this talk, I will discuss a clothing textile that is capable of dynamically gating infrared radiation through the fabric in response to personal thermal discomfort. We show that by simply coating triacetate-cellulose fibers with a thin layer of carbon nanotubes we can modulate the infrared radiation through the fabric by as much as 35% as a function of the relative humidity of skin. Both opportunities and challenges ahead will also be discussed if time permits.

Plenary Venue C8 (contributed)

Franconia Hall **Th 10:35 - 11:00**

Thermoelectric transport in polymer-functionalized semiconducting carbon nanotube films

Yoshiyuki Nonoguchi[1,2], Ami Takata[1], Chigusa Goto[1], Junichi Komoto[1], Tsuyoshi Kawai[1]

[1]*Nara Institute of Science and Technology*
[2]*JST PRESTO*

The application of carbon nanotubes in lightweight flexible thermoelectric materials has been demonstrated to keep pace with recent increased need for energy harvesting. However, there has been very little progress in understanding potential one-dimensional thermoelectric transport in nanotube films underlying the application. Here we report that semiconducting carbon nanotube films exhibit unique thermoelectric transport reflecting a quasi-one-dimensional band structure. Broadband absorption spectroscopy is utilized to link the thermoelectric properties of semiconducting carbon nanotubes to their electronic structures. Depending on doping level, the thermoelectric performance widely varies over the fifth-order conductivity range. Various controlling factors including polymer dispersants and chirality are examined for elucidating the intrinsic thermoelectric transport.

Plenary Venue C9 (contributed)

Franconia Hall **Th 11:00 - 11:25**

3D Al foam-enhanced graphene-based high voltage supercapacitor

Weizhong Qian[1]

[1] *Tsinghua University, Beijing, 100084,China*

Graphene, with high electrical conductivity, high surface area, exohedral surface and sufficient mesopore and high chemical stability, was proposed as an electrode of next generation EDLC supercapacitor with high energy density. Chemical vapour deposition method now offered graphene with high surface area, high yield, and high purity, making the fabrication of graphene-based supercapacitor more and more promising. However, low bulk density and large liquid intake of graphene bring unexpected great difficulties in fabricating an electrode sheet of graphene, with comparable property and performance to the conventional sheet of activated carbon with conventional processing method. This belongs to the important engineering of graphene, but is always neglected by scientists.

Here, we reported the use of 3D porous Al current collector to overcome the drawbacks of graphene in processing. Graphene-based supercapacitor (100 F-500 F soft pack) was prepared, which exhibited a volume energy density 3-4 times that of AC-based device with similar weight. We also discussed the improvement of ionic liquids electrolyte for the better low- temperature performance of supercapacitor.

Plenary Venue C10 (contributed)

Franconia Hall **Th 11:25 - 11:50**

Fast response Graphene/n-Si photodetector

Mattia Scagliotti[1,2], Matteo Salvato[1,2,3], Maurizio De Crescenzi[1,2], Nikolai G Kovalchuk[4], Ivan V Komissarov[4,5], Serghej L Prischepa[4,5], Daniele Catone[6], Lorenzo Di Mario[6], Maurizio Boscardin[7], Michele Crivellari[7], Paola Castrucci[1,2]

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[3]*CNR-SPIN Salerno, Università degli Studi di Salerno, Fisciano, I-84084, Italy*
[4]*Belarusian State University of Informatics and Radioelectronics, Minsk, 220013, Belarus*
[5]*National Research Nuclear University MEPhI, Moscow 115409, Russia*
[6]*Istituto di Struttura della Materia (ISM), CNR, Division of Ultrafast Processes in Materials (FLASHit), Rome, 00133, Italy*
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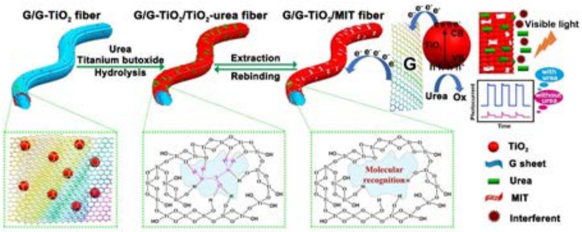
To surmount the limiting low efficiency in near UV and IR regions of Si photodetectors (PDs), and to improve its temporal response, we present a detector based on Graphene/n-Si hetero-junction. In this device graphene takes on a triple role: semi-transparent light window, Schottky junction constituent and photo charges collector. The designed PD multifinger geometry allows to obtain the typical I-V characteristics of a three terminals device, which can be used in photovoltaic (PV) and in photoconductive (PC) mode. To measure the PD ability in fast signals detection, a 35 femto-seconds pulsed laser system, has been used as light source by varying the incident wavelengths (from UV to IR) and energy. In the self-powered PC mode ($V_G = 0$) the measured rise time of the PD is ranged between 3 and 10 ns, that is comparable with commercial Si PDs. Moreover, applying a gate voltage $V_G = 0$, it is possible to make holes doping within the graphene and the PD external quantum efficiency hugely increases up to a value of 200%. Together, the rise time decreases down to a minimum value of about 1 ns, for all the investigated wavelengths. The obtained results are among the highest respect others graphene and carbon nanostructures-based devices.



Source-drain current I_{SD} vs. gate voltage V_G acquired in dark conditions for different values of V_{SD}. Inset: device schematic under illumination in PC mode.

Plenary Venue I14 (invited)

Franconia Hall **Th 11:50 - 12:15**

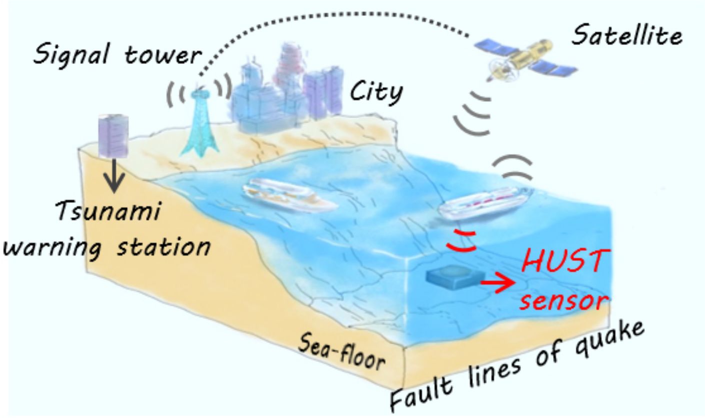
Advances in Structural Design of Three-dimensional Nanomaterials for the Extreme Environment Applications

Ming Xu[1]

[1] *School of Materials Science and Engineering, Huazhong University of Science and Technology, Wuhan 430074, China*

While downsizing the concept of structural design to nano-sized materials, their 3-D structures were conjugated in the specific way to improve the macro properties so as to meet the requirement of the potential applications [1-3]. Here, we demonstrated the CNT dry adhesive with the highest adhesion strength (~150N/cm^2) against almost all kinds of target surfaces by designing their adhesion surfaces to realize the nano-interlocking adhesion mechanism with rough asperities in heat [1]. Also, we fabricated self-powered, sea-water based electrochemical underwater pressure sensors for 1 mm to 30 m wave monitoring ()Figure 1)that show the sensitivity one order of magnitude higher than that of the most advanced oceanographic sensors in the report [4]. The concept of structural design would be extended to non-carbon nano-materials. By mimicking the human joint structure, we architected a super-elastic BN sponge possessing the operational temperature up to 1300 °C in oxygen.

[1] M. Xu et al. Science, 2010, 330, 6009
[2] M. Xu et al. Nat. Commun., 2016, 7, 13450
[3] X. Wan..,M. Xu & J. Shui et al, Nat. Catalysis 2019 (Online)
[4] A.Witze, Nature, 2017, 546, 466-468



Schematic of Self-powered, Sea-water Based Electrochemical Underwater Pressure Sensors for 1mm to 30m Wave Monitoring and its perspective use in Tsunami Early Warning System

Panorama 11 **Th 14:00 - 14:20**

Holey Single-Walled Carbon Nanotubes for Ultra-Fast Broadband Bolometers

Albert G. Nasibulin[1,4], Daria S. Kopylova[1], Fedor S. Fedorov[1], Alena ▯. Alekseeva[1], Evgenia P. Gilshteyn[1], Alexey P. Tsapenko[1], Anton V. Bubis[1], Artem K. Grebenko[1], Zakhar I. Popov[2], Pavel B. Sorokin[2], Yuriy G. Gladush[1], Anton S. Anisimov[3]

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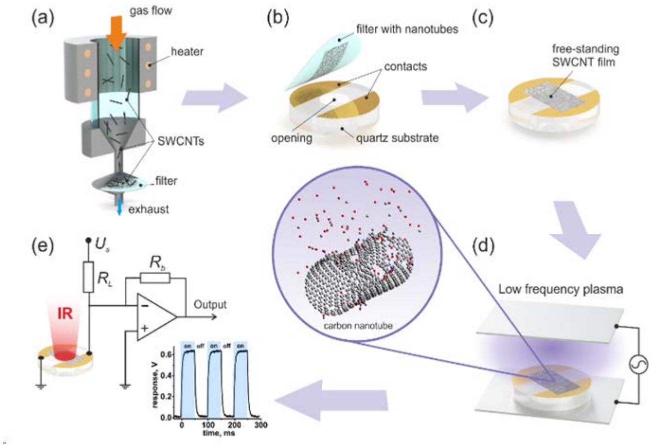
[2]*b. University of Science and Technology MISIS, Leninskiy prospect, 4, Moscow, 119049, Russia*
[3]*c. Canatu Ltd., Konalankuja 5, 00390, Helsinki, Finland*
[4]*d. Aalto University, Department of Applied Physics, 00076, Aalto, Finland*

Although carbon nanotubes have been already demonstrated to be a promising material for bolometric photodetectors, the sensitivity enhancement while maintaining the speed of operation remains a great challenge. Here, we present a holey carbon nanotube network, designed to improve the temperature coefficient of resistance for highly sensitive ultra-fast broadband bolometers. Treatment of carbon nanotube films with low frequency oxygen plasma allows fine tuning of electronic properties of the material. The temperature coefficient of resistance of our films is much greater than reported values for pristine carbon nanotubes, up to -2.8% K$^{-}1$ at liquid nitrogen temperature. The bolometer prototypes made of the treated films demonstrate high sensitivity in a wide IR range, short response time, smooth spectral characteristics and low noise level.



Fabrication of bolometer. a) aerosol CVD synthesis of SWCNTs; b) dry transfer onto a quartz substrate with an opening and Au contacts; c) formation of free-standing SWCNT films; d) oxygen plasma treatment; (e) bolometer prototype characterization.

Electronics Symposium SEI18 (contributed)

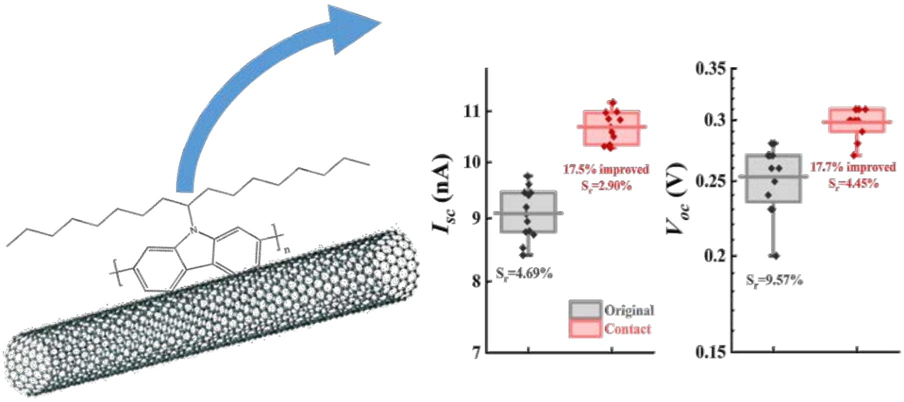
Panorama 11 **Th 14:20 - 14:40**

Improving Performance and Uniformity of Carbon Nanotube Network based Photodiodes via Yttrium Oxide Coating-and-decoating

Ze Ma[1], Jie Han[1], Sheng Wang[1], Lian-Mao Peng[1]

[1] *Key Laboratory for the Physics and Chemistry of Nanodevices and Department of Electronics, Peking University, Beijing, 100871, China*

Semiconducting single-walled carbon nanotube (SWCNT) thin film can be obtained by conjugated polymer wrapping sorting technique followed by solution deposition and can be utilized as channel materials of field-effect transistors and absorbing layer of photodiodes. However, after deposition process, there are still polymer molecules wrapping around nanotubes, remaining between nanotubes and remaining on the thin film surface, which will cause large nanotube-electrode resistance and tube-tube resistance. Here, we demonstrate an Yttrium oxide coating-and-decoating technique that can removes polymers only under electrodes and thus improves the performance of photodiodes without inducing new defects in device channel. Treating only contact area, the average short-circuit current of photodiode increases from 9.1 nA to 10.7 nA while the average open-circuit voltage increases from 0.25 V to 0.30 V. This method also improves device uniformity significantly.



Panorama 11 **Th 14:40 - 15:00**

Large Area Ion Sensitive Graphene Field Effect Transistors

Thomas Szkopek[1], Ibrahim Fakih[1], Farzaneh Mahvash[1], Boutheina Ghaddab[2], Alba Centeno[3], Amaia Zurutuza[3], Mohamed Siaj[2]

[1]*McGill University, Montréal, H3A0E9, Canada*
[2]*Université du Québec á Montréal, H2L 2C4, Montréal, Canada*
[3]*Graphenea Inc., San Sebastián, 20009, Spain*

Large-area graphene ion sensitive ion sensitive field effect transistors (ISFETs) have high mobility charge transport, reduced low-frequency noise with increasing transistor channel area, and enable facile integration with ion sensitive layers. Graphene ISFETs with an active area of approximately 1cm x 1cm have rms current noise as low as 5 ~ nA in a 60 Hz bandwidth, field effect mobilities up to 5000 $cm^2V^{-1}s^{-1}$ and quantum capacitance limited coupling between graphene channel and the sensing layer.

We have demonstrated graphene ISFETs selectively sensitive to H^+, K^+, Na^+, $NH_4^+$and Cl^-. In the case of H^+ sensing, metal oxides can be used to achieve Nernstian limited sensitivity with a 0.1 mpH resolution. Ion sensitive membranes based on ionophores can be used for selective sensing of other ionic species. For example, in the specific case of the K^+, real-time sensing was achieved using potassium ionophore III with a detection limit of 10^{-9}M [K^+], and a resolution of 10^{-3}log[K+]. Spiking experiments reveal good reversibility and stability. Graphene ISFETs are sufficiently sensitive and selective to measure the K^+ content of common beverages and blood samples.

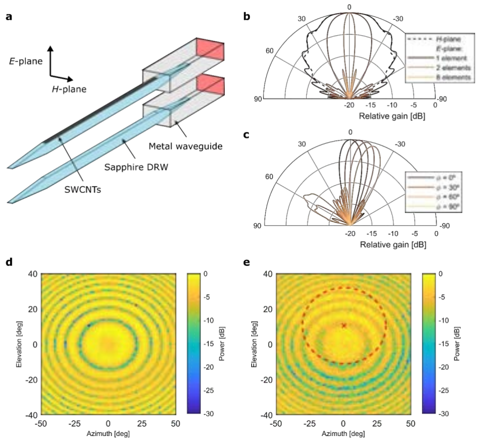
Panorama 11 **Th 15:00 - 15:20**

Thin Carbon Nanotube Layers for Terahertz Wave Applications

Dmitri Lioubtchenko[2], Serguei Smirnov[2], Mikhail Khodzitsky[3], Joachim Oberhammer[2]

[1]Center for Terahertz Research and Applications, Inst for High Pressure Physics, Warsaw
[2]Department of Micro and Nanosystems, KTH, Stockholm, Sweden
[3]Dep of Photonics and Optical Information Technologies, ITMO, Russia

The research and development of components in the 0.1-1.0 THz frequency region is extremely significant for a wide range of applications, such as telecommunication and imaging systems, material spectroscopy, medical imaging and treatments, etc. The state-of-the-art terahertz devices reveal serious problems with tunable materials. Carbon nanotubes offer unique properties due to their small dimensions and outstanding electrical properties that makes them very attractive for future THz applications. Here we introduce thin single-walled carbon nanotube (SWCNT) layers as a tunable impedance surface for millimeter and THz waves. SWCNT layers are integrated with dielectric rod waveguides. Their surface impedance, tuned by light, is shown to modify the wave propagation inside the waveguide. We experimentally demonstrate the phase shifting effect confirmed by numerical simulations. Additionally, we design and fabricate an antenna array of two dielectric waveguides, one covered in SWCNTs. The optically-controlled beam steering is enabled by SWCNTs and we provide directions for further device optimizations. These findings demonstrate thin SWCNT layers as an optically-reconfigurable element, suitable for broadband millimeter and THz wave communication systems.



SWCNT-based beam steering. a, Schematic geometry of the two-antenna array. b, c, Simulated and d, e, measured radiation patterns in the E and H-planes. The red cross and dashed circle are drawn as a guide to the eye to estimate the beam direction.

Electronics Symposium SEI21 (contributed)

Panorama 11 **Th 15:50 - 16:10**

Colloidal, Nanoelectronic State Machines Based on 2D Materials as Smart Aerosolized Probes and Recorders

Volodymyr Koman[1], Pingwei Liu[1], Daichi Kozawa[1], Albert Liu[1], Michael Strano[1]

[1]*Department of Chemical Engineering, Massachusetts Institute of Technology, USA*

A here-to-fore unexplored property of two-dimensional (2D) electronic materials is their ability to graft modular electronic functionality onto colloidal particles so as to access local hydrodynamics in fluids to impart mobility and enter spaces inaccessible to larger electronic systems. Herein, we demonstrate the design and fabrication of fully autonomous state machines (only 100x100x1 μm^3 in size) built onto a SU-8 particles powered by a 2D material-based photodiode. The on-board circuit connects a chemiresistor element and a memristor element, enabling the detection and storage of information after aerosolization, hydrodynamic propulsion to targets over 0.6 m away, and large area surface sensing of triethylamine, ammonia and aerosolized soot in inaccessible locations. An incorporated retro-reflector design allows for a facile position location using laser-scanning optical detection. Such state machines may find widespread application as probes in confined environments, such as the human digestive tract, oil and gas conduits, chemical and biosynthetic reactors, and autonomous environmental sensors.

Reference:

Nature Nanotechnology volume 13, pages 819–827 (2018).

Electronics Symposium SEI22 (contributed)

Panorama 11 **Th 16:10 - 16:30**

Enhancing optoelectronic performance of randomly oriented single walled carbon nanotube films for transparent and conducting applications

Alexey Tsapenko[1,2], Stepan Romanov[1], Daria Satco[1], Dmitry Krasnikov[1], Anastasia Goldt[1], Eugene Shulga[1], Zakhar Popov[3], Anton Anisimov[4], Pavel Sorokin[3], Esko Kauppinen[2], Albert Nasibulin[1,2]

[1]*Skolkovo Institute of Science and Technology, Nobel str. 3, 121205 Moscow, Russian Federation*
[2]*Aalto University, Department of Applied Physics, Puumiehenkuja 2, 00076 Espoo, Finland*
[3]*National University of Science and Technology "MISiS", Leninsky prospect 4, Moscow 119049, Russian Federation*
[4]*Canatu Ltd., Konalankuja 5, 00390, Helsinki, Finland*

Unique multifunctional nature of single-walled carbon nanotubes (SWCNTs) makes them nearly ideal candidate for applications in optoelectronics, including flexible and stretchable transparent conductive films (TCFs). Meanwhile, to be able to use all of these outstanding properties in modern transparent electrode applications, SWCNT-based TCFs have to demonstrate the optoelectrical performance at the level of the most dominant material for TCFs – indium tin oxide. This has not been achieved for SWCNTs yet and as a result limit their practical usage. Here, we propose various methods and techniques to enhance optoelectronic performance in a precise and controllable way, and thus, allowing to achieve the state-of-the-art results in the area of SWCNT-based TCFs. To realize that, we have shown the possibility to tune the film conductivity by means of doping parameter control, such as – temperature, film thickness, substrate, deposition techniques etc. Also, the understanding of the basic parameters of an ideal SWCNT film was presented along with the doping method comparison. Finally, the potential use of graphene as a flexible and transparent protective layer for the doped films was shown. This work was supported by Russian Foundation for Basic Research No. 18-32-00246.

Energy Symposium SEn17 (invited)

Franconia Hall **Th 14:40 - 15:00**

Construction of Carbon Interface for Electrical Energy Storage

Yanwu Zhu[1]

[1] *University of Science and Technology of China, Hefei, Anhui 230026, P. R. China*

Graphene and related materials have attracted much attention in the fields of electric energy storage. For the practical application in energy storage devices, tailoring the 3D carbon architectures is critical for achieving the comprehensively useful performance of the devices. In addition, constructing the carbon interface and understanding the interface is essential to further improve the performance. Herein our recent progress will be included in the talk, mainly focusing on the approach combining self-assembly and chemical processing developed for high volumetric performance of supercapacitor electrodes, high rate Li-ion battery electrodes and novel carbon monoliths with potentially new physical properties. Also, some recent progressing on the interface mechanisms towards understanding the kinetics of ions between graphene layers and probing the Li-ion deposition on single layer graphene will be discussed, based on ex-situ and in-operando techniques.

Energy Symposium SEn18 (contributed)

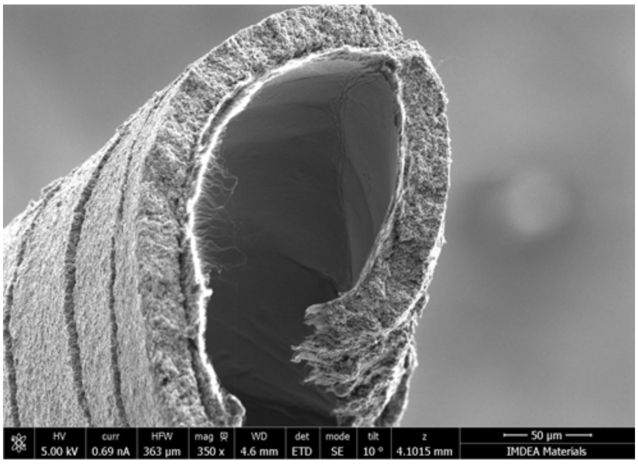
Franconia Hall **Th 15:50 - 16:10**

Operando characterisation of CNT fibre fabric-based electrodes and their application for high-toughness batteries

Juan Vilatela[1], Nicola Boaretto[1,2], Jesús Almenara[3], Anastasiia Mikhalchan[1], Rebeca Marcilla[2]

[1] *IMDEA Materials*
[2] *UC3M*
[3] *IMDEA Energy*

Macroscopic ensembles of nanocarbons, such as CNT fibres are characterized by a complex hierarchical structure combining crystalline regions with large porosity arising from imperfect packing of building blocks. Such structure is at the centre of a wide range of charge storage and transfer processes when CNT fibres are used as electrodes and/or current collectors1. This presentation starts with a description of a method to monitor structural descriptors of CNT fibres under in situ/operando electrochemical processes, based on wide and small angle X-ray scattering (WAXS/SAXS). It enables determination of parameters such as specific surface area, average pore size and average bundle size. In situ and ex situ WAXS/SAXS measurements during electrochemical swelling of CNT fibre electrodes continuously monitor the increase in effective surface area, in remarkable agreement with capacitance changes measured independently. The second part of the presentation presents result on the use of CNT fabrics as current collectors in battery electrodes, leading to superior specific capacity than commercial electrodes, combined with tensile toughness orders of magnitude above previous reports3. 1 Prog. Mat. Sci.; 2017, 89, 194-251; J. Mater. Chem. A; 2019, 7, 5305.3 Boaretto et al, submitted.



SEM micrographs of a battery electrode composite with CNT fibres

Panorama 13 **Th 14:00 - 14:40**

Electrostatically defined quantum devices in bilayer graphene

Luca Banszerus[1], Christoph Stampfer[1]

[1]*JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, 52074 Aachen Germany*

Graphene and bilayer graphene (BLG) are attractive platforms for quantum circuits. This has motivated substantial efforts in studying quantum dot (QD) devices based on graphene and BLG. The major challenge in this context is the missing band-gap in graphene, which does not allow confining electrons by means of electrostatics. A widely used approach to tackle this problem was to introduce a hard-wall confinement by etching the graphene sheet. However, the influence of edge disorder, turned out to be a road block for obtaining clean QDs. The problem of edge disorder can be circumvented in clean BLG, thanks to the fact that this material offers a tuneable band-gap in the presence of a perpendicularly applied electric field, a feature that allows introducing electrostatic soft confinement in BLG.

Here we present gate-controlled single, double, and triple dot operation in electrostatically gaped BLG. We show a remarkable degree of control of our device, which allows the implementation of two different gate-defined electron-hole double-dot systems with very similar energy scales. In the single dot regime, we reach the very few hole regime, extract excited state energies and investigate their evolution in a parallel and perpendicular magnetic field.

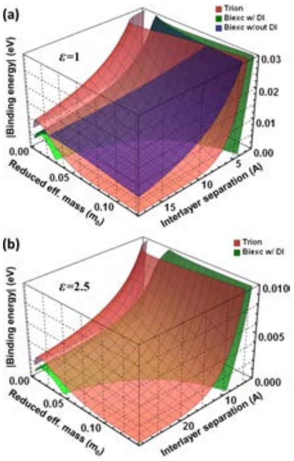
Panorama 13 **Th 14:40 - 15:00**

Interlayer Exciton Complexes in Planar Stacked Quasi-2D Heterostructures

Igor Bondarev[1], Maria Vladimirova[2]

[1]*Dept of Math and Physics, North Carolina Central University, Durham, NC 27707, USA*
[2]*Lab Charles Coulomb, Université de Montpellier, F-34095, Montpellier, France*

We discuss trion and biexciton complexes formed by interlayer (indirect) excitons in layered quasi-2D semiconductors. Indirect excitons – long-lived Coulomb-bound pairs of electrons and holes of different monolayers – were reported recently for bilayer graphene[1] and transition metal dichalcogenide systems[2]. We use the configuration space method[3] to derive the binding energies for the trion and biexciton complexes of indirect excitons as functions of the interlayer separation distance. The method captures essential kinematics of complex formation to reveal (and confirm recent observations[4]) that, despite a rapid decrease with distance, the binding energies of both complexes can be significant – up to a few tens of meV – for (typical) interlayer distances ~3-5 Å, with the trion always having a greater binding energy than the biexciton. Trions and biexcitons formed by indirect excitons control the formation of more complex Wigner-like electron-hole crystal structures which are of great interest for spin-optronics applications[5]. -- [1]J.I.A.Li, et al., Nat. Phys.13,751(2017); [2]M.Baranowski, et al., NL17,6360(2017); [3]I.V.Bondarev, M.R.Vladimirova, PRB97, 165419(2018), 1630006(2016); [4]APS Meeting 2018, Harvard group, unpublished; [5]J.S.Ross, et al., NL17,638(2017)



Binding energies of the biexciton and trion complexes as functions of the interlayer separation distance and the exciton reduced effective mass, calculated for (a) □ = 1 (with and with no long-range interaction terms included) and (b) □ = 2.5.

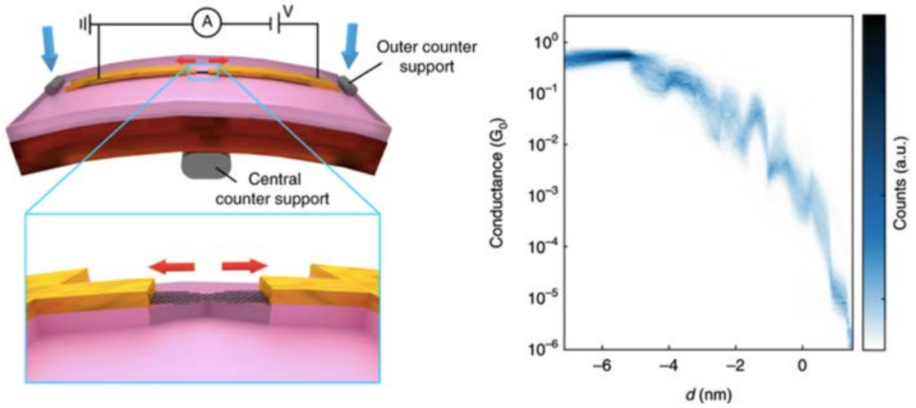
Panorama 13 **Th 15:00 - 15:20**

Mechanically Controlled Quantum Interference in Graphene Break Junctions

Sabina Caneva[1], Pascal Gehring[1], Martin Lee[1], Victor Garcia-Suarez[2], Amador Garcia-Fuente[2], Matthijs Hermans[1], Jaime Ferrer[2], Cees Dekker[1], Herre van der Zant[1]

[1] *Kavli Institute of Nanoscience, Delft University of Technology, Delft, The Netherlands*
[2] *Departamento de Física, Universidad de Oviedo, Oviedo, Spain*

Rich transport phenomena are predicted and have been experimentally confirmed in phase-coherent graphene nanoconstrictions, where the wave nature of electrons can give rise to various types of interference effects. Tuning the interference of electron waves has remained challenging primarily due to their manifestation at cryogenic temperatures in complex device architectures. Here we demonstrate mechanically controlled break junctions made from monolayer graphene and show that the electrical conductance of these bowtie-shaped nanoconstrictions displays pronounced oscillations at room temperature, with amplitudes that modulate over an order of magnitude as a function of sub-nanometer displacements. Surprisingly, the oscillations exhibit a period larger than the graphene lattice constant. Theoretical investigation shows that the periodicity originates from a combination of quantum-interference and lattice-commensuration effects of two graphene layers that slide across each other. The experimental results are in excellent agreement with charge-transport calculations and, importantly, provide direct experimental observation of Fabry-Pérot-like interference of electron waves that are partially reflected/transmitted at the edges of the graphene bilayer overlap region.



Left: Schematic of the graphene mechanically controlled break junction. Right: 2D histogram of conductance vs displacement

2D Materials Symposium S2D21 (contributed)

Panorama 13 **Th 15:30 - 15:50**

Room Temperature Initialisation and Readout of Intrinsic Spin Defects in a Van der Waals Crystal

Andreas Sperlich[1], A. Gottscholl[1], M. Kianinia[2], V. Soltamov[1], C. Bradac[2], C. Kasper[1], K. Krambrock[3], M. Toth[2], I. Aharonovich[2], V. Dyakonov[1]

[1]*Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg, Germany*
[2]*School of Mathematics and Physical Sciences, University of Technology Sydney, Ultimo, NSW 2007, Australia*
[3]*Departamento de Física, Universidade Federal de Minas Gerais (UFMG), Belo Horizonte, MG, Brazil*

Optically addressable spins in wide-bandgap semiconductors have become one of the most prominent platforms for exploring fundamental quantum phenomena. Although optically accessible spin states in 2D materials, such as hexagonal boron nitride (hBN) are theoretically predicted, they have not yet been observed experimentally. Here, employing rigorous electron paramagnetic resonance techniques and photoluminescence spectroscopy, we identify fluorescence lines in hBN associated with a particular defect, the negatively charged boron vacancy, and determine the parameters of its spin Hamiltonian. We show that the defect has a triplet (S = 1) ground state with a zero-field splitting of $\sim$3.5 GHz and establish that the centre exhibits optically detected magnetic resonance (ODMR) at room temperature and optically pumped spin polarization.

2D Materials Symposium S2D22 (invited)

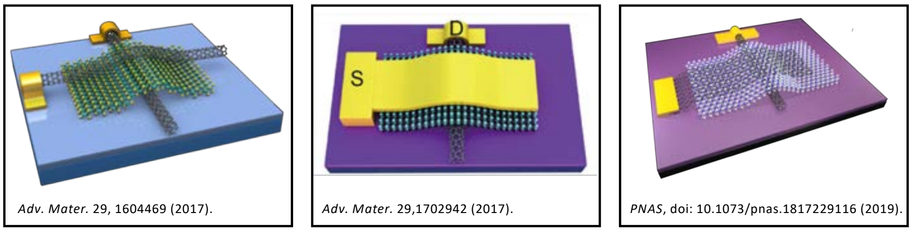
Panorama 13 **Th 15:50 - 16:10**

Mixed-dimensional van der Waals heterostructures based on carbon nanotubes and 2D materials

Yang Wei[1], Jin Zhang[1], Ke Zhang[1], Kaili Jiang[1], Shoushan Fan[1]

[1]*Department of Physics and Tsinghua-Foxconn Nanotechnology Research Center, Tsinghua University, Beijing 100084, P. R. China*

Mixed-dimensional van der Waals (vdW) heterostructures are important and promising, since low-dimensional nanomaterials, such as one-dimensional (1D) nanomaterials and layered 2D materials, have exhibited significance for their respective unique electronic and optoelectronic properties. Here, mixed-dimensional vdW heterostructures are developed with 1D carbon nanotubes (CNTs) and 2D semiconductors as building blocks. Some facile architectures were developed, such as vertical point heterostructure (VPH), CNT-confined vertical heterostructure (CCVH), and CNT–WSe_2–graphene heterostructure, in which 2D semiconductors are symmetrically sandwiched by two metallic SWCNTs, or asymmetrically sandwiched by a metallic SWCNT and a metal electrode/graphene. The VPH can be applied as photodetectors with ultra-high spatial resolutions, since it can map the Gaussian distribution of a focused laser beam. The CCVHs have reconfigurable transport properties, as the Fermi level of SWCNTs can be efficiently modulated by the gate voltage. The spatial resolution of CNT–WSe_2–graphene photodetector can be electrically switched between high-resolution mode and low-resolution mode. Therefore, the 1D/2D mixed heterostructures shows great potentials in future nanoelectronics and nano-optoelectronics.



Adv. Mater. 29, 1604469 (2017).

Adv. Mater. 29,1702942 (2017).

PNAS, doi: 10.1073/pnas.1817229116 (2019).

Figure 1. Mixed-dimensional van der Waals heterostructures with CNT and 2D materials.

2D Materials Symposium S2D23 (contributed)

Panorama 13 **Th 16:10 - 16:30**

A Dirac fermion wave reflector based on the laws of geometrical optics

Bernard Plaçais[1]

[1] *Laboratoire de Physique de l'ENS, 24, rue Lhomond, 75005 Paris, France*

Spectroscopy Symposium SSp6 (overview)

Panorama 12 **Th 14:00 - 14:40**

Optical Spectroscopy of Individual Carbon Nanotubes with Defined Chirality

Kaihui Liu[3]

[1]*Peking University, Beijing, 1000871, China,*

When the characteristic length of a material shrinks to 1 nm scale, many distinct physical phenomena, such as quantum confinement, enhanced many-body interactions and strong van der Waals inter-material couplings, will appear. To investigate the related fascinating low-dimensional physics, we need a tool to quantitatively link the atomic structures to the physical properties of these very small nano-materials. In this talk, I will introduce our recently developed in-situ TEM + high-sensitive ultrafast nano-optics technique, which combines capability of structural characterization in TEM and property characterization in nano-optics on the same individual nanomaterials. Several examples of using this technique to study the 1D carbon nanotube system will be demonstrated.

Spectroscopy Symposium SSp7 (invited)

Panorama 12 **Th 14:40 - 15:00**

Controlling the inner dielectric environment of carbon nanotubes to tune their optical properties

Sofie Cambré[1], Jochen Campo[1,2], Bea Botka[1], Wouter van Werveke[1], Wim Wenseleers[1], Jan Obrzut[2], Jeffrey A. Fagan[2]

[1]*Experimental Condensed Matter Physics, University of Antwerp, Belgium*
[2]*NIST, Materials Science and Engineering Division, Gaithersburg, USA*

The optical properties of single-wall carbon nanotubes (SWCNTs) are extremely sensitive to their external and internal environment. For example, filling of the endohedral cavity results in characteristic shifts and broadening of both the radial breathing mode vibrational frequency and the optical transitions.[1] Solvent ingestion effects are substantial, and can also be used to passivate the nanotube interior, by controlled filling prior to dispersion.[2]
Here, specific and tunable modification of the optical properties of SWCNTs is demonstrated through the direct encapsulation of more than 30 different guest molecules with widely varying dielectric constants. The spectroscopic analysis of these filled SWCNTs, in comparison to empty SWCNTs, demonstrates that the general effect of filler static dielectric constant on the SWCNTs' optical properties corresponds to a monotonic red shifting of the optical transitions with increased magnitude for higher dielectric constants. In addition to these spectral shifts, the filling also reveals a general increase of fluorescence intensity with lower dielectric constants.

[1] S Cambré et al Phys Rev Lett 104, 207401 (2010); S Cambré et al ACS Nano 6, 2649 (2012)
[2] J Campo et al Nanoscale Horizons 1, 317 (2016)

Spectroscopy Symposium SSp8 (contributed)

Panorama 12 **Th 15:00 - 15:20**

Temperature Change of Water Adsorption Layer on Suspended Single-walled Carbon Nanotube

Yoshikazu Homma[1], Yuta Saito[1], Yuichirou Tanaka[1], Genta Yamaguchi[1], Shohei Chiashi[2]

[1] *Department of Physics, Tokyo University of Science, Tokyo 162-8601, Japan*
[2] *Department of Mechanical Engineering, The University of Tokyo, Tokyo 113-8656, Japan*

Water adsorption with 2 molecular layers occurs on a SWCNT in atmosphere [1]. This is a 2D phase of water formed in van der Waals potential of the non-polar SWCNT surface. Because the hydrogen bonding arrangement in the layer is different from that of bulk water, the structure change at low temperature is of great interest. We investigated temperature change of the adsorption layer on suspended SWCNTs with various chiralities using photoluminescence spectroscopy at low temperatures. The emission energy exhibited type-dependent change, i.e., type-I and type-II showed constant decrease and increase, respectively, of emission energy with decreasing temperature. This indicated that SWCNTs were imposed compressive strain with decreasing temperature. Furthermore, the chiral angle dependence was not symmetric between type-I and type-II, which could be explained by the increase of dielectric constant of the adsorption layer due to an increase in the density with decreasing temperature. Thus, the combination of strain and environmental effects caused the complicated behavior of the temperature dependence of the emission energy. The 2D phase of water on the SWCNT surface can be regarded as a solid phase rather than a liquid phase.
[1] Y. Homma et al. Phys. Rev. Lett. 110, 157402 (2013).

Panorama 12 **Th 15:30 - 15:50**

Exciton Physics in Air-Suspended Carbon Nanotubes

Yuichiro Kato[1,2]

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[2]*Quantum Optoelectronics Research Team, RIKEN, Saitama 351-0198, Japan*

Electron-hole pairs form tightly-bound excitons in single-walled carbon nanotubes, and these excitons play a central role in optical processes. Air-suspended nanotubes, in particular, provide opportunities for elucidating the properties of excitons because of their pristine nature. The mobile excitons exhibit long diffusion lengths, and in combination with the increased scaling due to one-dimensionality, high diffusivity results in efficient exciton-exciton annihilation [1]. Interestingly, these excitonic processes give rise to antibunching at room temperature [2]. By integrating individual nanotubes into field-effect devices, carriers can be introduced to generate trions [3]. Measurements of photoconductivity have revealed field-induced activation of dark states as well as the continuum states [4]. Using split-gate devices, electroluminescence from cold excitons can be observed [5].

[1] A. Ishii, M. Yoshida, Y. K. Kato, Phys. Rev. B 91, 125427 (2015).
[2] A. Ishii, T. Uda, Y. K. Kato, Phys. Rev. Appl. 8, 054039 (2017).
[3] M. Yoshida, A. Popert, Y. K. Kato, Phys. Rev. B 93, 041402(R) (2016).
[4] T. Uda, M. Yoshida, A. Ishii, Y. K. Kato, Nano Lett. 16, 2278 (2016).
[5] N. Higashide, M. Yoshida, T. Uda, A. Ishii, Y. K. Kato, Appl. Phys. Lett. 110, 191101 (2017).

Spectroscopy Symposium SSp10 (invited)

Panorama 12 **Th 15:50 - 16:10**

Shaping Nanotubes and Nanowires with Surfaces for Electronics and Optoelectronics

Ernesto Joselevich[1]

[1] *Weizmann Institute of Science, Rehovot 76100, Israel*

The large-scale assembly of nanotubes (NTs) and nanowires (NWs) with controlled geometries on surfaces remains one challenge toward their integration into practical devices. Following our earlier work on the guided growth of carbon nanotubes, we reported the growth of perfectly aligned, millimeter-long, horizontal NWs of various semiconductor materials with controlled crystallographic orientations on different substrates. The growth directions and crystallographic orientation of the NWs are controlled by their epitaxial relationship with the substrate, as well as by a graphoepitaxial effect that guides their growth along surface steps and grooves. We demonstrated the massively parallel self-integration of NWs into circuits via guided growth. Here we will show how guided nanowires with complex morphologies and heterostructures can be used for the bottom-up fabrication of nano-optoelectronic devices, including photodetectors, photodiodes and photovoltaic cells. Lastly, we also show how surfaces induce the spontaneous self-organization of carbon nanotube coils, which could be used as electromagnets and dynamos. These findings highlight the potential of surface-guided growth as a general approach for the large-scale integration of NTs and NWs into a wide range of functional systems.

Panorama 12 **Th 16:10 - 16:30**

Decay Dynamics and Diffusion Properties of Bright and Dark Excitons in Air-Suspended Carbon Nanotubes

Akihiro Ishii[1,2], Hidenori Machiya[1,3], Yuichiro K. Kato[1,2]

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[2]Quantum Optoelectronics Research Team, RIKEN, Saitama 351-0198, Japan
[3]Department of Electrical Engineering, The University of Tokyo, Tokyo 113-8656, Japan

We investigate exciton dynamics of parity-odd bright state and parity-even dark state by performing time-resolved photoluminescence measurements on defect-free as-grown carbon nanotubes. The emission decay curves exhibit bi-exponential behavior, where the fast and slow decay components arise from the dynamics of bright and dark excitons, respectively. We analyze such exciton dynamics using a three-level model including the effects of end quenching by measuring chirality-identified nanotubes with different suspended lengths [Fig. 1]. We find that bright excitons have lifetimes of ~80 ps and diffusion lengths of ~400 nm, consistent with the known values. In comparison, dark excitons have much longer lifetimes in the order of nanoseconds, and their diffusion lengths are too long to experimentally determine. We also observe chirality dependence of diffusion coefficient and bright-dark transition rate, giving further insight into the nature of excitons.

References

[1] A. Ishii, H. Machiya, Y. K. Kato, manuscript in preparation.
[2] A. Ishii, T. Uda, Y. K. Kato, Phys. Rev. Appl. 8, 054039 (2017).
[3] A. Ishii, M. Yoshida, Y. K. Kato, Phys. Rev. B 91, 125427 (2015).

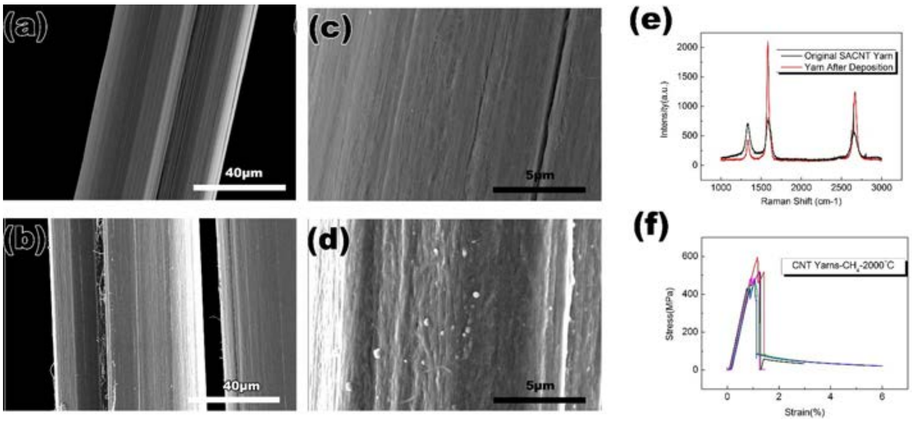

Fig.1 Emission decay curves obtained from (9,8) nanotubes with various lengths ranging from 0.5 μm (purple) to 4.2 μm (red). The gray line is the instrument response. (inset) Schematic of the three-level model for exciton decay dynamics.

NanoBio Symposium SNB6 (invited)

Panorama 10 **Th 14:00 - 14:20**

The advantages of carbon nanomaterials for bone tissue engineering

Eri Hirata[1]

[1]*Graduate School of Dental Medicine, Hokkaido University, Sapporo 060-8586, Japan*

Carbon nanomaterials (CNMs), including carbon nanotubes (CNTs) carbon nanohorns (CNHs) and graphene, have gained great attention in the scientific community due to their unique physico-chemical properties, which could also be promising in many biomedical-related fields. Because of their high biocompatibility, use of CNMs in biomedical applications is widely anticipated. We have been studying CNMs for bone tissue engineering.

We previously reported that CNT-coated collagen sponges have a favorable biocompatibility profile for bone tissue. Biodistribution of CNTs locally implanted in mice was also investigated by near-infrared (NIR) fluorescence imaging and transmission electron microscopy (TEM). The mechanism of the bone formation by CNHs is also discussed.

In this presentation, the advantages of using carbon-based nanomaterials in bone tissue engineering will be shown.

Panorama 10 **Th 14:20 - 14:40**

Carbon Nanotubes impact Microglia function and phenotype

Silvana Fiorito[1,2]

[1] *Inst. Traslational Pharmacology, CNR -Via Fosso del Cavaliere 100 - 00133 Rome, Italy*
[2] *Dept. Clinical Medicine, Sapienza University, 00185 Rome, Italy*

CNTs have been recently investigated for applications in nervous tissue engineering. Microglia are considered as the brain's resident immune cells that are activated in response to inflammatory stimulations and neurological injuries. Microglia "M1" phenotype is involved in the regulation of brain development by enforcing, through the production of pro-inflammatory molecules, the elimination of damaged neural cells. Microglia "M2" phenotype enhances neuronal survival through the release of trophic and antiinflammatory factors and cytokines and is involved in neurogenesis. We demonstrated that electro-conductive MWCNTs (a-MWCNTs) increase significantly the release of proinflammatory factors (NO, iNOS) and cytokines (IL-1b,TNF-a) by microglia after 24 h exposure. This activity decreased at 48 h while a shift to an increase of antiinflammatory cytokines (IL-10 and TGF-b1) and neurotrophic factors (mNGF) occurred. In a-MWCNT exposed cells, the "M2" phenotype was particularly expressed at 48 h, and most of them were found to be bipolar/rod-shaped with a neuro-protective role. The transition to "M2" phenotype microglia and the release of anti-inflammatory cytokines and neurotrophic factors seem extremely important to support the capacity of these CNTs to modulate microglia behavior

NanoBio Symposium SNB8 (contributed)

Panorama 10 **Th 14:40 - 15:00**

Quantitative evaluation of the biodegradation of single-wall carbon nanotubes in the mouse lung and liver

Minfang Zhang[1], Ying Xu[1], Mei Yang[1], Masako Yudasaka[1,2], Toshiya Okazaki[1]

[1]*National Institute of Advanced Industrial Science and Technology (AIST)/Tsukuba, Japan*
[2]*Meijo University, Nagoya, Japan*

Carbon nanotubes (CNTs) have been demonstrated as promising nanomaterials for a wide range of applications from materials and electronics to nanomedicine. However, the toxicity of CNTs has not been fully understood especially the long-term toxicity and the degradation in vivo. Recently, we have developed a quantification method to investigate the biodistribution of CNTs in the mouse by using NIR optical absorption. With this method, we have quantitatively investigated the fate of single-wall CNTs (SWNTs) in the lung and the liver after single intravenous injection into mice. Our results showed that almost SWNTs in the lungs and that of about 15 wt % in the liver were removed within 60 days. The measurement results of cytokines of TGF-β1, IL-6, INF-γ, and TNF-α in blood plasma and tissue lysates indicated there are no significant differences between the groups of control and SWNTs injected mice, suggesting the low toxicity of SWNTs.

NanoBio Symposium SNB9 (contributed)

Panorama 10 **Th 15:00 - 15:20**

Synthetic Molecular Recognition Optical Nanocarbon Sensors for Diagnostics

Daniel Heller[1,2], Januka Budhathoki-Uprety[3]

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[3]North Carolina State University, Raleigh, NC, 27606, USA

We investigated a synthetic molecular recognition optical nanosensor for the quantitative measurement of proteins in patient biofluids. The sensor was comprised of photoluminescent single-walled carbon nanotubes cloaked with a carboxylate-functionalized polycarbodiimide polymer--materials that afford the relative ease of production, storage, handling, stability, and robustness as compared to antibodies used in current methods. The rapid sensor response under ambient conditions in minimally processed urine samples suggests that this sensor may facilitate diagnosis in point-of-care and resource-limited settings. We also found that the nanocarbon sensor can be integrated into a matrix material, potentially opening new opportunities for the engineering of point-of-care and wearable devices for clinical and field uses.

NanoBio Symposium SNB10 (invited)

Panorama 10 **Th 15:30 - 15:50**

Molecular Perceptron: Perception-based Biosensing using DNA-wrapped Carbon Nanotube Arrays

Ming Zheng[1]

[1]*National Institute of Standards and Technology, Maryland 20899, USA*

In this talk, I will present our recent work in developing new spectroscopy and separation method to obtain DNA sequences that are capable of resolving different CNT structures. I will then present a multiplex sensing scheme we call “molecular perceptron”, which is based on an array of DNA-CNT hybrids to mimic human perception systems for biosensing applications.

NanoBio Symposium SNB11 (contributed)

Panorama 10 **Th 15:50 - 16:10**

Functionalized CNT-based sensors platform for breath analysis application

Sonia Freddi[1,2], Stefania Pagliara[1,2], Giovanni Drera[1,2], Aleksei Emelianov[3,4], Ivan Bobrinetskiy [3,5], Daria Kopylova [6], Maria Chiesa[1], Paolo Montuschi[7], Albert Nasibulin[6], Luigi Sangaletti[1,2]

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[2] *Surface Science and Spectroscopy Lab @ I-Lamp, Brescia, Italy*
[3] *National Research University of Electronic Technology, Moscow, 124498, Russia*
[4] *P.N. Lebedev Physical Institute of the Russian Academy of Sciences, Moscow, 119991, Russia*
[5] *BioSense Institute, University of Novi Sad, Dr Zorana Djindjica 1a, 21000 Novi Sad, Serbia*
[6] *Skolkovo Institute of Science and Technology, Moscow 143026, Russia*
[7] *Fondazione Policlinico A. Gemelli, Largo Francesco Vito, 1, 00168 Roma, Italy*

Breath analysis is a powerful method in the diagnostic of many diseases, since it allows the detection of the most common volatile organic compounds (VOCs), and it is expected to be a non-invasive and a real-time monitoring technique. The effort to develop methods and devices for breath analysis is quite intense nowadays, and, among the devices for breath testing, electronic noses may become an important resource in the diagnostics of some diseases or in health screening programs.

An array of 8 CNT sensors, functionalized with organic molecules, has been produced to explore applications in the field of breath analysis. The array was exposed to a set of target gas molecules relevant to specific diseases (e.g. ammonia, nitrogen dioxide, hydrogen sulfide, benzene, acetone, ethanol…), and the data analysis was carried out on the basis of the principal component analysis (PCA) approach. Then, tests on the exhaled breath from healthy volunteers and volunteers with chronic obstructive pulmonary diseases (COPD) have been carried out, and the capability of this sensors array to discriminate the breath fingerprint of healthy and sick patients has been demonstrated.

NanoBio Symposium SNB12 (contributed)

Panorama 10 **Th 16:10 - 16:30**

Protein recognition using functionalized fluorescent single-walled carbon nanotubes

Gili Bisker[1,2,3]

[1]Department of Biomedical Engineering, Tel Aviv University, Israel
[2]Tel Aviv University Center for Nanoscience and Nanotechnology
[3]The Center for Physics and Chemistry of Living Systems at Tel Aviv University

Single-walled carbon nanotubes (SWCNTs) have unique optical and physical properties, and they benefit from the ease of surface functionalization and biocompatibility. Semiconducting SWCNTs fluoresce in the near-infrared (nIR) part of the spectrum, which overlaps with the tissue transparency window. The SWCNTs fluorescence is sensitive to the environment, and depending on the surface functionalization, subtle changes in the proximity of the nanotube can result in significant spectral modulations. Hence, SWCNTs can be utilized as optical sensors enabling real-time optical detection. I will present two recent discoveries of protein detection using SWCNTs functionalized with variants of poly(ethylene glycol). Using high-throughput screening against a panel of human blood proteins, we have discovers sensors for the proteins fibrinogen and insulin. The recognition also occurs in serum environment, showing that the SWCNTs sensors work in this complex environment despite the potential nonspecific adsorption. These results open new avenues for synthetic recognition of biological macromolecules, and hold great promise for medical and clinical applications.

Reference

1. Gili Bisker et. al., ACS Sensors, 3(2), 367-377 (2018).
2. Gili Bisker et. al., Nature Communications, 7 (2016).

Abstracts Thursday (Poster)

P001 **Th 17:00 - 18:30**

Superdurabe and Superelastic Carbon Nanotubes on the Macroscale

Yunxiang Bai[1], Rufan Zhang[1], Fei Wei[1]

[1] *Beijing Key Laboratory of Green Chemical Reaction Engineering and Technology, Tsinghua University, Beijing, 100084, China.*

Superstrong materials with outstanding fatigue-resistance are in great demand in a variety of high-end applications. An ultrahigh tensile strength of over 100 GPa of individual CNTs has been demonstrated. Nevertheless, to our best knowledge, no experimental and corresponding theoretical law study have been simultaneously carried out to investigate the intrinsic fatigue behavior of defect-free CNTs on the macroscale. Herein, an acoustic-resonance-test (ART) system was designed to investigate the tensile fatigue behavior of individual centimeters-long defect-free CNTs. An ultrahigh fatigue-resistance (without failure after being applied a stress of 95% of the CNT static strength of over 100 GPa for over 10^7 cycles), as well as a supertoughness about 8 GJ/m^3, could be reached at the same time, and CNTs could recover their original shape with very fast speed even at a near-threshold strain. We ascribe the simultaneously obtained various mechanical superiorities of CNTs to the unprecedented low-dimentional defect-free highly-symmetric entire-surface-carbon covalent structure. Our results shine light on more reliable CNT devices, engineering applications and provide an analysis framework to develop the superstrong materials with superdurable property as well.

P003 **Th 17:00 - 18:30**

The electrical and thermal transport at the interface between Sb2Te3 and graphene heterostructures

Seongkyun Kim[1], Seongkyun Kim[2], Wonjae Jeon[3], Krishna P.Dhakal[1], Jeongyong Kim[1,4], Seunghyun Baik[2,4]

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[2] *School of Mechanical Engineering, Sungkyunkwan University, Suwon 16419, Korea*
[3] *Institute of Advanced Machinery and Technology, Sungkyunkwan University, Suwon 16419, Korea*
[4] *Center for Integrated Nanostructure Physics, Institute for Basic Science (IBS), Suwon 16419, Korea*

Hetero-structured 2-dimensional materials have received considerable attention recently. The electrical and thermal transport at the interface of such devices plays an important role in the device performance. Here we directly synthesized single-crystalline Sb_2Te_3 nanoplates (NPs) on graphene by the solvothermal method based on the lattice similarity. Interestingly, the size of Sb_2Te_3 NPs increased as the grain size of graphene increased. The electrical transport was investigated by conducting atomic force microscopy, and the thermal transport was characterized by Raman thermometry. The Ohmic contact was realized between the Sb_2Te_3 NP and graphene. However, a limited thermal boundary conductance was observed. The thermal transport mechanism was investigated by the lattice and acoustic mismatch analysis. Both the electrical and thermal contact was poor when Sb_2Te_3 NPs were simply transferred on graphene, demonstrating the importance of interface construction method for device performance. A recent progress in the laboratory will also be presented.

P005 **Th 17:00 - 18:30**

Unravelling Effect of Carbon Nanotube Powders by Highly Viscous Liquids

Kazufumi Kobashi[1], Atsuko Sekiguchi[1], Takeo Yamada[1], Toshiya Okazaki[1]

[1]*AIST, CNT-Application Research Center, Tsukuba, 305-8565, Japan*

Commercialized CNT powders have been vigorously used in recent years. However, many of the CNT dispersing processes unexpectedly led to deterioration in the qualities and the inhomogeneous states in matrices. Here unravelling CNT powders prior to distributing them in matrices would be crucial to fully utilize the intrinsic CNT properties.

Thus we investigated unravelling effect of as-grown CNT powders by viscous liquids. A simple method used is agitating Super Growth-CNT powders at rt by a stir bar in solvents with various viscosities like alcohols, silicone oils, ionic liquid, ketone, hydrocarbons, aprotic polar solvents, and water. Regardless of solvent polarity, more viscous liquids gave more blackish suspensions, indicative of more unravelled CNT particles. Interestingly a blackish suspension was made in propylene glycol at rt, but not obtained at 65 °C with the decreased solvent viscosity. By NMP and DMF with low viscosities, a blackish suspension was not formed, while they are known as good solvents for CNTs (Fig. 1a). These results clarified the unravelling effect by viscous liquids. To quantitatively verify this finding, we measured CNT particle numbers in the suspensions by particle image analyzer, revealing higher numbers with higher solvent viscosities (Fig. 1b).

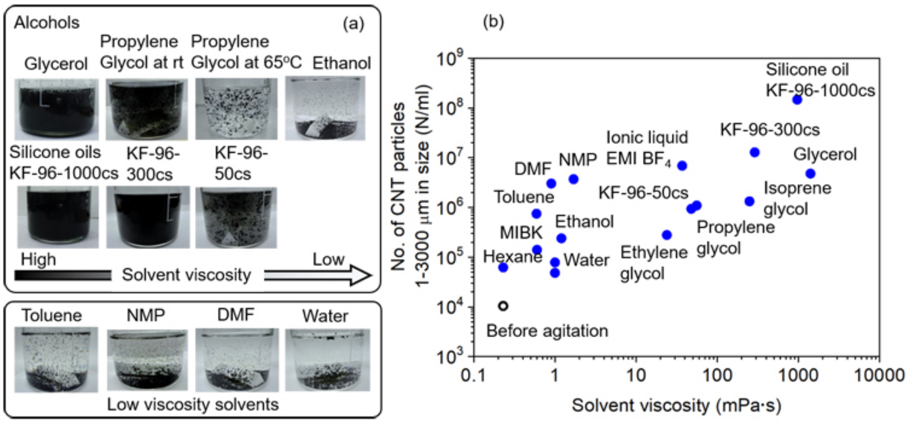

Fig. 1 (a) Photos of CNT suspensions agitated in solvents with various viscosities at CNT concentration of 0.01wt% by a stir bar for 3h, and (b) relationship of CNT particle number in the suspensions and solvent viscosity.

Plenary Venue Poster

P007 **Th 17:00 - 18:30**

A Mass-scale Growth of Carbon Nanofiber Mats over Copper Catalysts

Jarrn-Horng Lin[1], Chung-Hsuan Hsiao[1]

[1]*National University of Tainan, Taiwan.*

Carbon nanomaterials were widely used in flexible and wearable electronics, however, how to fabricate several components using lay-by-layer assembling at low temperatures in flexible and wearable electronics still remains great challenges. Herein, we explore a simple method to directly fabricate CNF mats on any substances, e.g. carbon fiber, copper foil, silicon wafer, and slide glass, using copper catalysts at 200 °C under a stream of argon-diluted acetylene. Thermal sublimation of copper precursors on substrates at 150-190 °C, then follow a heat-treatment at 200-250 °C with a stream of argon-diluted acetylene. Sublimation conditions, treated temperatures for the formation of amorphous carbons, and growth parameters in the generation of CNF mats are discussed. As our findings, this approach can lead to the integration of CNF mats on any substrates at low temperatures and promisingly benefit applications in flexible and wearable electronics.

P009 **Th 17:00 - 18:30**

Carbon Nanotube Film Gate in Vacuum Electronic Devices

Peng Liu[1]

[1] *Tsinghua University*

A superaligned carbon nanotube (SACNT) film can act as an ideal gate electrode in vacuum electronics due to its low secondary electron emission, high electron transparency, ultrasmall thickness, highly uniform electric field, high melting point, and high mechanical strength. We used a SACNT film as the gate electrode in a thermionic emission electron tube and field emission display prototype. The SACNT film gate in a thermionic emission electron tube shows a larger amplification factor. A triode tube with the SACNT film gate is used in an audio amplification circuit. The SACNT film gate electrode in field emission devices shows better field uniformity. The field emission display prototype is demonstrated to dynamically display Chinese characters.

P011 **Th 17:00 - 18:30**

Photo-driven nanoactuators based on carbon nanocoil and vanadium dioxide bimorph

He Ma[1]

[1] *Beijing University of Technology, College of Applied Science, Beijing*

Photo-driven actuators are highly desirable in various smart systems owing to the advantages of wireless control and possible actuation by solar energy. Miniaturization of photo-driven actuators is particularly essential in micro-robotics and micro-/nano-electro-mechanical systems. However, it remains a great challenge to build up nano-scale photo-driven actuators with competitive performance in amplitude, response speed, and lifetime. In this work, we developed photodriven nanoactuators based on bimorph structures of vanadium dioxides (VO_2) and carbon nanocoils (CNCs). Activated by the huge structural phase transition of VO_2, the photo-driven VO_2/CNC nanoactuators deliver a giant amplitude, a fast response up to 4500 Hz, and a long lifetime more than 10,000,000 actuation cycles. The excellent photothermal conversion efficiency of CNCs enables a low light-triggering threshold of VO_2/CNC nanoactuators. Our photo-driven VO_2/CNC nanoactuators would find potential applications in nano-scale electrical/optical switches and other smart devices.

P013 **Th 17:00 - 18:30**

In situ TEM observation of CNT formation via plastic deformation

Hideki Masuda[1], Yu Kikuchi[1], Kanade Matsuo[1], Toshihiko Fujimori[2], Takeshi Hikata[2], Soichiro Okubo[2], Yoshikazu Ito[1], Jun-ichi Fujita[1]

[1]*Univ. of Tsukuba, Ibaraki, 305-8573, Japan*
[2]*Sumitomo Electric Industries, Ltd., Osaka, 554-0024, Japan*

Demand for ultra-long CNTs has been increasing to apply CNT to bulk assemblies while maintaining the high strength of individual CNTs. We focused on incorporating plastic deformation into the CVD synthesis process, using the shear stress of gas laminar flow. Here we demonstrated the CNT formation through the tensile deformation while heating of a hollow carbon structure.
We sampled hollow carbon structures as an intermediate product of the CNT synthesize process using the mist CVD from ferrocene and ethanol. The sample was fixed between a gold substrate and a gold tip which are installed in a home-made TEM sample holder equipped with a piezo manipulator. Fig. 1 is a time series of TEM images capturing the tensile deformation process of the hollow carbon structure under the joule heating. As the tip (right side) moved in the direction of the arrow (in Fig. 1(a)), the structure extended from 60 nm (Fig. 1(a)) to 120 nm (Fig. 1(d)) in length, while the maximum width decreased from 8.5 nm to 7.1 nm. Finally, the narrowest width became 2.5 nm as shown in Fig. 1(d). We have identified that the CNT can be formed from the elongation and the thinning of the hollow carbon structures under the joule heating.

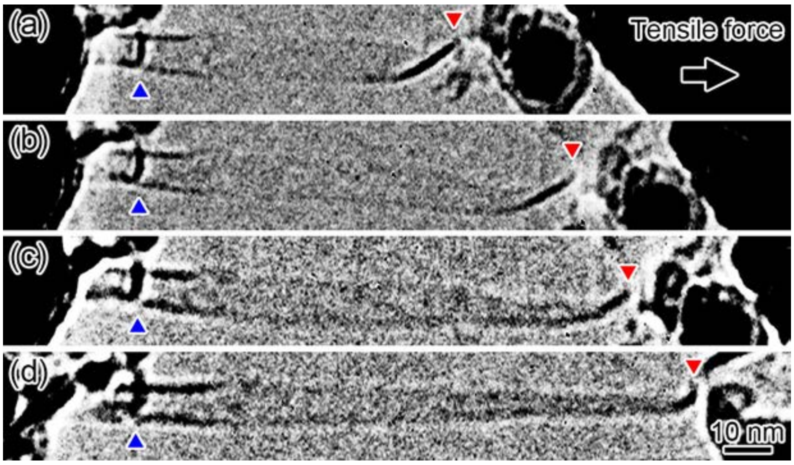

Fig. 1. Time-sequence TEM images observed during the tensile deformation process of a hollow carbon structure.

Plenary Venue Poster

P015 **Th 17:00 - 18:30**

First Steps towards Bottom-up Synthesis of Graphene Nanoribbon from Fluorinated Precursors

Valeria Milotti[1], Ann-Kristin Steiner[2], Thomas Pichler[1], Konstantin Amsharov[2]

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[2]*Department of Organic Chemistry, Friedrich Alexander University Erlangen-Nuremberg, 91058 Erlangen, Germany*

Graphene nanoribbons have been produced and tailored on metal substrates via a bottom up approach from organic precursors, which paves the way to their application in nanoelectronics after transfer to insulating substrates. Quantum confinement of the macromolecules leads to the creation of peculiar band structures, strongly influenced by the topological characteristics of the ribbons. Therefore, it is important to be able to exactly engineer the ribbons, in order to precisely tune their electronic, optical and magnetic properties. Here, we present recent progress in achieving atomically precise bottom-up synthesis of nanoribbons without the presence of a metal catalyst, by using fluorinated precursors to exploit cyclodehydrofluorination as reaction for surface-assisted synthesis [1,2], and/or by using the chemically stable conditions inside carbon nanotubes as reaction environment [3]. We use resonance Raman spectroscopy as probe to analyse these nanocarbon structures via their spectral fingerprint.

This work is supported by the FWF project P27769-N20 and by the Vienna Doctoral School.

[1] Amsharov, Phys. Stat. Solidi B 2016, 253, 2473.
[2] Kolmer et al., Science 2019, 363, 57-60.
[3] Kuzmany et al., Phys. Status Solidi RRL 2017, 11, 1700158.

P017 **Th 17:00 - 18:30**

Reductive Alkylation of s-SWNTs

Kerstin Müller[1], Martina Wederhake[1], Friedrich Schöppler[1], Tobias Hertel[1,2]

[1]*Institute of Physical and Theoretical Chemistry, Julius Maximilian University, Würzburg, 97074, Germany*

[2]*Röntgen Center for Complex Material Systems, Julius Maximilian University, Würzburg, 97074, Germany*

Impurities in semiconductors can play a key role for enabling device functionality, for example by acting as donors or acceptors for semiconductor doping or by modifying photophysical properties in beneficial ways. Specifically, the introduction of near infrared emissive defect states in covalently functionalized semiconducting single-wall carbon nanotubes (s-SWNTs) has led to the realization of single photon sources at room-temperature and at telecom wavelengths.[1] However, the mechanism underlying such functionalization is generally not well understood.

To elucidate reaction pathways for the reductive alkylation of s-SWNTs we have thus investigated functionalization kinetics using photoluminescence (PL) and absorption spectroscopy. The experiments suggest that the reductive alkylation is a follow-up reaction which presumably undergoes a SN2 reaction as primary alkyl halides lead to a much higher functionalization degree compared to secondary ones and especially tertiary ones.

Besides by means of this new kind of reductive alkylation[2] we find that we can even functionalize with different solvent molecules (figure 1).

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[2] H. Kwon, Department of Chem. and Biochem, Maryland, 2016.

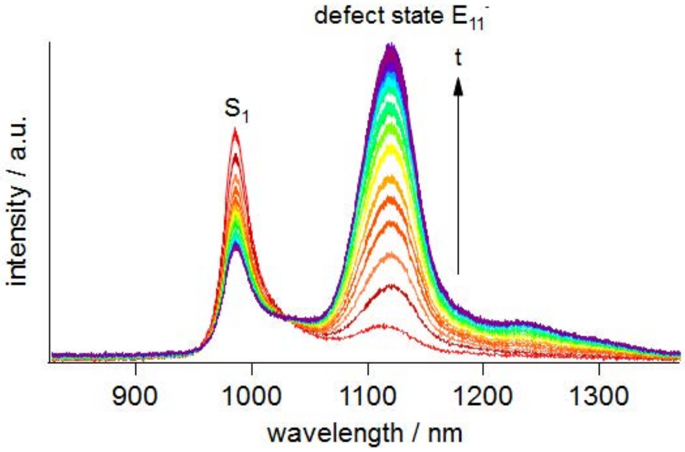

Fig. 1: PL spectra of alkylated s-SWNTs showing the increase of an emissive defect state with increasing reaction time.

Plenary Venue Poster

P019 **Th 17:00 - 18:30**

Quantifying doping levels in carbon nanotubes by optical spectroscopy

Florian Oberndorfer[1], Klaus H. Eckstein[1], Melanie M. Achsnich[1], Friedrich Schöppler[1], Tobias Hertel[1,2]

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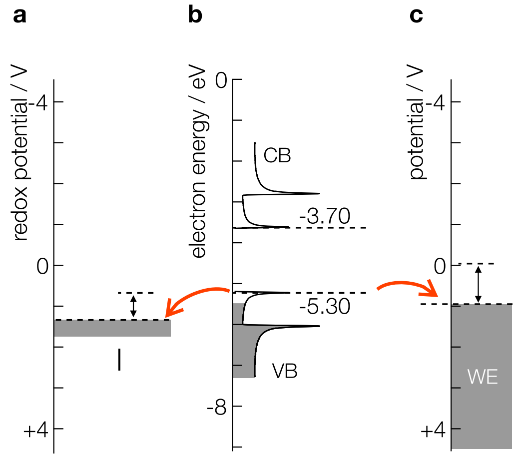
The ability to control doping is essential for the integration of semiconductor materials into device technologies. However, the means for quantification of doping levels often lags behind the technological requirements. Here, we describe efforts toward a quantitative determination of doping levels in semiconducting carbon nanotubes (s-SWNTs). A comparison of changes in the optical absorption spectra of redox- or electrochemically doped s-SWNTs revealed no dependence on the doping scheme over a broad spectral- and doping-range. Carrier densities are determined from changes of exciton oscillator strength and band position using a band filling or - alternatively - an exciton confinement model with quantitatively similar results.



a) For redox- and c) for field-induced doping of s-SWNTs with valence and conduction band alignment indicated on the same energy or potential axis in b). The direction of charge transfer is determined by differences in redox potential ΔE or by the sign of the potential difference U between SWNT and a nearby working electrode.

P021 **Th 17:00 - 18:30**

Selective dry pick-up of CVD grown CNTs for integration in 2D van der Waals heterostructures

Taoufiq Ouaj[1], Christoph Stampfer[1,2]

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In the last years, the integration of different 2D materials such as e.g. graphene, hexagonal boron nitride (hBN) and transition metal dichalcogenides into stacked van der Waals (vdW) heterostructures led to interesting devices allowing studying highly interesting phenomena, such as superconductivity, ballistic transport or proximity induced spin orbit coupling. Thus, vdW stacking might also be an interesting venue for 1D carbon nanotubes (CNTs) opening the door of combining 2D and 1D systems, not only interesting for substantially increasing CNT device quality. In this work, we present a technology, which allows to integrate CNTs in a 2D materials stack. We grow the CNTs by a ferritin-based CVD process on SiO_2. Atomic force microscopy and confocal Raman microscopy are used directly after growth for localization and pre-characterization of specific CNTs. Using our dry transfer techniques, the selected CNTs are encapsulated in exfoliated hBN crystals. As a next step the influence of the different substrates on the electronic properties is investigated by confocal Raman spectroscopy, which also allows to select individual CNTs for contacting with Cr/Au electrodes. Such devices enable the investigation of the substrate influences on quantum transport through individual CNTs.

P023 **Th 17:00 - 18:30**

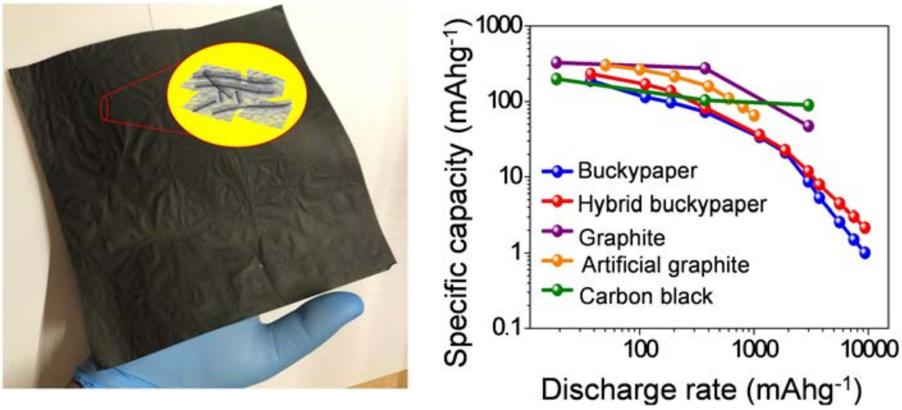
Highly conductive auxetic CNT-graphene hybrid buckypaper

Shashikant Patole[1]

[1] *Department of Physics, Khalifa University of Science and Technology, P.O. Box 127788, Abu Dhabi, UAE*

A combination of carbon nanotubes (CNTs) and graphene in the form of macroscopic hybrid bucky paper (HBP), have unique properties that can be exploited for many emerging applications. However, lack of an inexpensive, simple, scalable process to convert CNT and graphene powder into HBP disdains its common use. Here, we present a simple, inexpensive and scalable approach for the synthesis of HBP via wet-filtration-zipping. The electrical, electrochemical and mechanical performance (tensile, mode I and mode III) of synthesized HBP are evaluated. An overall, increase of 247% of electrical conductivity is observed for HBP (50% graphene and 50% CNTs) compare to BP (100% CNTs). As a negative electrode for lithium-ion batteries, HBP shows 50% higher specific capacity and 848% lower charge transfer resistance compared to BP. The graphene content in the HBP influences the mechanical performance giving an auxetic structure to HBP with large negative Poisson's ratio. A green-chemistry approach, flexibility in accommodating any other 1D and 2D materials, and scalability of the method demonstrate the novelty of the work for industrial scale application.

Reference: S. P. Patole et. al, Scientific Reports 8, 12188 (2018).



Photograph with schematic showing the hybrid buckypaper (HBP). The plot shows the rate capability of HBP and BP at various discharge rates.

P025 **Th 17:00 - 18:30**

One-dimensional nanoobjects with alternating chains and polycyclic graphene-like regions

Andrey Popov[1], Alexander Sinitsa[2], Irina Lebedeva[3], Andrey Knizhnik[4], Dimas G. de Oteyza[5,6,7]

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[2]*National Research Centre Kurchatov Institute, Moscow 123182, Russia*
[3]*CIC nanoGUNE, San Sebastián 20018, Spain*
[4]*Kintech Lab Ltd., Moscow 123298, Russia*
[5]*Donostia International Physics Center, San Sebastián 20018, Spain*
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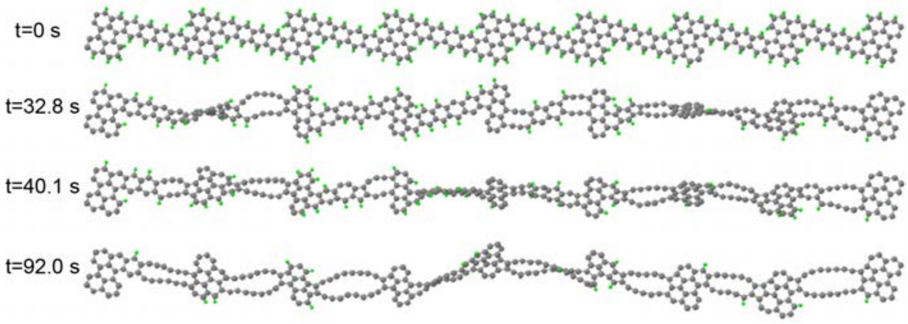
Since the direct observation of atomic carbon chain formation from graphene, their mechanical and electronic properties have attracted considerable interest. Recently we have proposed the method to produce carbon chains by heating of graphene nanoribbons (GNRs) [1]. Here the synthesis of one-dimensional nanoobjects with alternating chains and polycyclic graphene-like regions under electron irradiation of GNRs in HRTEM is proposed and studied by molecular dynamics (MD) simulation. For this purpose a possible scheme of synthesis of GNRs with a periodically alternating width is proposed. In MD study the effect of electron irradiation is simulated by the CompuTEM algorithm. The version of the first-generation reactive Brenner potential previously fitted by us [1] to describe formation of carbon chains, vacancy migration and pristine graphene edges is used. Two parameters of the potential are additionally changed to reproduce also the energies of various graphene edges terminated by hydrogen. The simulations reveal formation of quasiperiodic nanoobjects with alternating chains and polycyclic graphene-like regions for the considered GNRs. The atomistic mechanism of formation of these nanoobjects is discussed.

1. AS Sinitsa, IV Lebedeva, AM Popov, AA Knizhnik, Carbon 140, 543(2018)



Simulated structure evolution of the graphene nanoribbon with edges terminated by hydrogen atoms (shown in green) under 80 keV electron irradiation in HRTEM.

Plenary Venue Poster

P027 **Th 17:00 - 18:30**

Optical absorption in the two-dimensional hexagonal materials

Fenda Rizky Pratama[1], M. Shoufie Ukhtary[1], Riichiro Saito[1]

[1]*Department of Physics, Tohoku University*

Two-dimensional (2D) hexagonal materials, such as h-BN, silicene, & MoS_2have promising applications in valleytronics and spintronics due to the occurrence of valley polarization (VP) and circular dichroism (CD). The electronic structure of the 2D materials can be generally written by the Haldane model. Recently, Ghalamkari et al. [J. Phys. Soc. Jpn. 87 063708 (2018)] showed by the the dipole approximation that VP as well as perfect CD occur exclusively in the material with the Haldane Hamiltonian at the energy gap of the K and K' points. However, to obtain the optical absorption probability as a function of the photon energy, we require a more general approach. By using the Kubo formula, we calculate the longitudinal and the Hall optical conductivities of the Haldane model as a function of the photon energy. We found that the VP and perfect CD can be explained by the properties of the Hall conductivities of the Haldane materials, and VP and perfect CD can occur simultaneously in the materials depending on the photon energy, because the energy gaps at K and K' points can be different. We generalize our formula to include the absorption of elliptically polarized light and the depolarization effect in the materials, where the Hall conductivity enhances the depolarization effect.

P029 **Th 17:00 - 18:30**

Multifunctional Polymeric Acid Doping, Anti-Reflection, and Encapsulation of Carbon Nanotube-Si Solar Cells with Record-High Efficiency and Stability

Yang Qian[1], Il Jeon[1], Ya-Lun Ho[1], Esko I. Kaupinnen[2], Jean-Jacques Delaunay[1], Shigeo Maruyama[1,3]

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[2] *Department of Applied Physics, Aalto University School of Science*
[3] *National Institute of Advanced Industrial Science and Technology*

Carbon nanotubes (CNTs) is a promising material for energy applications. The single-walled carbon nanotubes (SWNTs) films, which are constructed from SWNTs, have been regarded as the alternative to Indium Tin oxide (ITO) films. One application of the SWNT films is the CNT-Si solar cells. The unique configuration of CNT-Si solar cells eliminates high-temperature diffusion and element doping process as well as minimizing the charge carrier recombination loss at the Si interface. Moreover, the performance of CNT-Si solar cells can be further improved by tailoring the SWNT films through chemical modifications, such as chemical doping, anti-reflection coating, and encapsulation.

In this work, we propose a novel type of polymeric acid, Nafion®, with a multifunction of anti-reflection, long-term p-doping, and exceptional encapsulation for CNT-Si solar cells. A simple process improved the power conversion efficiency (PCE) from 9.5% to 14.4%. Thanks to the intrinsic chemical robustness of Nafion, the Nafion-applied CNT-Si solar cells demonstrated superior device stability against ambient environment, UV, water, and acid. The mechanisms for the Nafion-applied CNT-Si solar cells will be discussed through various characterization and simulation methods.

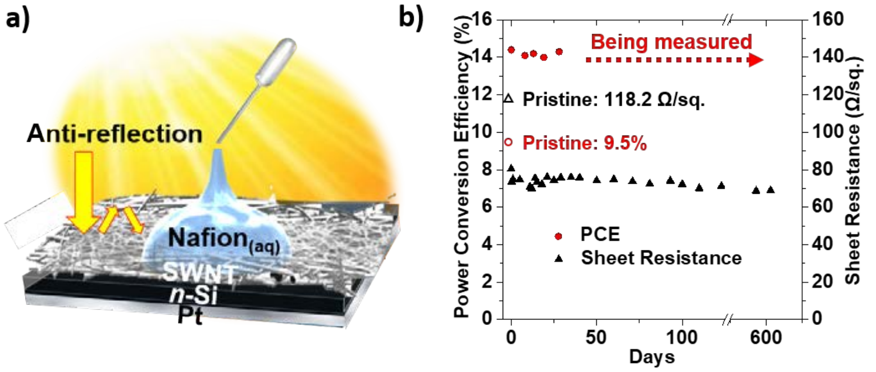

Fig.1 a) Schematic of Nafion-applied CNT-Si solar cells. b) Stability measurement of Nafion-applied CNT-Si solar cells and SWNT films under ambient environment.

P031 **Th 17:00 - 18:30**

Contact Induced Phase Separation of Alloy Catalyst for Efficient Carbon Nanotube Growth

Lu Qiu[1,2], Feng Ding[1,2]

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[2] *Center for Multidimensional Carbon Materials, Institute for Basic Science, Ulsan, 44919, Republic of Korea*

The high efficiency of alloy catalyst for carbon nanotube (CNT) growth has been a long-term puzzle and deep insights into the mechanism is crucial for catalyst design. In this letter, via density functional theory-based molecular dynamic (DFT-MD) simulations, we report a CNT-catalyst contact induced phase separation of alloy catalyst and its effects on CNT growth. During CNT growth, its growth front tends to be in contact with the more active metal, and therefore, a phase separation of the alloy particle which contains both active and less active metal will be induced. Careful atomic simulations reveal three key advantages of using alloy catalyst in CNT growth: (i) the strong interaction between CNT and the active metal atoms stabilizes the open end of the CNT; (ii) the active metal attracts carbon precursors to quickly diffuse to CNT's growth front for fast CNT growth; and (iii) the depletion zone near the less active part of the catalyst prevents the poisoning of the catalyst. The finding paves the way for designing alloy catalyst for efficient CNT growth.

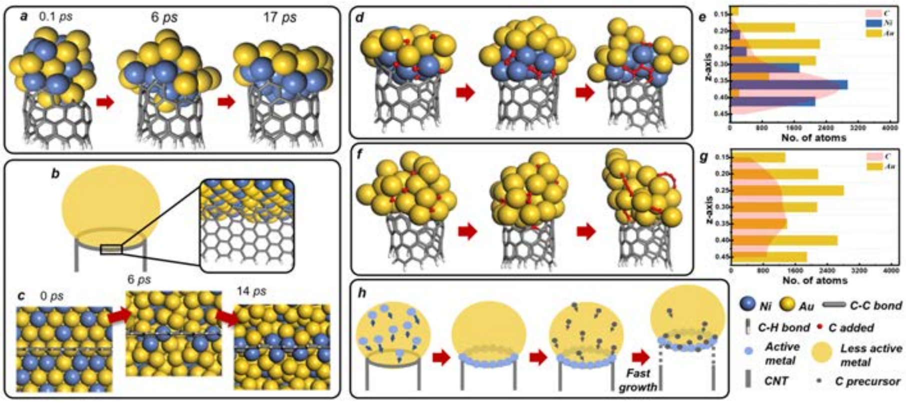


Fig. 1 Phase separation of alloy catalysts on CNT in small (a) and large (b-c) systems. (d-e) Directional carbon diffusion on alloy catalyst. (f-g) Random carbon diffusion on pure metal catalyst. (h) Schematic diagram of phase separation.

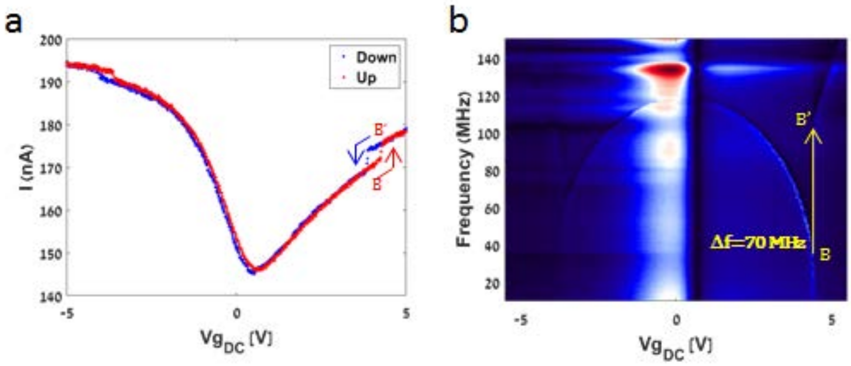
P033 **Th 17:00 - 18:30**

Snap-Through Buckling Bi-Stability in Suspended Carbon Nanotube Resonators

Sharon Rechnitz[1], Tal Tabachnik[1], Michael Shlafman[1], Shlomo Shlafman[1], Yuval Yaish[1]

[1] *Technion - Israel Institute of Technology*

Mechanical bi-stability based on snap-through (ST) buckling is a well-known phenomenon in micro-electromechanical systems (MEMS) which serves as the underlying mechanism for many practical applications such as switches, actuators, sensors, filters, and memory elements, to name a few. Here, we report the first realization of a suspended carbon nanotube (CNT) based bi-stable resonators exhibiting ST buckling phenomena. Both the static and dynamic responses of the system were obtained through conductance and resonance frequency measurements, respectively. In both measurements, non-linear effects such as jumps, hysteresis, softening and hardening, and super and sub-harmonic excitations were observed. Apart from these resonators being the smallest bi-stable electromechanical system based on ST buckling to date, our devices could also serve as excellent sensors with ultrahigh sensitivities, reaching electrostatic tunability values beyond 100MHz/V, which are also attractive for the realization of mechanical quantum-bits. Finally, we developed a comprehensive theoretical model based on the Euler-Bernoulli curved beam equation and obtained excellent agreement with the experimental results.



Conductance (a) and resonance frequency (b) measurements of a typical device exhibiting snap-through behavior. The large abrupt mechanical ST transition results both in a change in the conductance and a ”jump” in the resonance frequency of the device

P035 **Th 17:00 - 18:30**

Modeling of graphene-based conductors

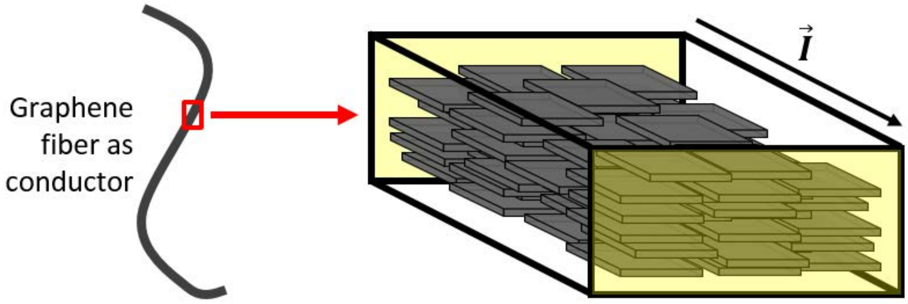
Leo Rizzi[1,2], Andreas Zienert[1,3], Jörg Schuster[1,3], Martin Köhne[2], Stefan E. Schulz[1,3]

[1]*Faculty of Electrical Engineering and Information Technology, TU Chemnitz, Reichenhainer Str. 70, 09126 Chemnitz, Germany*
[2]*Robert Bosch GmbH, Robert-Bosch-Campus 1, 71272 Renningen, Germany*
[3]*Fraunhofer ENAS, Technologie-Campus 3, 09126 Chemnitz, Germany*

Graphene-based conductors such as films or fibers aim to transfer graphene's extraordinary properties to the macroscopic scale. As a new form of efficient electrical conductors, they show great potential for large-scale applications. Graphene-based conductor materials are lightweight, corrosion-resistant, mechanically strong and highly conductive. Since they rely on graphite as their raw material, they promise to be a cost-efficient and sustainable alternative to metals.

While lots of experimental work on graphene-based conductors has been published, there is a lack of simulations and modeling approaches. Supported by theoretical considerations and finite element analysis, we developed a network simulation method to model the electrical conductivity of 2D-based materials. The method considers all the relevant microscopic parameters such as graphene flake conductivity, interlayer conductivity, packing density, and flake size.

Our results offer production guidelines and enable the systematic optimization of high-performance graphene-based conductor materials. A generalization of the model to any conductor based on two-dimensional materials is straightforward.



Simulation of a graphene fiber segment

P037 **Th 17:00 - 18:30**

Analysis of Furnace Gas Evolved During Carbon Nanotube Fibre Production

James Ryley[1], James Ryley[1], John Bulmer[1], Adarsh Kaniyoor[2], Thurid Gspann[2], Martin Sparkes[1], William O'Neil[1], James Elliott[2]

[1] *1. Institute for Manufacturing, University of Cambridge, CB3 0FS, UK*
[2] *2. Department of Materials Science and Metallurgy, University of Cambridge, CB3 0FS, UK*

The direct-spinning continuous carbon nanotube fibre production process developed at Cambridge has recently been enhanced by in-line infra-red (FTIR) spectrographic analysis visualising its reactor's inputs. Progress in understanding the reaction process is sought by live sampling of reactor gas in-situ and an analysis of the compounds found within under different conditions and settings. Of particular interest is discovering whether the presence of particular chemical species indicate high quality CNT production.

Focusing on the carbon precursors toluene, thiophene and ferrocene, we can now show the live in-situ gas composition of the furnace, as sampled from different tube depths, describing how the quantities of detectable reagents and breakdown products evolve down the furnace including their stability over time under reaction conditions. Practical applications of these findings are discussed with respect to chemical control feedback, the timing and role of thermal decomposition and the effect of different reagent delivery methods. Finally, using measured mechanical strength, electrical conductivity and Raman spectroscopy assessments of purity; we relate the properties of different fibre samples to the gasses observed during spinning and theorise reaction mechanics.

P039 **Th 17:00 - 18:30**

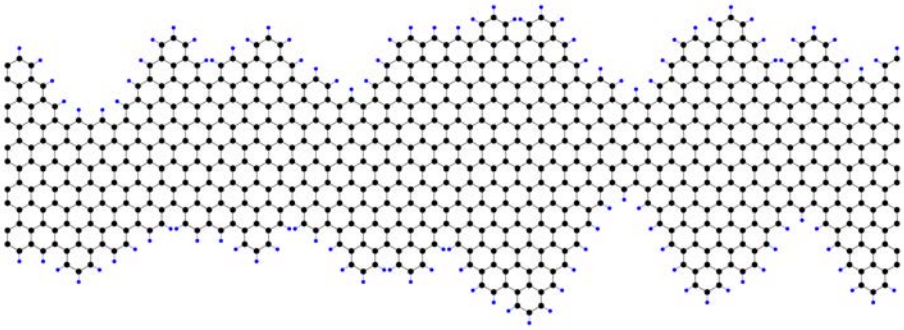
Electron transport through graphene nanoribbons with edge roughness

Jörg Schuster[1,2,3], Fabian Teichert[3,4], Tom Rodemund[1,4]

[1] *Fraunhofer Institute for Electronic Nanosystems – ENAS, 09126 Chemnitz, Germany*
[2] *Center for Microtechnologies, TU Chemnitz, 09107 Chemnitz, Germany*
[3] *Dresden Center for Comp. Materials Science - DCMS, TU Dresden, 01062 Chemnitz, Germany*
[4] *Institute of Physics, TU Chemnitz, 09107 Chemnitz, Germany*

Graphene nanoribbons (GNRs) are promising candidates for electronic applications. However, edge roughness is known to limit their performance. We use a density-functional-based tight-binding model and quantum transport theory based on an efficient implementation of the recursive Green's function approach to calculate the conductance of rough GNRs at the mesoscopic length scale.

Based on our very efficient computational approach we are able to perform statistical studies on large ensembles of GNRs with random edges. We calculate the conductance loss due to edge roughness of various strength for ribbons with varying width and chirality. Similar to other low-dimensional systems like CNTs we can analyze the roughness induced conductance losses in terms of strong localization. Hence, the conductance depends exponentially on the length of the system which is characterized by the localization length. We demonstrate how the localization length can be expressed as a function of roughness, GNR width and chirality. As an alternative interpretation of our data we study the localization length as a function of the total contour length of the rough ribbon edges and the fraction of armchair and zigzag type edges.



Model of a zigzag GNR (width = 5 unit cells) with edge roughness as it is used in our statistical study.

Plenary Venue Poster

P041 **Th 17:00 - 18:30**

Draw your doodles here.

Plenary Venue Poster

P043 **Th 17:00 - 18:30**

CNT Supported Mn-doped ZnO Nanoparticles as Competent Visible Light-Active Photocatalyst

Ahmed Shawky[1], Reda M. Mohammed[1,2]

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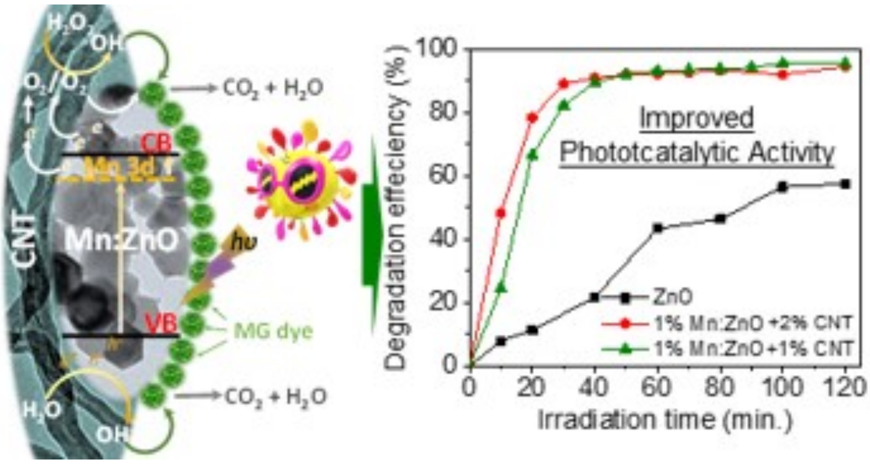
[2]Chemistry Department, Faculty of Science, King Abdulaziz University, P.O. Box 80200, Jeddah 21589, Saudi Arabia

Photocatalysis is photoreaction process occurs in the presence of semiconductor resulting in an electron-hole pair generation. These carriers able to generate free radicals undergo secondary oxidation reactions. ZnO is a well-known photocatalyst long time ago. However, the large band gap and low surface area are major problems for the real industrial applications. Doping of ZnO with transition metal is one of the effective ways to reduce the band gap to the visible light regime. On the other hand, Carbon nanotubes (CNT) represents an excellent carbon member which can introduce a higher surface area of ZnO. Also, CNT can improve the photocatalytic activity due to the ease of charge transfer from the ZnO surface and reduce recombination.

In this regard, we introduce our recent work on the incorporation of CNT during synthesis of Mn-doped ZnO nanoparticles. The CNT induce a decrease in the band gap of ZnO and improve the charge transfer according to our investigations. The photocatalytic activity was applied for the degradation of Malachite green (MG) dye as an industrial model. The degradation efficiency reached more than 95% after just 2h under bulb light illumination. The photocatalytic mechanism and degradation kinetics will be discussed in some details.



Schematic representation of the photocatalytic degradation of MG dye using CNT supported Mn-doped ZnO (left) showing the effect of adding CNT on the photodegradation efficiency (right)

P046 **Th 17:00 - 18:30**

High-throughput Preparation of Wafer-Scale Highly Uniform Carbon Nanotube Films for Applications of Electronics and Optoelectronics

Wei Su[1,2], Dehua Yang[1,2], Jiaming Cui[1], Shilong Li[1,2], Xiaojun Wei[1,3], Weiya Zhou[1,2,3], Huaping Liu[1,2,3], Sishen Xie[1,2,3]

[1] *Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China*
[2] *School of Physics Science, UCAS, Beijing 100049, China*
[3] *Songshan Lake Materials Laboratory, Dongguan, Guangdong 523808, China*

Single-wall carbon nanotube (SWCNT) has great potential applications in electronics and optoelectronics because of its excellent properties. To meet the practical application of SWCNTs in electronics circuits, wafer-scale SWCNT films with uniform electrical property are essentially crucial. Here, we report an innovative method for high-throughput preparation of wafer-scale SWCNT films with controllable density and uniform electrical property, in which $NaHCO_3$was employed to enhance the interaction between substrate and SWCNTs. With the technique, a 4-inch SWCNT film can be prepared within 10 mins, and the linear density can be adjusted from several to ~50 per micrometer. When utilizing single-chirality SWCNTs, high uniformity of density and electrical characteristics was confirmed by AFM and SWCNT transistor arrays. Clearly, the work established a new method for the high-efficiency preparation of wafer-scale uniform SWCNT films, paving a way for the application of SWCNTs in digital integrated circuits.

This work is supported by the National Key R&D Program of China (Grant 2018YFA0208402), the National Natural Science Foundation of China (Grants 51472264,11634014, 51820105002, 51872320, 51561022), and the Key Research Program of Frontier Sciences, CAS (Grant QYZDBSSW-SYS028).

P048 **Th 17:00 - 18:30**

Threshold voltage tuning by controlled doping for low-power complementary carbon nanotube integrated circuits on flexible substrate

Fu-Wen Tan[1], Jun Hirotani[1], Yoshiyuki Nonoguchi[2], Shigeru Kishimoto[1], Yutaka Ohno[1,3]

[1]*Department of Electronics, Nagoya University, Nagoya 464-8603, Japan*
[2]*Division of Materials Science, NAIST, Takayama, Ikoma, Nara 8916-5, Japan*
[3]*Institute of Material and Systems for Sustainability, Nagoya Univ., Nagoya 464-8601, Japan*

Flexible electronics can be realized by combining the remarkable properties of carbon nanotube thin-film transistors (CNT TFTs) and low-power complementary metal-oxide semiconductor (CMOS) technology. Despite reports on n-type doping for CNT TFT CMOS, threshold voltage variability and hysteresis of pristine p-type devices remain as challenging issues [1-2]. In this work, deliberate doping of both p- and n-type TFTs and passivation procedures were carried out for stable CMOS circuit operation. Bottom-gated complementary TFTs with semiconductor-enriched CNTs as the channel material were fabricated on a flexible substrate. Before doping, uniform p-type characteristics were confirmed on all 252 devices. Then, we performed n-type doping by spin-coating potassium hydroxide/benzo-18-crown-6-ether on selective devices, followed by atomic layer deposition of an Al_2O_3 passivation layer. Next, silver-bis(trifluoromethane-sulfonyl)imide was spin-coated to tune the threshold of p-type TFTs, and then passivated with polymethyl-methacrylate and Al_2O_3. We evaluated more than 100 CNT CMOS inverters with a yield of 95.4 %, low operation voltage of 0.5 V, and average power consumption of 18 nW. [1] M.L. Geier et. al., Nano Lett. 13, 4810 (2013). [2] J. Tang et al., Nat. Nanotechnol. 1, 191 (2018).

P050 **Th 17:00 - 18:30**

Understanding the Encapsulation of Organic Salts in Single-Walled Carbon Nanotubes. Band-Gap Opening in Metallic SWNTs.

Julia Villalva[1], Belén Nieto-Ortega[1], Mariano Vera-Hidalgo[1], Luisa Ruiz-González[2], Enrique Burzurí[1], Emilio M. Pérez[1]

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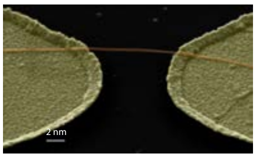
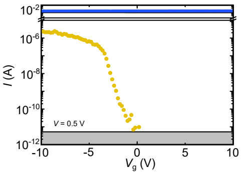
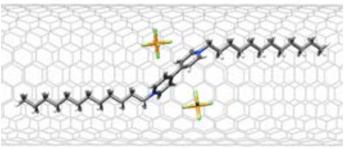
[2] *Departamento de Química Inorgánica, Universidad Complutense de Madrid, Madrid (Spain)*

Carbon nanotubes (CNTs) are one of the most promising one-dimensional nanoscale materials. Interestingly, their optical, electronic, and mechanical properties can be modulated on demand via controlled chemical modification. The encapsulation of viologen derivatives into metallic single-walled carbon nanotubes (SWNTs) results in the opening of a band gap, making the SWNTs semiconducting. Raman spectroscopy, thermogravimetric analysis, and aberration-corrected high-resolution transmission electron microscopy confirm the encapsulation process. Through the fabrication of field-effect transistor devices, the change of the electronic structure of the tubes from metallic to semiconducting upon the encapsulation is confirmed. The opening of a gap in the band structure of the tubes was not detected in supramolecular controls.







P052 **Th 17:00 - 18:30**

Towards microwave optomechanics using a superconducting carbon nanotube weak link

Marco Will[1], Jukka-Pekka Kaikkonen[1], Dmitry Golubev[1], Yongping Liao[2], Patrik Laiho[2], Thanniyil Sebastian Abhilash[1], Pertti Hakonen[1]

[1]*Low Temperature Laboratory, Dept. of appl. Phys., Aalto University, Espoo, 02150, Finland*
[2]*Dept. of appl. Phys., Aalto University, Espoo, 02150, Finland*

Utilizing the ultra-high sensitivity of a superconducting single-walled carbon nanotube (SWCNT) sensor to probe the quantum ground state is a promising experimental approach for investigations of macroscopic quantum phenomena. However, reproducible and eliable fabrication of such devices is still to be shown due to the demands on high temperature stable materials that the SWCNT growth requires and the crucial role the contact resistance plays for inducing superconductivity into the SWCNT. We approach the challenge with suspended, 300nm long SWCNT contacted on MoRe leads. Good transparency of the superconductor-nanotube contacts allows observation of proxomity induced supercurrents of up to 50 nA, tuneable by gate induced charge. Additionally, we have developed a method to pick-up and place individual suspended SWCNT selectively on metal-electrodes. Using such weak links in an optomechanical microwave setting, coupling energies on the order of 100 kHz can be reached between the mechanical resonator and the electrical cavity.

P054 **Th 17:00 - 18:30**

Poly(p-Styrene-Sulfonic Acid) as Dispersant and Stable Dopant for Carbon Nanotubes

Rongbin Xie[1], Suguru Noda[1,2]

[1]*Department of Applied Chemistry, Waseda University, Tokyo, 169-8555, Japan*
[2]*Waseda Research Institute for Science and Technology, Waseda University, 169-8555, Japan*

Carbon nanotubes (CNT) films have been widely applied in the fields of electronics, capacitors, and batteries due to the unique structure, high conductivity and stability. Generally, the solution fabrication of high-quality CNT films needs several steps, including dispersion of CNT in surfactant solution, filtration to form the film, removal the surfactant and doping treatment. Obviously, such complicate process cost lots of time and expense. Moreover, the sheet resistance of CNT films doped with nitric acid increased a lot after a few days. Therefore, it is essential to develop a simple and efficient method for facile fabrication and stable doping of CNT films.
Herein, we applied the repetitive dispersion-filtration method [1] to CNT using poly(p-styrene-sulfonic acid) (PSS) aqueous solution (Figure 1). Almost complete dispersion of CNT aggregates (>90%) was achieved within 3 cycles. CNT films were then prepared via vacuum filtration without any additional strong acid, showing low sheet resistances of 125 and 66 Ω/sq at 90% and 82% optical transmittances, respectively. Notably, these films showed high long-term stability for >1000 h. PSS is a promising dispersant and dopant for CNT.

[1] H. Shirae, et al., Carbon 91, 20 (2015).

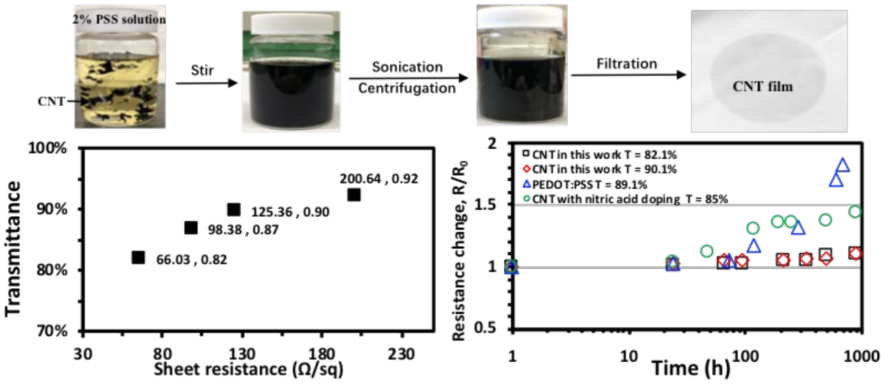


Figure 1. The fabrication procedure, performance and stability of CNT films using PSS as dispersant and dopant.

P056 **Th 17:00 - 18:30**

Charge Modulation Spectroscopy of Semiconducting SWCNT Networks

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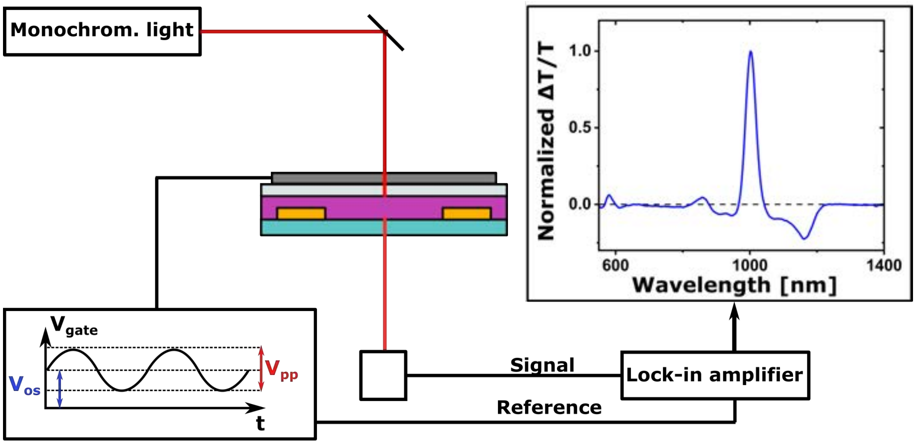
Solution-processed networks of semiconducting single-walled carbon nanotubes (SWCNTs) are promising candidates for electronic circuits, as they combine high charge carrier mobilities with mechanical flexibility. However, fundamental aspects such as the influence of the composition of the SWCNT network on charge transport in field-effect transistors remain unclear. Here, we investigate charge accumulation and transport in two model systems: networks of only (6,5) SWCNTs and networks with five different semiconducting nanotubes (selected from HipCO SWCNTs) using charge-modulated absorption and photoluminescence spectroscopy. Charge modulation spectroscopy is ideally suited to study the nature and distribution of mobile (not trapped) carriers in working transistors. We find that mobile charges are predominantly located on and move through those SWCNTs with the smallest bandgaps, even if they represent only a small proportion of the network. In agreement with previous experimental and theoretical studies (ACS Appl. Mater. Interfaces 2016, 8, 5571 & Phys. Rev. Mater. 2017, 1, 046003) the mobile carrier distribution changes with applied gate voltage. Our findings highlight the importance of the network composition for charge transport in SWCNT thin films and thus device performance.



Schematic of the experimental principle of charge modulation spectroscopy.

P059 **Th 17:00 - 18:30**

Thermal and electrical characteristics of epoxy composites with graphite platelets coated by amorphous carbon and ceramic particles

Solbi Shin[1]

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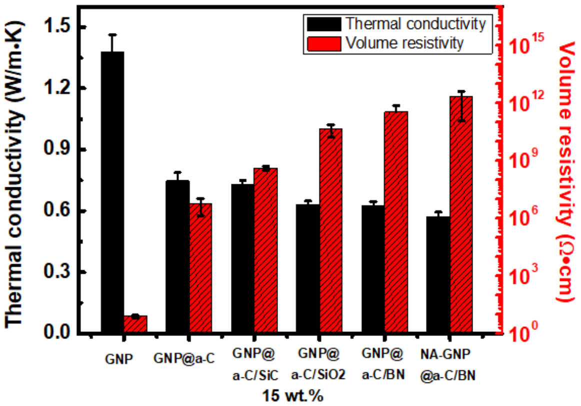
As devices become smaller, heat dissipation characteristics of electrical components are more emphasized. Recently, carbon nanomaterials such as graphite nanoplatelets (GNPs) and graphene are popular as thermally conductive fillers for polymer composites. However, needs of heat-dissipating but electrically insulating materials have been increasing in many devices. This study has developed thermally conductive but electrically insulating epoxy composites by incorporation GNPs. We introduced functional groups to the surfaces of GNPs by acid treatment to improve their chemical interaction with polymer. Here, GNPs treated with nitric acid were denoted by NA-GNPs. For this purpose, GNPs were mixed with poly (melamine-co-formaldehyde) methylated (PMF), followed by heat treatment at 400 °C in nitrogen. The PMF layers were converted to amorphous carbon (a-C) layers over the surface of NA-GNPs (NA-GNPs@a-C) by heat treatment, forming insulating layers on the GNP surface. During this process, boron nitride particles with size of a µm range were added to improve electrical insulation of NA-GNPs (NA-GNPs@a-C/µ-BN). Until 20 wt.% loading of the NA-GNPs@a-C/µ-BN fillers, the epoxy composites maintained electrical insulation while performing good thermal conductivity.



Thermal conductivities and volume resistivities of epoxy composites loaded with 15 wt.%

P061 **Th 17:00 - 18:30**

Electrochemical Measurements of Polyaniline with and without MWNTs

Fahima Djefaflia[1,2], Ouanassa Guellati[1,2], Ilyes Terrab[1], Fahima Djefaflia[1,2] , Assia Nait-Merzoug[1,2], Aicha Harat[1], Simon Detriche[3], Zineb Mekhalif[3], Mohamed Guerioune[1]

[1]*LEREC laboratory, Badji Mokhtar university, BP. 12, 23000 Annaba, Algeria*
[2]*Mohamed Cherif Messadia university, BP. 1553, 41000 Souk-Ahras, Algeria*
[3]*Laboratoire de Chimie et d'Électrochimie des Surfaces (CES), FUNDP rue de Bruxelles 61, B-5000 Namur, BELGIUM*

The electrochemical storage of energy - super-capacitors - has today become a major social and economic issue, which is expected to make much progress, whether in the field of nomadic applications (electronic, portable, automotive) or stationary (renewable energies storage).

Our aim in this investigation is focused on the electrochemical characterization of nano-PANI conductive polymers and their nanocomposites reinforced with MWNTs as electroactive nanomaterials in super-capacitor type energy storage devices.

Electrochemical measurements have shown a pseudo-capacitive or faradic behavior of these nano-PANI and its nanocomposites with very important specific capacities. As well as, we proved that the reinforcement of these PANI nanofibers by functionnalized O-MWNTs greatly improved the specific capacity from 346 F/g (for PANI nanofibers) to 743 F/g (for PANI/O-MWNTs). These results showed the electrochemical performance of these PANI nanofibers synthesized using hydrothermal process which presents a simple method and less expensive; as well as of their nanocomposites synthesized through in-situ polymerization.

P063 **Th 17:00 - 18:30**

Modification of graphite derivatives by solution plasma

Hae Kyung Jeong[1]

Solution plasma is applied to graphite and thermally reduced graphite oxide in ambient conditions in order to improve their dispersion. Changes in morphology, oxygen functional groups, defects, decomposition temperatures, oxygen to carbon atomic ratio, conductivity, stability, and degree of dispersion are systematically investigated by using scanning electron microscopy, Fourier transformed infrared spectroscopy, Raman spectroscopy, Thermogravimetric analysis, X-ray photoelectron spectroscopy, Zeta potential analyzers, and ultraviolet-visible spectrophotometry. Dramatic enhancement of the dispersion after the simple plasma treatment is introduced without evident change of conductivities. This simple, easy, economical, and eco-friendly plasma method could functionalize and reform material efficiently in many application fields.

P065 **Th 17:00 - 18:30**

Effect of liquid phase plasma irradiation in hydrogen production by photocatalytic water splitting with Ni-TiO_2/carbon nanotube

Sang-Chul Jung[1], Seo Jin Ki[2], Kay-Hyeok An[3], Yoong Ahm Kim[4]

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[2]Department of Environmental Engineering, Gyeongnam National University of Science and Technology, 33 Dongjin-ro, Jinju 52725, Republic of Korea
[3]Department of Nano & Advanced Materials Engineering, Jeonju University, 303 Cheonjam-ro, Jeonju 55069, Republic of Korea
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Hydrogen evolution by water photocatalysis using liquid phase plasma system was disserted over metal-loaded TiO_2 photocatalysts. Carbon nanotube was applied as a support for the metal-loaded TiO_2 nanocrystallites. Photocatalytic activities of the photocatalysts were estimated for hydrogen production from water. Hydrogen was produced from the photodecomposition of water by liquid phase plasma irradiation. The rate of hydrogen evolution was improved by the metal loading on the TiO_2 surface. TiO_2 nanocrystallites were incorporated above 40 wt% onto the carbon nanotube support. The carbon nanotubes could be applied as a useful photocatalytic support for the fixation of TiO_2. Hydrogen evolution was enhanced by the Ni loading on the TiO_2 nanocrystallites supported on the carbon nanotube. Hydrogen evolution was increased apparently with addition of the alcohols which contributes as a kind of sacrificial reagent promoting the photocatalysis.

P067 **Th 17:00 - 18:30**

Site-dependent doping mechanism and thermoelectric properties of Sb-doped $SnSe_2$

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[2]*Department of Chemistry, Pohang University of Science and Technology, Pohang 37673, Korea*

We report thermoelectric transport properties of Sb-doped $SnSe_2$compounds. Two types of Sb doping, cation-exchanged $(Sn_{0.96}Sb_{0.04})Se_2$and anion-exchanged $Sn(Se_{0.96}Sb_{0.04})_2$, were performed in this experiment. All the compounds were prepared by conventional melting and annealing process, followed by the consolidation using spark plasma sintering. The resulting compounds were characterized to be a homogeneous phase of layered hexagonal structure (JCPDS # 89-3197) without any secondary phase. Since Sb is a group-V element, it must serve as a donor when occupying the Sn site and should act as an acceptor when occupying the Se site. However, the cation-exchanged compound exhibited decreased n-type electrical conductivity as compared with undoped $SnSe_2$compound, while the anion exchanged compound exhibited increased n-type electrical conductivity. These contradictory doping effects were also observed in Seebeck coefficients. The mechanism is under investigation based on density functional theory calculations, and detailed thermoelectric transport properties of the compounds will be presented.

P069 **Th 17:00 - 18:30**

Enhancement of carbon nanotube yarn based thermoelectric properties by interfacial graphene like layers converted from residual amorphous carbon

Kazuki Omoto[1], Hirotaka Inoue[1], Shogo Iemoto[1], Masaki Hada[1,2], Taisuke Hasegawa[3], Takeshi Nishikawa[1], Yoshifumi Yamashita[1], Satoshi Maeda[3,4], Yasuhiko Hayashi[1], Paneer Selvam Karthik[1]

[1]*Okayama University,Okayama 700-8530,Japan*
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Wearable thermoelectric generators (TEGs) are required to possess features of ultralight, flexible, durable, non-hazardous, chemically stable and low cost. TEG based on carbon nanotube (CNT) yarn responds to those requirements and has high Seebeck coefficient; S and high electrical conductivity; σ. Although the thermal and electrical properties of CNT yarns are affected by the post-high-temperature process, the phenomena underlying the improvement of properties has not been clarified yet. Here, we present TE properties of high temperature treated CNT yarns and computational analysis of the structural changes of the interface between CNTs by the global reaction route map method.The σ, S and power factor; PE of as-prepared CNT yarn shows 25 μV/K, 532 S/cm and 33 μW/mK^2, respectively. Although there is a slight decrease of the σ both S (103 μV/K) and PE (473 μW/mK^2) are increased drastically by Joule heating at 2000 K for 1 min. Raman characterization of the joule-heated CNT yarn, we observed the G* peak indicating the presence of graphene or graphite. The computation analysis reviled that the residual amorphous carbon in the interface between CNTs changes into the graphene-like structure. Our results indicate that the improvement of TE properties is due to graphene layers.

P071 **Th 17:00 - 18:30**

InP/ZnS quantum dots application in inverted solar cell

Anna Pidluzhna[1], Pavlo Stakhira[1], Glib Baryshnikov[2,3]

[1]*Lviv Polytechnik National University, St.Bandery st. 12, Lviv 79013 Ukraine*
[2]*Bohdan Khmelnytsky National University, 18031, Cherkasy, Ukraine*
[3]*KTH Royal Institute of Technology, 10691, Stockholm, Sweden*

A wide list of recent scientific reports confirm the immense potential for QDs application in photovoltaics, light emitting devices and in many ecological and bio medical applications. A big progress in QD application in photovoltaics was attained in the field of II-VI semiconductors, Cd-containing in particular. But cadmium compounds are known to be toxic one. Therefore the search for safer and less harmful materials but with the same properties at least is very urgent point. Thus InP is a good candidate for a development in photovoltaics because it demonstrates suitable optical properties combining size-tunable emission in the visible and near-infrared spectral range and low intrinsic toxicity.
Thus, the purpose of this work was to synthesis InP/ZnS QD with the one-step one pot synthesis method which does not require additional component injections and among others comply more with cost requirements. Here, for the first time for our knowledge, we investigated the applicability of the synthesised InP/ZnS nanocrystals in inverted solar cells formed with step-by-step procedure which combines thermal vacuum deposition method and spin-coating technique. The overall scheme of the inverted structure is ITO/PCBM/QD/P3HT/MoO_3/Al and its photovoltaic behaviour demonstrated.

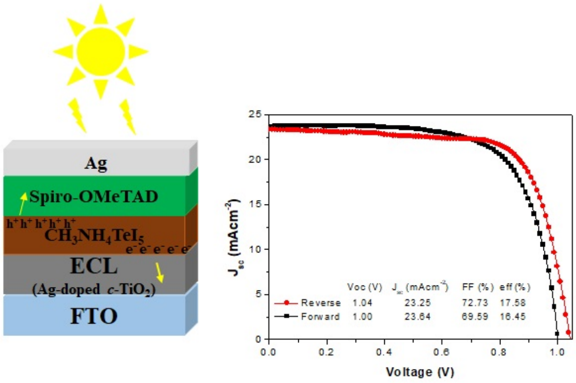
P073 **Th 17:00 - 18:30**

Assistant Prof.

Someshwar Pola[1]

[1] *Department of Chemistry, Osmania University*

A set of three 4,4',4",4"'-(pyrene-4,5,9,10-tetrayl)tetrakis(N,N-diphenylaniline)and its derivatives have efficiently been prepared and analyzed by mass spectrometry , 1H/13C NMR spectroscopy and elemental analysis. The optical properties of the pyrene derivatives were used to monitoring the ratio of dialkyl triphenylamine to pyrene and examined by UV/vis spectroscopy and cyclic voltammetry. Moreover, the in-situ synthesis of the electron-transporting layer (ETL) characterized by XPS and SEM-EDX analyses. The pyrene products were functioning as hole-transporting materials (HTMs) in fabricating mesoporous $TiO_2/CH_3NH_3TeI_5$/HTMs/Ag solar cells. The pyrene centered analog revealed a short-circuit current density of 23.25 mA/cm^2, an open-circuit voltage (Voc) of 1.04 V, and a fill factor of 72.7% under a brightness of 1 sun (100 mW/cm^2), resulting in a total power conversion efficiency of 17.6%. The overall performance is correlated benchmark material such as Spiro-OMeTAD, and however, the Voc is marginally lower. Thus, this freshly synthesized pyrene derivative encirclements potential as an HTM for extremely efficient hybrid tellurate based solar cells.



Device structure and I-V curve of the New tellurate system

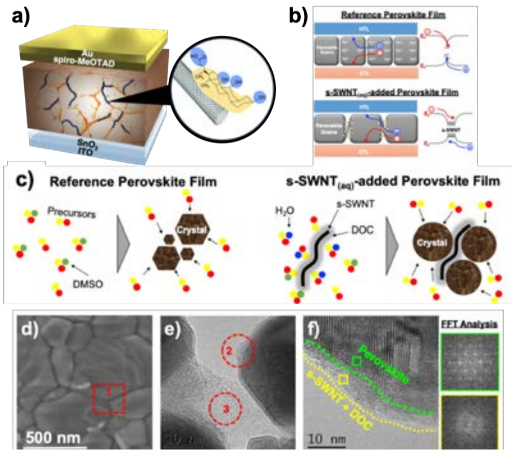
P075 **Th 17:00 - 18:30**

Semiconducting Carbon Nanotubes for grain engineering in perovskite solar cells

Seungju Seo[1], Il Jeon[1], Rong Xiang[1], Takeshi Tanaka[2], Jin-Wook Lee[3], Donguk Suh[1], Ryosuke Nishikubo[4], Akinori Saeki[4], Shohei Chiashi[1], Junichiro Shiomi[1], Hiromichi Kataura[2], Yang Yang[3], Yutaka Matsuo[1,5], Shigeo Maruyama[1,6]

[1]*Department of Mechanical Engineering, The University of Tokyo, Japan*
[2]*Nanomaterials Research Institute, AIST, Japan*
[3]*Department of Materials Science and Engineering, University of California, USA*
[4]*Department of Applied Chemistry, Osaka University, Japan*
[5]*University of Science and Technology of China, China*
[6]*Energy NanoEngineering Lab, AIST, Japan*

Grain size control and boundary passivation of perovskite films are the key to obtaining highly efficient perovskite solar cells. In order to accomplish both goals, semiconducting single-walled carbon nanotubes are added to perovskite films as additives, functioning both the crystal growth templates and charge bridges between the perovskite grains. The resulting perovskite films display more uniform and larger crystal grains compared with conventional films owing to long and flexible single-walled carbon nanotubes, retarding the crystal growth and functioning as the cross-linker between perovskite grains. In addition, sodium deoxycholates attached on the carbon nanotubes passivated the grain boundaries by forming Lewis adducts. Thanks to the improved quality of the photoactive layers by using semiconducting carbon nanotubes, a power conversion efficiency of 19.5% was obtained which is higher than 18.1% of reference devices with no additives.



Illustrations of (a) PSC in this work, (b) MAPbI3 films w. (above) & wo. s-SWNT (below), (c) the role of water and s-SWNT additives during the perovskite growth. (d) SEM and (e)(f) TEM images of the s-SWNT-added MAPbI3 film with the FFT analysis.

P077 **Th 17:00 - 18:30**

Uniform coating of nano-carbon layer on SiO$_x$ in aggregated fluidized bed as high-performance anode material

Zhexi Xiao[1], Chunhui Yu[1], Fei Wei[1]

Carbon layer coating is a facile method to improve the electrochemical performance of SiOx. However, few strategies promise a uniform coating. The fluidized bed reactor with high heat and mass transfer efficiency to ensure uniform coating, requires large particles to achieve smooth fluidization. In this study, we bound the raw powders together to form loose secondary particles with a diameter of $\sim$100 µm, which were supposed to be both fluidized smoothly and also returned to their original size after carbon coating, to achieve a uniform carbon layer coating of $\sim$15 nm on commercial SiO$_x$ powders with a preferable graphitization degree (ID/IG = 1.0) and low surface area ($\sim$2 m2 g^{-1}). The SiO$_x$@C composites delivered a high initial coulombic efficiency (75.1%), an excellent cyclability (83% capacity retention rate for 500 cycles at 1 A g^{-1}), and a superior rate capability (907.7 mAh g^{-1} at 2 A g^{-1}). The more than 10^6 increase in electronic conductivity and 10^4 increase in Li+ diffusion were responsible for the improvement of electrochemical performance. The resistance of the carbon layer to hydrogen fluoride (HF) erosion was observed. This method is suitable for the scaled-up production of anode materials and is expected to be applied to other materials.

P079 **Th 17:00 - 18:30**

Advanced Nanocarbon Energy Materials for Lithium-Sulfur Batteries

Qiang Zhang[1]

Among various promising candidates with high energy densities, lithium-sulfur (Li-S) batteries with a high theoretical capacity and energy density are highly attractive;1-2 while the commercial application of Li-S batteries still faces some persistent obstacles, such as the low electrical conductivity of sulfur and lithium sulfide and the dissolution of polysulfides. The introduction of nanocarbon into the field of Li-S batteries sheds a light on the efficient utilization of sulfur by improving the conductivity of the composites and restraining the shuttle of polysulfides. In this presentation, the concept for the rational design of nanocarbon for energy storage is explained. The advances in the use of advanced energy materials in the cathode, separator, and anode is explained.3-4 New insights on the relationship between the nanostructure and the electrochemical performance are presented.

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P002 **Th 19:00 - 21:00**

Growth mechanism of multi-millimeter-tall single-wall carbon nanotube forests using Fe/Gd/Al catalysts

Hisashi Sugime[1], Rei Nakagawa[2], Toshihiro Sato[2], Cinzia Cepek[3], Suguru Noda[2]

[1]*Waseda Institute for Advanced Study, Waseda University*
[2]*Department of Applied Chemistry, Waseda University*
[3]*Istituto Officina dei Materiali-CNR, Laboratorio TASC*

Growth of single-wall CNT forests by CVD is an attractive for making applications. However, the growth termination by deactivation of catalysts is an obstacle. To realize longer growth lifetime, engineering catalysts is crucially important. To date, Fe-Gd catalyst on Al_2O_3 layer was reported to realize the growth lifetime of 13h and 22-mm-tall multi-walled CNT (MWCNT) forest at the growth temperature of 780 °C [1]. However, the growth rate is relatively low as ~0.5 μm s^{-1}, and the possibility of using Gd for SWCNT growth was not discussed in detail. In this work, we applied the Fe/Gd/Al catalyst to the growth of SWCNT forests, and systematically studied the mechanism behind the enhanced growth (Fig. 1a). By optimizing the catalyst condition, we achieved a high initial growth rate of ~2 μm s^{-1} and long catalyst lifetime of ~50 min at 800 °C. Correspondingly, the areal mass continued increasing up to ~8 mg cm^2 in 60 min (Fig. 1b). It was found that Gd layer with the thickness of less than 1 nm is effective when it is deposited between Fe and Al layers. The Raman spectra showed the radial breathing mode (RBM) peaks from the top to the bottom of the CNT forests, which suggests the continuous growth of SWCNTs.

References
[1] W. Cho et al., Carbon 72, 264 (2014).

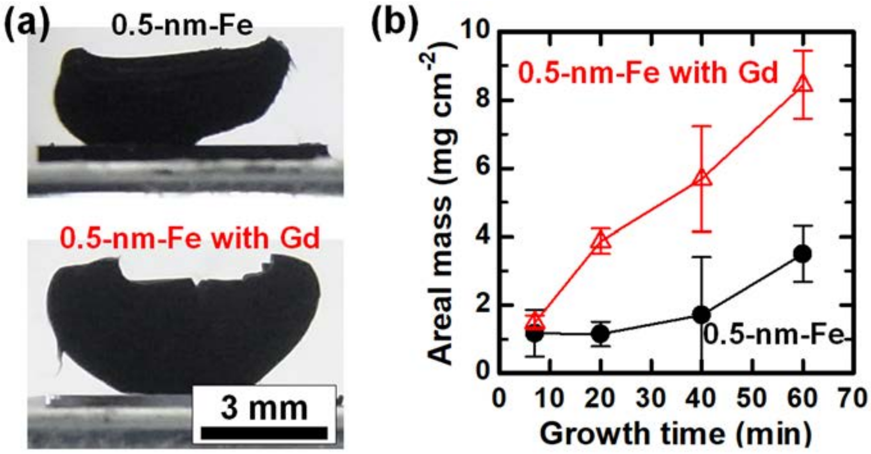

Fig. 1. (a) SWCNT forests grown using Fe/Al or Fe/Gd/Al catalysts. (b) Areal mass of the SWCNT forests with two different catalysts.

P004 **Th 19:00 - 21:00**

Ultrafast Transport of Water Molecules through Centimeter-long Carbon Nanotubes

Silei Sun[1], Zhenxing Zhu[1], Boyuan Shen[1], Yunxiang Bai[1], Rufan Zhang[1], Fei Wei[1]

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Transportation of small molecules through nanochannel, such as water flowing through nanowires, may exhibit emerging physics such as superlubricity[1]. Recent theoretical researches have further predicted the extraordinary transport of water molecules through CNTs, whereas there still lacks reliable experimental evidence[2]. Here we use centimeter-long ultralong CNTs as a model channel to probe the transportation properties of water as well as deuteroxide molecules, by combining the structural characterization and mass spectrometry analysis. The dependence of CNTs' structures, including chirality and defect distribution on the water transport was firstly investigated. We exhibited the ultrafast transport of water molecules inside the nanotube with the flow rate as high as 200-2000 μm/s, peculiarly faster than the transport in bulk analogues. The result reveals that the water transport process inside carbon nanotubes is complex. The water velocity of encapsulating an empty tube and transferring in a full tube has significant difference. Our results demonstrated that this ultrafast transportation through CNTs can be important for developing high-speed transmission devices, such as molecule nanosyrines.

Ref:
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P006 **Th 19:00 - 21:00**

Flexible terahertz camera with microscale free-standing carbon nanotube film array

Daichi Suzuki[1], Koji Ishibashi[1], Yukio Kawano[2]

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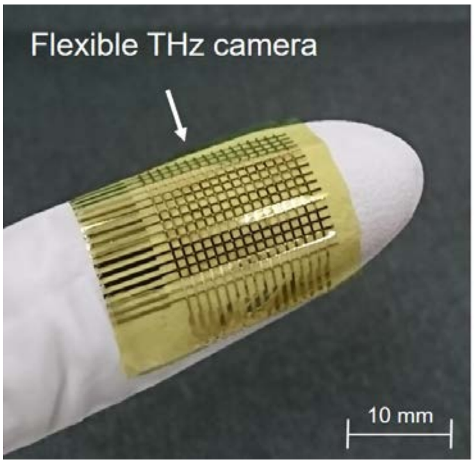
Carbon nanotube (CNT) films have been utilized for a wide variety of applications such as thermoelectric generators, broadband photo-sensors and reinforcing materials. In order to accelerate the CNT-based research, development of synthesis/processing and application of CNT films is one of the key issues. Here we report a novel self-align filtration process of a microscale free-standing CNT film array and its application to terahertz (THz) imaging. By using the free-standing shape of the CNT film, we could enhance the detection sensitivity by the reduction in the THz-induced thermal diffusion into substrates. Additionally, the free-standing CNT film array enabled us to fabricate THz cameras through simple two processes: electrode evaporation from front and rear side of the film. In contrast to conventional fabrication processes, this method can eliminate complicated processes such as lithography and chemical deposition/etching that restrict the adaptable range of CNT films. By utilizing the self-align filtration process, we developed a flexible THz camera and demonstrated real-time nondestructive imaging of industrial products. We expect that this simple fabrication process of a microscale free-standing CNT film array will promote the nanocarbon science to the practical use.



Photographic image of the flexible THz camera with microscale free-standing CNT film array.

P008 **Th 19:00 - 21:00**

Non-volatile optical memory with suspended graphene nanoribbons

Hiroo Suzuki[1,2], Toshiro Kaneko[1], Toshiaki Kato[1]

[1]*Department of Electronic Engineering, Tohoku University, Sendai 980-8579, Japan*
[2]*JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany*

Graphene nanoribbons (GNRs) combine the unique electronic, optical and spin properties of graphene with a transport gap, which makes them an attractive candidate material for the channels of next-generation transistors. Up to now, we developed a novel method based on the advanced plasma CVD method with nanoscale Ni catalyst (Ni nanobar) for directly fabricating suspended GNRs devices [1-2].

In this study, we will present optical non-volatile memory device with suspended GNR [3]. We measured high stable persistent photoconductivity (PPC) in the suspended GNR device, which is a phenomenon that photocurrent persists for a long time even after stopping photoirradiation. Utilizing PPC, we presented a repeatable operation of optical memory by combing writing and erasing memory by photo and gate voltage. The mechanism of PPC was also systemically investigated by surface analysis of oxide Ni and optical measurements. Based on these measurements, we reached a model of PPC involving the photo-protonation reaction in an interface between GNR and oxide Ni layer.

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Plenary Venue Poster

P010 **Th 19:00 - 21:00**

Quantitative measures of crystallinity in carbon nanotubes and its influence on mechanical behaviour

Krister Svensson[1], Mattias Flygare[1]

[1]*Department of Physics, Karlstad University, SE-65188 Karlstad, Sweden*

Different fabrication methods for production of carbon nanotubes will provide materials with different levels of crystallinity. As crystallinity is qualitatively known to have a direct influence on material properties, this raises the need for standardized quantitative analysis.

Here we have use transmission electron microscopy and electron diffraction to obtain quantitative information about crystallite sizes in individual nanotubes and its influence on the mechanical behaviour. The crystallinity of arc-discharge grown tubes was found to be high enough for the crystallite sizes to exceed the circumference of the tubes. This enables the formation of continuous graphene-like cylinders that constitute the nanotube walls. In contrast, the crystallite sizes for catalytically grown tubes are notably small, smaller than the tube circumference, implying that here the walls are made from a patchwork of small graphene-like grains.

The difference in atomic structure has profound effects on the mechanical behaviour, and one should really treat these as two distinctly different materials. This type of quantitative information, together with a classification system for different material qualities, will be vital for a successful utilization of carbon nanotube materials in applications.

P012 **Th 19:00 - 21:00**

Carrier density control of SWCNTs by chemical doping for electric power generation by electrolyte solution flow

Takeshi Tanaka[1], Guowei Wang[1], Atsushi Hirano[1], Hiromichi Kataura[1]

[1] *Nanomaterials Research Institute, National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Ibaraki 305-8565, Japan*

Electric power can be generated by moving an electrolyte droplet on a thin film of single-wall carbon nanotubes (SWCNTs); however, the power is not so high at present. To improve the efficiency, the carrier density of the film should be controlled precisely. In this study, we tried to control the number of organic dopant molecules inside SWCNTs. We used DPSQ* and PBI** as hole and electron dopant molecules, respectively, and coronene as a dummy molecule to control the number of the dopants. Figure shows the schematic illustration of how the dopant density inside SWCNTs can be controlled. Before doping, endcaps of SWCNTs (EC1.5, Meijo Nano Carbon) were removed by heating in air. Subsequently, the SWCNTs were refluxed in 1,4-dioxane for 3 h with different ratios of dopant and dummy molecules pre-dissolved therein. After the reflux process, the SWCNTs were washed for many times to remove excess dopant molecules outside the SWCNTs. We confirmed the different degrees of dopant encapsulation in SWCNTs using optical absorption spectroscopy. Details will be discussed in the presentation. This work was supported by JST CREST Grant Number JPMJCR16Q2, Japan.

*DPSQ: 2,4-bis[4-(N,N-diphenylamino)-2,6-dihydroxyphenyl] squaraine

**PBI: N,N’-bis(3-pentyl)perylene-3,4,9,10-bis(dicarboximide)

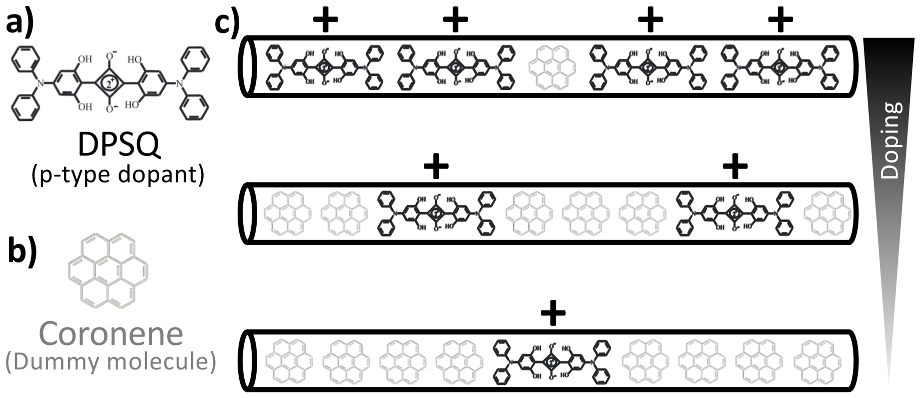

Figure The molecular structures of DPSQ (a) and coronene (b). Schematic illustration of the carrier density control of SWCNTs (c).

P014 **Th 19:00 - 21:00**

Effects of tungsten catalyst addition on the properties of direct-spun CNT materials

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Conventionally, Cambridge's floating catalyst CVD direct-spinning method uses iron, in the form of ferrocene, as the sole source for the metal catalytic particles on which the nanotubes grow [1]. However, work by other groups on fixed-catalyst CVD growth of CNTs has shown that the addition of tungsten to the catalytic transition metal in quantities up to 50 at% has the effect of narrowing the chiral angle distribution of the nanotubes produced [2]. In this work, we use several techniques, including Raman spectroscopy, thermogravimetric analysis, electron microscopy, and 4-probe conductivity measurements, to investigate the effects of incorporating different amounts tungsten from two different sources – namely tungsten hexacarbonyl and bis(cyclopentadienyl)tungsten(IV) dihydride – into the conventional ferrocene-based feedstock.

[1] Li, Kinloch, and Windle, Science Vol. 304, Issue 5668, pp. 276-278 (09 April 2004).
[2] Yang, et al., Nature Vol. 510, pp. 522–524 (26 June 2014).

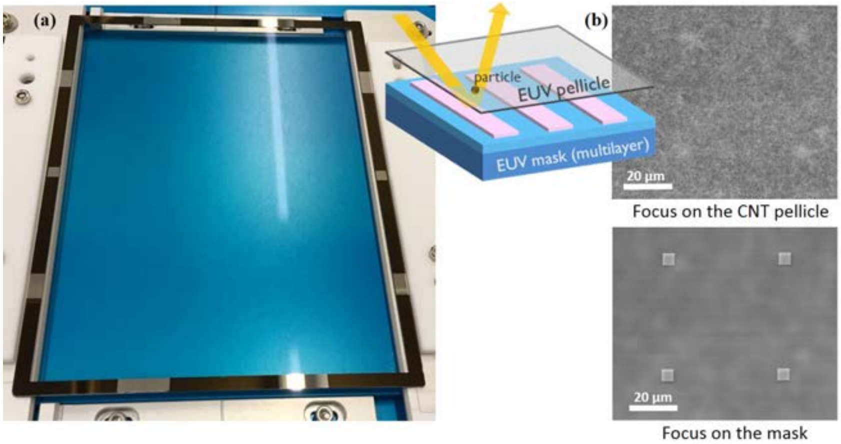
P016 **Th 19:00 - 21:00**

Free-standing carbon nanotube films for extreme ultraviolet pellicle application

Marina Y. Timmermans[1], Marina Mariano[1], Ivan Pollentier[1], Cedric Huyghebaert[1], Emily E. Gallagher[1]

[1]*imec, Kapeldreef 75, 3001 Leuven, Belgium*

A pellicle is required to enable high volume semiconductor manufacturing with extreme ultraviolet (EUV) lithography. A pellicle is a thin membrane suspended above the photomask to protect it from any fall-on particles. We propose free-standing (FS) membranes comprised of either SW or MWCNTs, to be used as a core material for the EUV pellicle. The very high EUV transmission of such films is attractive for the pellicle application where the loss of every EUV photon is translated into the reduction of scanner throughput. High transmission of CNT films in the range of 190-250 nm enables through-pellicle mask inspection. Data suggest that e-beam mask metrology may also be possible. FS CNT films are robust during handling even at the full pellicle size of 12x15 cm^2 supported by a silicon border with thin edges. The ability of such porous CNT films to stop particles as a function of film density was measured. Thermal stability of FS CNT films in vacuum was shown for EUV source power equivalent above 1 kW. The primary remaining challenge for the application of CNT pellicles is its chemical stability in the presence of a hydrogen plasma found in the EUV scanner. We explore coating FS CNTs with thin films to protect the CNTs while preserving high EUV transmission and mechanical stability.



(a) Free-standing CNT film at full pellicle size and schematics of EUV pellicle assembly on the photomask.(b) SEM images demonstrating the capability of through pellicle mask inspection.
[1] Timmermans et al, J. Micro/Nanolith. MEMS MOEMS 17(4), 2018

P018 **Th 19:00 - 21:00**

Bifacial Raman Enhancement on Monolayer Two-Dimensional Materials

Lianming Tong[1], Na Zhang[1], Jingjing Lin[1], Wei Hu[2], Liangbo Liang[3], Rui Wang[4], Xue Luo[1], Yi Luo[2], Xiaohui Qiu[4], Jin Zhang[1]

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Understanding the charge interaction between molecules and two-dimensional (2D) materials is essential for the design of functional devices. This interaction leads to not only the modulation of the opto-electronic properties of materials, but also the Raman scattering enhancement of molecules. Here, we show the bifacial Raman enhancement of molecules on monolayer graphene and hexagonal boron nitride (h-BN). Taking advantage of the atomically thick layered structure, we show that both surfaces of 2D materials can interact with molecules and simultaneously enhance their Raman scattering. A different enhancement was observed for monolayer graphene and h-BN. The intensity decrease of particular Raman modes of copper phthalocyanine (CuPc) on both surfaces of h-BN suggests that z-dipoles exist and are partially canceled out between the two interfaces, while the twice Raman intensities of CuPc on both surfaces of graphene compared to that on one surface evidenced the charge transfer process. These results provide an approach to modify 2D materials by bifacial adsorption of molecules, and the findings can inspire the design of functional 2D material-based devices.

P020 **Th 19:00 - 21:00**

Tunable properties of pristine and filled single-wall carbon nanotubes assembled in macrostructures

Alexander Tonkikh[1,2], Victor Tsebro[3,4], Ekaterina Obraztsova[2,5], Valentina Eremina[1,2], Ivan Kondrashov[1], Esko Kauppinen [6], Andrey Chuvilin[7,8], Elena Obraztsova[1,2]

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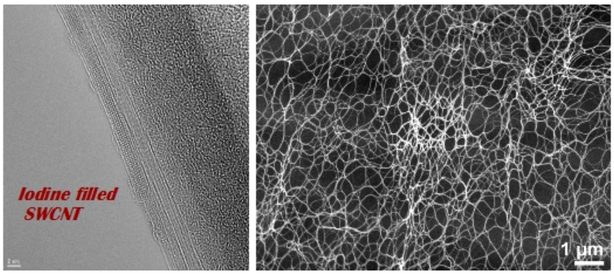
[2] *A.M. Prokhorov General Physics Institute, RAS, 38 Vavilov Street, 119991 Moscow, Russia.*
[3] *P.N. Lebedev Physical Institute, RAS, 53 Leninsky Prospect, 119991 Moscow, Russia.*
[4] *Kapitza Institute for Physical Problems, RAS, 2 Kosygina Street, 119334 Moscow, Russia*
[5] *Shemyakin and Ovchinnikov Institute, RAS, 16/10 Miklukho-Maklaya Str, 117871 Moscow Russia*
[6] *Depart. of Applied Physics, Aalto University, P.O. Box 15100, FI00076 Espoo, Finland*
[7] *CIC nanoGUNE Consolider, Tolosa Hiribidea 76, 20018 Donostia-San Sebastian, Spain*
[8] *IKERBASQUE Basque Foundation for Science, Maria Diaz de Haro 3, E-48013 Bilbao, Spain*

At the moment, namely the assembled structures (films, buckypaper, and fibers) are used and most integrated for making various devices (displays, diodes, detectors, etc.). Therefore, there is a need to tune the properties of such structures for specific technological tasks and applications.

In this work, we present a comprehensive study of the formation of assembled structures based on pristine and modified SWCNTs [1]. We show the effect of diameters, ratio of metal and semiconductor nanotubes and filling of the internal channels of nanotubes on the properties of the assembled structure as a whole.

Another important direction is to study the interaction of assembled SWCNTs or their hybrids with external factors. In this area, we have studied optical and transport properties of assemblies of pristine or filled SWCNTs. This is important for control of the stability and property modifications of both the macrostructures and the nanostructures formed inside single-walled carbon nanotubes.

The work was supported by RFBR project 18-29-19113-mk, grant No 311533 of Academy of Finland, Russian Federation President Program for young scientist MK-3140.2018.2. Also, the reported study was funded by RFBR and Moscow city Government according to the research project No 19-32- 70004.



HRTEM image (left) of SWCNT filled with iodine; SEM image (right) of aerosol-grown SWCNT films [1]. [1] Nanoscale, 2019, DOI: 10.1039/C8NR10238D

Plenary Venue Poster

P022 **Th 19:00 - 21:00**

Aerosol doping of single walled carbon nanotubes

Alexey Tsapenko[1,2], Stepan Romanov[1], Daria Satco[1], Dmitry Krasnikov[1], Anastasia Goldt[1], Anton Anisimov[3], Albert Nasibulin[1,2]

[1]*Skolkovo Institute of Science and Technology, Nobel str. 3, 121205 Moscow, Russian Federation*
[2]*Aalto University, Department of Applied Physics, Puumiehenkuja 2, 00076 Espoo, Finland*
[3]*Canatu Ltd., Konalankuja 5, 00390, Helsinki, Finland*

Being a unique material with diverse exceptional properties, single-walled carbon nanotube (SWCNT) still need an improvement of their conductivity for numerous applications. Among various techniques, adsorption doping with HAuCl4 dissolved in ethanol is the most efficient way to enhance it. Unfortunately, the dopant deposition is yet not sufficient for roll-to-roll production of largely uniform flexible and stretchable transparent conductive films (TCFs). Thus, precise control of dopant formation on top of the SWCNTs is a highly desirable tool for both theoretical studies and emerging mass production technologies. First, will allow to understand the nature of doping mechanism, including nanoparticle aggregation role. The second, may positively influence the resulting film morphology and optoelectronic values. To realize it, we introduced and utilized a controllable aerosol doping approach. The volumetric uniformity of the films was confirmed at an each process step. Also, peculiar thickness dependent scattering effect was uncovered. Finally, based on the precise doping level change and unique peak position control, we optimized the doping set-up for TCF applications with low equivalent sheet resistance values. This work was supported by Russian Science Foundation No. 17-19-01787.

P024 **Th 19:00 - 21:00**

Influence of CNT’s Length on Polymer based CNT composites

Shuntaro Tsuchiya[1], Toshiyuki Yasuhara[1]

[1]*Nippon Institute of Technology*

Nanocarbon materials are well known to have excellent property. Generally, fiber length and dispersion are important factors on the properties of Fiber Reinforced Plastic (FRP). It is said that CNT have especially high aspect ratio. And also, properties of CNT’s composites usually have close relationships between length and dispersion. However, both dispersion and length of CNTs inside of composites are very difficult to observe or evaluate. In this study, the influence of length of single wall carbon nanotube (SWCNT) in polymers on properties of polymer based SWCNT composites was investigated.
Fiber lengths of CNTs were measured by SEM observation. Then, the relationships between properties and CNT length were investigated. Secondly, CNT were kneaded with polypropylene (PP) using a mechanical melt mixer. Mixer which has twin screw named elliptical blade was used. The blades were modified to increase in strain rate. As a result, In the case of high rotation speed, tensile strength of composite specimens decreased at all mixing conditions. Therefore, molecular chains of polypropylene and CNT seem to be shortened by high strain rate. In case of using small gap blade, dispersion of CNT was improved by the cause of increase of shear stress and strain rate.

P026 **Th 19:00 - 21:00**

Edge plasmon in graphene ribbon

M. Shoufie Ukhtary[1], Maruoka Masato[1], Riichiro Saito[1]

[1] *Department of Physics, Tohoku University, Japan*

Surface plasmon (SP) is an oscillation of charge density followed by the propagation of electromagnetic (EM) wave on a surface. The SP in graphene forms a truly 2D plasmon and it is tuneable by gate voltage. However, if we consider the region in the vicinity of edge, there will be an accumulation of charges near the edge. This accumulation of charges can also oscillate collectively and form so-called the edge plasmon with the EM fields localized near the edge. The edge plasmon is distinct mode from the 2D plasmon and the EM fields is localized near the edge, not uniform across the surface.

In this work, we discuss the edge plasmon in graphene ribbon with finite width by solving the electric potential analytically using the Lorentz gauge. We show that the frequency of edge plasmon depends on the width and the Fermi energy of graphene. More importantly, we also found that the electric field of edge plasmon on the surface of graphene rotates as a function of time, in contrast to case of 2D plasmon. The reason of the rotation is that the phase difference between the electric fields in the direction parallel and perpendicular to the edge due to localization of electric fields near the edge. As a result, the induced current is also rotating on the surface.

P028 **Th 19:00 - 21:00**

A thermodynamic study of SC surfactant adsorption and SDS co-adsorption on SWNT surfaces

Markus Voelckel[1], Ivonne Vollert[1], Friedrich Schöppler[1], Tobias Hertel[1]

[1] *Julius-Maximilians-Universität, Würzburg, 97074, Deutschland*

Surfactants play an important role in the solubilization, purification and separation of single-wall carbon nanotubes (SWNT). Aqueous mixtures of ionic surfactants like sodium dodecyl sulfate (SDS) and sodium cholate (SC) are commonly used for isolation of SWNTs with different properties. Still, the mechanisms underlying selectivity and interactions between adsorbed surfactants and different SWNTs are not well understood.

Here we present an investigation of surfactant (co-)adsorption on different SWNTs using small changes in the fluorescence spectra of dispersed SWNTs as a local probe of changes in the structure of the surfactant adsorbate layers. Such changes are used to determine thermodynamics and cooperativity of SWNT-surfactant micellization, providing new insights into the origins of surfactant selectivity [1].

Our investigations reveal that SWNTs with a smaller diameter generally form thermodynamically more stable SC micelles. The admixture of SDS is found to alter the Gibbs free energy of SWNT-SC micelles by formation of mixed SDS-SC adsorbate layers. Small SDS mass fractions induce stabilization of SC-SWNT micelles while larger SDS concentrations destabilize these micelles.

[1] F. F. Bergler, S. Stahl, A. Goy, F. Schöppler, T. Hertel, Langmuir 2016, 32, 9598-9603.

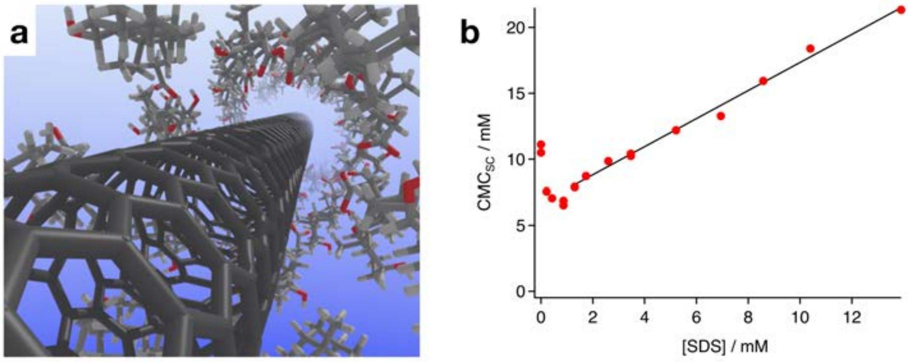


Fig. 1: a) Schematic illustration of adsorbed SC on a (6,5) s-SWNT. b) Shift of the CMC with increasing SDS concentration.

Plenary Venue Poster

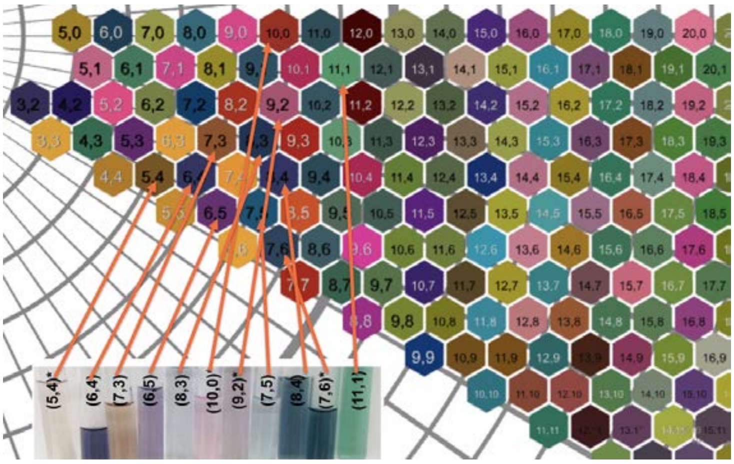
P030 **Th 19:00 - 21:00**

Color of single-walled carbon nanotubes

Nan Wei[1], Ying Tian[2], Yongping Liao[1], Qiang Zhang[1], Aqeel Hussain[1], Saeed Ahmed[1], Erxiong Ding[1], Abu Taher Khan[1], Fengrui Yao[3], Kaihui Liu[3], Hua Jiang[1], Esko Kauppinen[1]

[1]*Department of Applied Physics, Aalto University School of Science, Puumiehenkuja 2, 00076 Aalto, Finland*
[2]*Department of Physics, Dalian Maritime University, Dalian, Liaoning 116026, China.*
[3]*School of Physics, Collaborative Innovation Center of Quantum Matter, Peking University, Beijing 100871, China*

We report the colorful nature of single-walled carbon nanotubes. The colours of 466 species are calculated, covering all species that has been experimentally prepared. The relationship between optical absorption and color of SWCNTs is experimentally verified. We found good agreement between the calculated colours and samples of previous experiments. A method for taking photographs with more accurate colour is proposed. The results show that the most colourful SWCNTs are yet to be prepared.



Part of calculated colors of carbon nanotube helicities and one of the experimental data (Piao et al. ACS Nano 10, 5252–5259 (2016)) as verification.

P032 **Th 19:00 - 21:00**

Electrochemical properties of 3D graphene sponge fabricated from graphene oxide

Zizhao Xu[1], Chikako Ishiguro[1], Ahmad Ibadurrahman[1], Yuta Nishina[2], Yoshihiro Kobayash[1]

[1] *Osaka University*
[2] *Okayama University*

Single-layer graphene exhibits excellent properties for electric and thermal conductance, but is easy to stack to form graphite structure, resulting in degradation of these properties. We have addressed it by fabricating 3D graphene sponge with single-layer properties[1]. In this work, we examine electrochemical features of the 3D graphene to elucidate the performance.

Graphene oxide(GO) sponge was prepared as reported previously[1] and were thermo-treated at 400/1500ºC in Ar or Ar+ethanol (named as GS400-Ar, GS1500-Et, and so on). To control layer spacing, some samples are prepared from mixture of GO and cellulose nanofiber (GCS400-Ar, GCS1500-Et). Electrode activity is evaluated by analyzing cyclic voltammetry (Fig. 1(a)). The scan rate dependence of anodic peak potential in voltammogram (Fig. 1(b)) indicates that more defective samples (GS400/1500-Ar) exhibit reversible behavior. Contrary to expectation by superior current for higher conductivity, irreversible behavior is observed from less defective and spacing-controlled samples (GS1500-Et and GCS1500-Et). These results suggest that controlled formation of artificial defects in defect-free graphene sponge is a promising strategy to develop high-performance electrode materials.

[1] Z. Xu et al., PS050, NT18 (2018, Beijing).

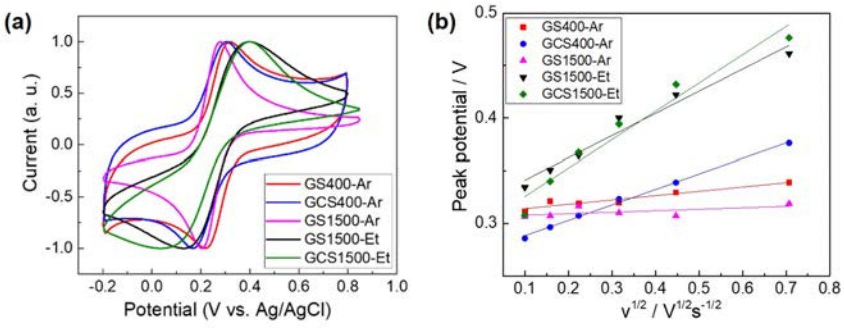


Fig. 1 (a) Cyclic voltammogram (CV) with scan rate v=100mV/s observed from various graphene sponge samples (b) Correlation between the peak anodic potential in the CV and scan rate (v1/2).

P034 **Th 19:00 - 21:00**

Surface-Enhanced Raman Spectroscopy of Individual Single-Walled Carbon Nanotubes

Juan Yang[1], Chenmaya Xia[1], Daqi Zhang[1], Henan Li[1], Sheng Li[1], Haoming Liu[1], Ruoming Li[1], Yan Li[1]

[1] *College of Chemistry and Molecular Engineering, Peking University, Beijing 100871, China*

Surface-enhanced Raman scattering (SERS) spectroscopy can enhance weak signal and expand the resonance window. However, detection of off-resonance single-walled carbon nanotubes (SWNTs) by SERS remains challenging due to the difficulties in locating the SWNTs exactly at the hot spots. Here, we report a method to in-situ form closely spaced polyhedral gold nanocrystals (AuNCs) on suspended SWNTs. The fact that the edges of the AuNCs attach to the SWNTs ensures the location of SWNTs at the hot spots. Consequently, we achieve enormous enhancements of the Raman signal of the SWNTs that are two orders of magnitude higher than any previous values. This enables the detection of many off-resonance SWNTs and also several new Raman bands of the SWNTs.
Moreover, We show that single molecules (SM) encapsulated inside the SWNT and located at the hot spot can be unambiguously detected. We then monitor those SERS fingerprints as the single molecule undergoes a chemical reaction inside the SWNTs. The encapsulation of the single molecules inside the SWNT reduces the vast complexities caused by the SM signal fluctuations, and may help to achieve a fundamental understanding of the SM behavior and SM reactivity.

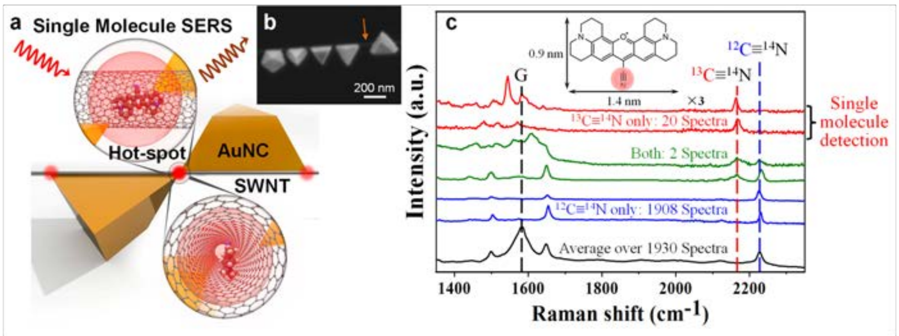


Fig.1 Schematics (a), SEM image (b), and SERS spectra (c) of the AuNCs-SWNT nanocomposite with a single rhodamine 800 molecule encapsulated inside the SWNT and located at the hot spot.

P036 **Th 19:00 - 21:00**

Nanotube-based High-Brightness Fluorophores for Flow Cytometry

Yoke Khin Yap[1], Nazmiye Yapici[1, 2], Rodney Oakley[1, 2], Xiuling Liu[1], Dongyan Zhang[1]

[1]*Department of Physics, Michigan Technological University, USA*
[2]*StabiLux Biosciences, Inc, USA.*

High-brightness fluorophores (HBFs) based on carbon nanotubes (CNTs) and boron nitride nanotubes (BNNTs) will be discussed for biomarker identification on live cells. These HBFs are several thousand times brighter than regular dyes, suggesting for a promising new application of nanotubes for counting and sorting of rare cells in immunology, cancer, and stem cell research. Flow cytometry is a laser fluorescence-based technique indispensable for clinical and research laboratories. The performance of flow cytometry is limited by "autofluorescence" and "spill-over". Here, we demonstrated that CNTs and BNNTs can be used to create HBFs to overcome these issues. These HBFs can be conjugated with antibodies to specifically recognize bio molecules on T cells. Binding efficiencies above 97% have been achieved. Furthermore, the fluorescence brightness of each HBFs is more than 2000X brighter than commercial fluorophores. We also found a significant brightness difference between fluorophores made of CNTs and BNNTs. The theoretical basis of the HBF design, and detailed experimental results will be discussed in the meeting.

Yoke Khin Yap acknowledge funding supports from National Science Foundation (DMR 1266910, IIP 1738466).

Plenary Venue Poster

P038 **Th 19:00 - 21:00**

Photoluminescence Spectra from Single-Walled Carbon Nanotubes on hexagonal Boron Nitride

Satoshi Yotsumoto[1], Tatsuro Ogamoto[1], Tatsuya Murai[1], Hayato Arai[1], Taiki Inoue[1], Rong Xiang[1], Shigeo Maruyama[1,2], Shohei Chiashi[1]

[1]*Department of Mechanical Engineering, The University of Tokyo, Tokyo 113-8656, Japan*
[2]*Energy NanoEngineering Lab., AIST, Ibaraki 305-8656, Japan*

Photoluminescence (PL) spectroscopy is one of the important methods to analyze optical properties of single-walled carbon nanotubes (SWCNTs). SWCNTs which emit PL on substrates are needed in the field of optoelectronics devices of SWCNTs, and PL emission from SWCNTs on hexagonal boron nitride (h-BN) were recently reported [1]. In this study, SWCNTs were synthesized on h-BN by using CVD method and their PL spectra were investigated. Multilayered h-BN was prepared on silicon substrates by mechanical exfoliation. The catalyst particles were prepared only on the silicon substrates and not on h-BN. Ethanol was used as the carbon source of SWCNT growth. SWCNTs on h-BN were observed by scanning electron microscope (SEM) and atomic force microscope (AFM). We obtained PL maps of SWCNTs with different chiralities and compared them with those of air-suspended SWCNTs [2] and surfactant-wrapped SWCNTs [3]. It was found that the optical transition energy of SWCNTs on h-BN was redshifted compared with that of surfactant-wrapped SWCNTs due to the environmental effects.

[1] J. C. Noé et al., Nano Lett. 18, 4136 (2018).
[2] J. Lefebvre and P. Finnie, Phys. Rev. Lett. 98, 167406 (2007).
[3] S. M. Bachilo et al., J. Am. Chem. Soc. 125, 11186 (2003).

P040 **Th 19:00 - 21:00**

High-Efficiency Growth of Single-Wall Carbon Nanotubes with Uniform Structures

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[1]*Center for Multidimensional Carbon Materials, Institute for Basic Science, UNIST-gil 50, Ulju-gun, Ulsan 44919, Korea*
[2]*Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, Wenhua Road 72, Shenyang 110016, China*
[3]*School of Material Science and Engineering, Ulsan National Institute of Science and Technology, UNIST-gil 50, Ulju-gun, Ulsan 44919, Korea*

Single-walled carbon nanotubes (SWCNTs) with uniform structure are highly desired for fabricating high-performance electronic devices.1 Great efforts have been devoted to synthesizing SWCNTs with specific chirality or conductivity.2,3 However, up to now, the yields of most synthesized SWCNTs with uniform structures are normally quite low. Comparing with single metallic catalysts, bimetallic catalysts have advantages in controlled growth of SWCNTs. Here we report a bimetallic particle catalyzed chemical vapor deposition (CVD) SWCNT growth. High density SWCNTs networks with a narrow chirality distribution are obtained by using specially designed bimetallic nanoparticles as catalysts. It is found that the growth-efficiency and structural uniformity are highly depended on the catalysts-composition ratio.

1. Franklin, A. D.,. Nature 2013, 498 (7455), 443-444.
2. Liu, C.; Cheng, H. M.,. J. Am. Chem. Soc. 2016, 138 (21), 6690-6698.
3. Wang, X.; He, M. S.; Ding, F.,. Mater. Today 2018, 21 (8), 845-860.

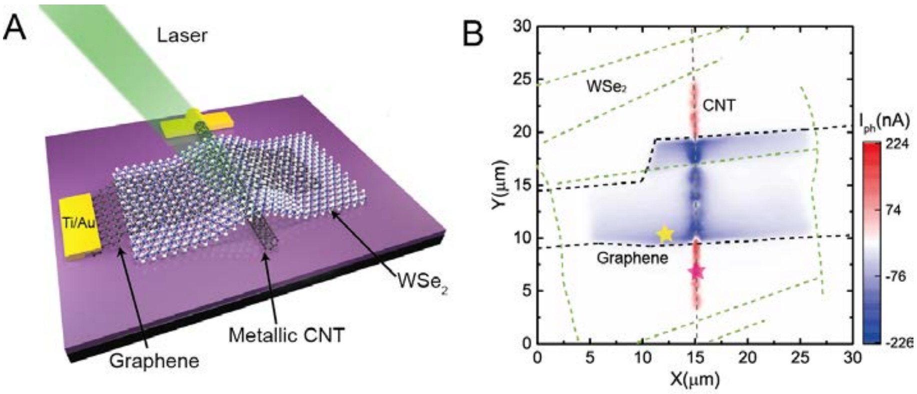
P042 **Th 19:00 - 21:00**

Electrical control of spatial resolution in mixed-dimensional heterostructured photodetectors

Ke Zhang[1], Yang Wei[1], Kaili Jiang[1], Shoushan Fan[1]

[1]*Department of Physics and Tsinghua-Foxconn Nanotechnology Research Center, Tsinghua University, Beijing 100084, China*

Low-dimensional nanomaterials, such as one-dimensional (1D) nanomaterials and layered 2D materials, have exhibited significance for their respective unique electronic and optoelectronic properties. Here we show that a mixed-dimensional heterostructure with building blocks from multiple dimensions will present a synergistic effect on photodetection. A carbon nanotube (CNT)– WSe_2–graphene photodetector is representative on this issue. Its spatial resolution can be electrically switched between high resolution mode (HRM) and low-resolution mode (LRM) revealed by scanning photocurrent microscopy (SPCM). The reconfigurable spatial resolution can be attributed to the asymmetric geometry and the gate-tunable Fermi levels of these low-dimensional materials. Significantly, an interference fringe with 334 nm in period was successfully discriminated by the device working at HRM, confirming the efficient electrical control. Electrical control of spatial resolution in CNT–WSe_2–graphene devices reveals the potential of the mixed-dimensional architectures in future nanoelectronics and nano-optoelectronics.



(A) Schematic illustration of the CNT–WSe_2–graphene heterostructure. (B) A representative SPCM image of the heterostructure device taken at VG = VDS = 0 V (laser wavelength, 520 nm; power, 24 μW; spot size, ∼1 μm).

P044 **Th 19:00 - 21:00**

Ultralong Carbon Nanotubes: Structures, Synthesis and Properties

Rufan Zhang[1]

[1] *Tsinghua University*

Ultralong carbon nanotubes (CNTs) usually refer to the horizontally aligned CNT arrays with lengths up to centimeters or even decimeters grown on flat substrates by chemical vapor deposition. With the optimized growing conditions, we successfully synthesized half-meter long CNTs. They have perfect structures and extraordinary electrical and mechanical properties. In addition, Optical visualization of individual ultralong CNTs by chemical vapour deposition of titanium dioxide nanoparticles was realized. Moreover, we found the macroscale superlubricity in centimeters long perfect double-walled CNTs under ambient conditions. Recently, CNT bundles with defect-free, neat, unifom oriented, continuous, and stress free structure were successfully prepared, which showed a tensile strength over 80 GPa.

P045 **Th 17:00 - 18:30**

Synthesis and electrical properties of 1D-2D van der Waals heterostructures via van der Waals epitaxy

Boyuan Shen[1], Fei Wei[1]

[1] *Department of Chemical Engineering, Tsinghua University*

Epitaxial growth of 2D layered materials via van der Waals (vdW) interaction has opened up an unprecedented opportunity to design nanoscale heterostructures with perfect interfaces and no invasive structure destruction. However, there is no effective method to fabricate 1D/2D vdW heterostructures with the epitaxial growth on 1D materials. Here we report a bottom-up strategy for 1D/2D vdW heterostructures based on the 1D ultralong carbon nanotubes (ULCNTs). The anthracene and molybdenum oxide (MoO_3) were used to form 2D hexagonal structure on single ULCNTs by the vapor deposition. The heterostructures were characterized by optical microscopy, Raman spectroscopy, scanning electron microscopy (SEM) and transmission electron microscopy (TEM). The growth rates, numbers and orientations of the layered hexagonal crystals could be accurately controlled. And the mechanism of 1D-2D transition was conjectured based on the lattice distortion in radial direction. These results can help us understand the epitaxial process on the abrupt 1D interfaces and pave the way for the fabrication of perfect vdW heterostructures in diverse dimensionalities for further applications in electronic devices and nano-electromechanical systems (NEMS).

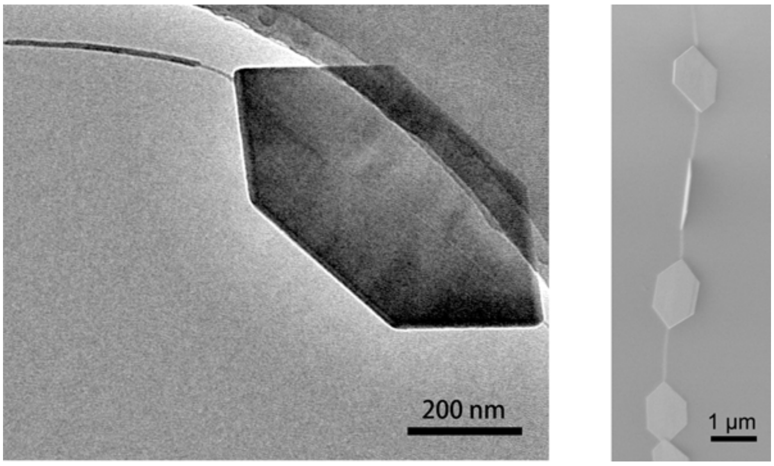


Figure 1 TEM and SEM images of CNT/α-MoO_3 heterostructures

P047 **Th 17:00 - 18:30**

Highly Ordered Metallic Phase of Indium on SiC(0001)

Maximilian Bauernfeind[1], Jonas Erhardt[1], Jörg Schäfer[1], Ralph Claessen[1]

[1]*Physikalisches Institut and Röntgen Research Center for Complex Material Systems, Universität Würzburg, D-97074 Würzburg, Germany*

For the monolayer growth of two-dimensional topological insulators (2D-TIs) on the insulating SiC(0001) substrate, the strong interaction between the deposited layer and the substrate dangling bonds (DBs) plays a pivotal role and drastically affects the electronic structure of the system. Especially 2D-TIs with fragile topology, e.g. quasi-freestanding stanene, require a passivated substrate to cancel out such interactions that are detrimental for the topological properties [1]. Indium with its three valence electrons is such a passivation candidate and leads to metallic or insulating phases on various semiconducting surfaces. Here we report first results of a highly ordered indium phase on SiC(0001). Scanning tunneling microscopy (STM) reveals a Kagome-like superstructure tentatively assigned as a $(4\sqrt{3} \times 4\sqrt{3})$R30° reconstruction. Additionally, scanning tunneling and angle-resolved photoelectron spectroscopy (STS and ARPES) show a band structure distinct from pristine SiC and reveal a metallic character with a pronounced electron pocket, indicative of a 2D electron gas. Interestingly, despite the large unit cell observed in STM and low-energy electron diffraction, the corresponding Brillouin zone is not effective in the ARPES band structure.

[1] D. Di Sante et al., Physical Review B 99, 035145 (2019)

P049 **Th 17:00 - 18:30**

Optical characterization of ion implanted monolayer transition metal dichalcogenides

Minh Bui[1], Jhih-Sian Tu[1], Manuel Auge[2], Sven Borghardt[1], Eoghan O'Connell[3], Ursel Bangert[3], Hans Hofsäss[2], Beata Kardynał[1]

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Monolayers (MLs) of transition metal dichalcogenides are a new class of two-dimensional semiconductors that draw much attention due to their unique band structure and geometry, resulting in exciting physical properties. Deterministic doping is a desirable pathway to exploit those properties, analogously to bulk semiconductors. In this contribution, low energy ion implantation was used to incorporate dopant atoms into MoS_2 MLs. Optical properties of the implanted MLs were investigated with Raman, reflectance and photoluminescence spectroscopies. The prototypical system of Se-implanted MoS_2 was prepared with ion energies ranging from 10 to 25 eV and fluence from 0.1 to 5 ions per chalcogen atom in the top layer. With S atoms being substituted by Se, MoS_2 is converted to $MoSe_{2x}S_{2(1-x)}$ while no free charge carriers are created. Evidence of implantation levels higher than required for doping, up to 20%, is shown. The ion energy is found to be a compromise between implantation success rate and defect formation. We also identify the most likely defects, and treatments for healing these defects are discussed.

P051 **Th 17:00 - 18:30**

Hyperelastic material models for graphene and blue phosphorus

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Two new hyperelastic material models are presented for graphene and single layer blue phosphorus [1, 2, 3]. They are nonlinear and can capture anisotropic material behavior. A set of DFT simulations, two perpendicular uniaxial stretches and one pure dilatation test, is designed for the calibration of the model. The models are then implemented in the rotation-free shell formulation of [4].

These material models are then used for studying indentation of graphene and blue phosphorus sheets [1, 3], torsion, bending and modal analysis of carbon nanotubes and carbon nanocones [5], and modal analysis of graphene and blue phosphorus sheets [5, 3]. The results are compared with atomistic results and they are in good agreement.

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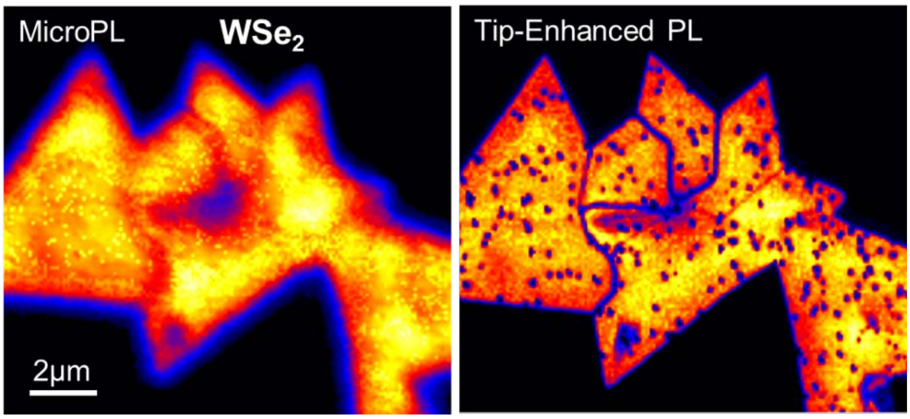
P053 **Th 17:00 - 18:30**

Know more about your 2D Material with Tip-enhanced Raman spectroscopy and Photoluminescence combined with other Scanning Probe Microscopy Methods

Jana Kalbacova[1], Marc Chaigneiau[1], Andrey Krayev[1]

New two dimensional materials are on the rise. After the wonder material graphene, new materials such as MoS_2, $MoSe_2$, WSe_2 have an intrinsic bandgap and as such are opening new doors for semiconductor applications. Raman spectroscopy offers information on the chemical structure of materials but cannot provide information on the electronic properties such as surface potential or photocurrent of our sample. Co-localized measurements combining scanning probe microscopy (SPM) with Raman spectroscopy can already bring a wealth of information; however, further improvements can be obtained by a tip that will act as an antenna and amplify the Raman signal and thus breaking the diffraction limit in a method called Tip-enhanced Raman spectroscopy (TERS). Typically spatial resolution of 10 – 20 nm can be achieved. In this contribution, we investigate different 2D materials by a combination of TERS, tip-enhanced photoluminescence, Kelvin probe microscopy, and other SPM methods to show very locally for example doping variations or defects that would otherwise go unnoticed with other macro- and microscopic techniques.



Comparison of conventional photoluminescence (microPL) and tip-enhanced photoluminescence of WSe_2.

P055 **Th 17:00 - 18:30**

Exploring How To Chemically Tune The Properties Of Graphene Covered With Hydroxyl And Epoxy Groups From First-Principles Calculations

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Within the field of two-dimensional crystals, the study of graphene oxide (GO) has two mainly research interests. Chemical reduction of GO for production of graphene and its great application potential in different fields, such as (opto)electronics, sensors, energy storage. Besides, its properties mainly depend on the oxidation level, making its study rich in terms of physics and possible applications.
In this work, combining a statistical model with DFT calculations, we study the incomplete oxidation of graphene for hydroxyl and epoxy oxidant groups. The chemically tunable properties are described as a function of the amount of hydroxyl and epoxy groups. A complete scenario of energetics and phase stability is developed, yielding insight into the structure, electronic and optical properties of graphene oxide. A tendency to agglomeration of oxygen-containing groups is found, independently of their relative proportion. Finally, we discussed the dependence of the optical absorbance on composition and temperature of a fully oxidized GO phase and demonstrated a strong influence of the relative amount of –OH and –O– groups on the calculated absorption spectra.

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P057 **Th 17:00 - 18:30**

Optical gain in nanographene molecules and modulation of their optical properties by peripheral substituents

Francesco Scotognella[1], Giuseppe M. Paternò[2], Qiang Chen[2], Xiao Ye Wang[3], Junzhi Liu[1], Silvia Motti[1], Annamaria Petrozza[3], Xinliang Feng[1,4], Guglielmo Lanzani[2], Klaus Müllen[2], Akimitsu Narita[4], Francesco Scotognella

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The potential application in photonics of large polycyclic aromatic hydrocarbons, also called nanographene molecules, has remained largely unexplored. Here we show the optical gain properties of dibenzo[hi,st]ovalene and the low power threshold when the molecule is embedded in an inert polymer matrix [1]. Ultrafast transient absorption helps to elucidate the stimulated emission in this material. Moreover, we study the modulation of the nonlinear optical properties of dibenzo[hi,st]ovalene as a function of the peripheral substituents [2].

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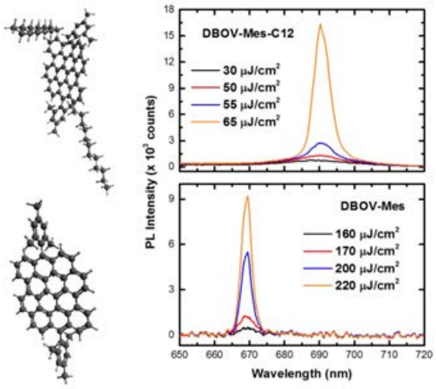

(Left) Optimized geometries of DBOV-Mes-C12 and DBOV-Mes. (Right) Photoluminescence spectra as a function of the laser energy density for DBOV-Mes-C12 and DBOV-Mes.

P058 **Th 19:00 - 21:00**

Hot electrons modulation of third harmonic generation in graphene

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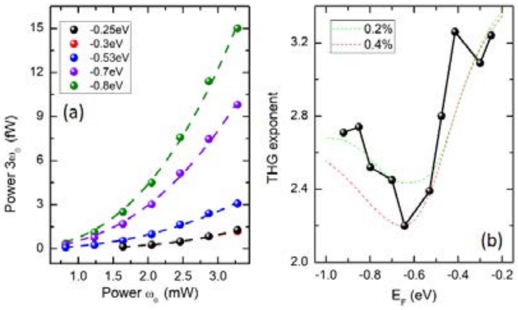
We perform power-dependent third harmonic generation (THG) measurements on gated single layer graphene (SLG) and show that hot-electrons induce a large deviation from the expected cubic power-law. Fig.1(a) plots the experimental THG power dependence for incident photon energy$\hbar\omega$=0.69 eV and for different EF values of the SLG device. Fig.1(b) plots the THG exponent as a function of EF. The dotted lines in Fig.1(b) are the theoretical values of the THG exponent, calculated as follows: (i) we derive the electronic temperature (Te) as a function of incident power considering two values of the residual absorption α=0.2% and 0.4%. α originates from intra-band electronic transitions enabled by disorder when EF»$2\hbar\omega$; (ii) we use these to calculate the third-order optical conductivity σ(3) as a function of incident power ; (iii) we calculate the theoretical THG intensity given the power-dependent value of σ(3). We find that the THG exponent varies between $\sim$2 and 3.4, with a non-monotonic behavior as a function of EF and with a minimum at EF$\sim$0.6eV. An increase of the incident power affects Te and □(3) and this induces deviations from the expected cubic power-law in SLG. This work shows that hot-electrons significantly alter the third-order nonlinear optical response of SLG.



(a) THG power dependence in SLG for different values of EF. (b) THG exponent as a function of EF. The black line and spheres represent experimental data. The dotted lines are theoretical results for different values of the SLG residual absorption.

P060 **Th 19:00 - 21:00**

Prediction of low temperature valley polarization characteristics in 2D semiconductors using machine-learning approach

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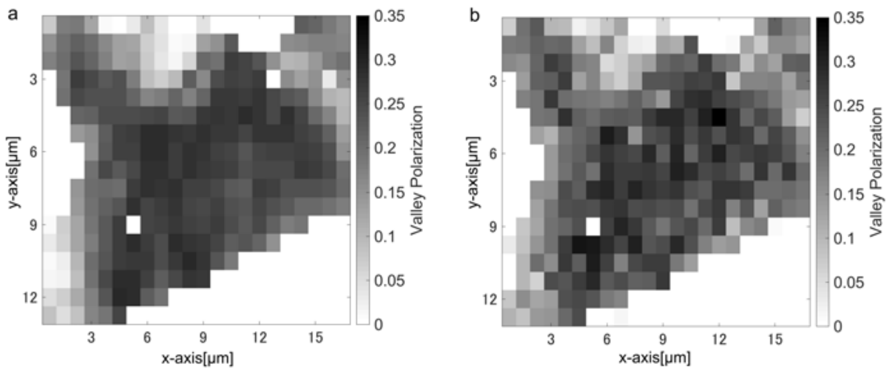
Monolayer (1L-) transition metal dichalcogenides (TMDCs) such as 1L-WSe$_2$ show valley polarization (VP) of excitons under irradiation of circularly polarized light at low temperature (LT). This unique characteristic has offered new possibility of information processing in future optoelectronics technologies called valleytronics. When we measure the VP as a function of position at LT, VP normally shows spatially inhomogeneous distribution as shown in Fig. 1(a). This spatial inhomogeneity is highly problematic not only for fundamental scientific researches but also for applications of these materials in valleytronic devices. Thus, a rapid screening method of the local VP distribution is strongly desired for the sample's quality inspection. Here, we demonstrate machine-learning-based prediction of the VP of 1L-WSe$_2$ at LT only from the information of their photoluminescence (PL) spectra at room temperature (RT). Predictive random forest models were grown for the VP at LT (30K) using the information of PL spectra at RT (300K). We gave local information at each position on a new sample at RT to the learned tree and successfully predicted the local VP at 30K as shown in Fig. 1(b). The results suggest that random forest method is a suitable approach for this problem.



(a)Experimental and (b)predicted spatial distributions of exciton valley polarization in a mechanically exfoliated 1L-WSe$_2$ on a SiO$_2$/Si substrate.

P062 **Th 19:00 - 21:00**

Tunable electronic and magneto-optical properties of monolayer arsenene from GW0 approximation to large-scale tight-binding simulations

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Monolayers of group VA elements have attracted great attention with the rising of black phosphorus. Here, we derived a simple tight-binding model for monolayer grey arsenic, referred as arsenene (ML-As), based on the first-principles calculations within the partially self-consistent GW0 approach. The resulting band structure derived from the six p-like orbitals coincides with the quasi-particle energy from GW0 calculations. In the presence of a perpendicular magnetic field, ML-As exhibits two sets of linear Landau levels with respect to the magnetic field strength and level index. Our numerical calculation on the optical conductivity spectrum of ML-As also reveals that the obtained optical gap is very close to the GW0 optical gap and it can be effectively tuned by external magnetic field. Thus, our proposed TB model paves a new way in describing the electronic structure of ML-As and can be used for further large-scale studies of the electronic, optical and transport properties.

P064 **Th 19:00 - 21:00**

Orientation-Dependent Chiral Raman Response of two-dimensional ReS_2

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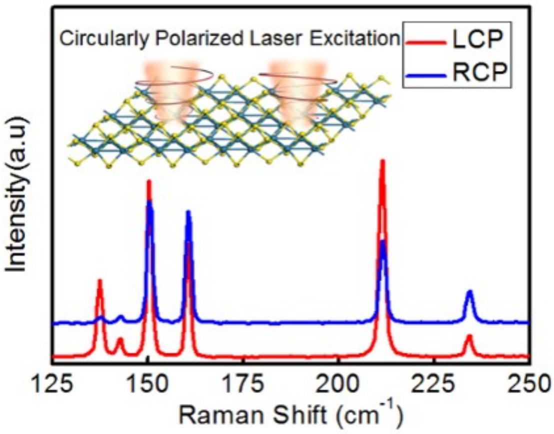
The Raman tensor of a crystal is dependent on the symmetries of the crystal and the Raman-active vibrational mode. The intensity of a particular mode is determined by the Raman selection rule, which involves the Raman tensor and the polarization configurations. However, for the triclinic ReS_2, the symmetry is lower and only has an inversion center, so the 2D ReS_2 has different vertical orientations. Herein, we report the anomalous chiral Raman response of 2D layered triclinic ReS_2, and showed large circular intensity differential (CID) of Raman scattering. The origin of the chiral response was attributed to formalism of Raman tensor. Considering the electron-photon and electron-phonon interaction in Raman process, the Raman tensor elements will include the real parts and imaginary parts. The off-diagonal elements are the key factors in the chiral Raman response. These findings may help to identify the vertical orientation of low symmetry crystals and further understand the Raman scattering process in 2D materials of low-symmetry.



P066 **Th 19:00 - 21:00**

fabrication of graphene nanoribbons via wrinkles in ultral clean graphene

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Acquiring clean and complete 2D materials is fundamental for the fabrication of devices and transfer process of 2D materials is also an essential step in the fabrication of nanodevices. Especially for graphene grown by chemical vapor deposition, transfer process is inevitable. In the transfer process of graphene, copper foil is etched by etchant, and ferric chloride or ferric nitrate is widely used as copper etchant. As the polymer support, methyl methacrylate (PMMA) is introduced in transfer of 2D materials such as graphene and molybdenum disulfide. However, we find contaminants, such as metal particles and residue PMMA, are introduced in the transfer process, decreasing the properties and yield of devices. Here we develop a new copper etchant, the solution mixed with hydrochloric acid, hydrogen peroxide and water. The amount of metal particles and PMMA residue can be significantly reduced by using the new etchant, which makes the ultra-clean graphene easy to obtain and high performance graphene-based electronic devices possible. Utilizing the ultra-clean graphene on substrate, we can easily find, even control the wrinkle of graphene, furthermore acquiring the clean carbon nanoribbon by etching the graphene.

P068 **Th 19:00 - 21:00**

Flexible visible-light-driven photoelectrochemical biosensor based on molecularly imprinted graphene/TiO_2 fiber for ultrasensitive urea detection

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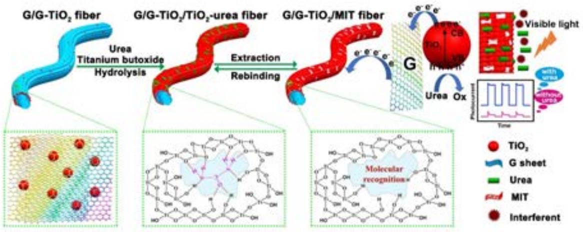
Flexible fiber-shaped microelectrode biosensors have aroused intensive attention due to the promising use for monitoring personal healthcare. However, challenges still exist in the pursuit of combination of high sensitivity and selectivity. Herein, a facile and effective strategy to solve these problems was proposed by developing a novel fiber-shaped photoelectrochemical urea biosensor (PUB) based on highly flexible graphene (G) fiber. The remarkable combined features of the resulting PUB with high surface roughness, good transmittance and superior molecular recognition could contribute to good adsorption capacity, convenient light absorption and selective detection, thus boosting a wide linear range from 0.01 to 1500 µM and a low detection limit of 1 nM. Meanwhile, rapid response, outstanding selectivity and perfect working performance during bending were available as expected. This research provides useful guidelines for designing and fabricating flexible microelectrode biosensors with high sensing performance toward future uses.



Schematic illustration of fabrication process for PUB and detection mechanism of its photoelectric response

P070 **Th 19:00 - 21:00**

Manipulating transition-metal dichalcogenide monolayers with proximity effects

Lanqing Zhou[1], Sven Borghardt[1], Beata Kardynal[1]

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Transition-Metal Dichalcogenides (TMDs) monolayers have been shown to exhibit many interesting physical properties related to their crystal structure and strong spin-orbit interactions. In addition, being only three atomic planes thin, their properties can be manipulated using proximity fields generated when they are placed in contact with functional molecules or films. Here we interface tungsten diselenide monolayers with thin films of chromium trichlotride and chromium tribromide. Both chromium trihalides are layered materials which are electronic insulators that are also ferromagnetic at low temperatures. As such, they can be used as functional substrates for the monolayer WSe_2 to introduce energy splitting of the spin states in K and K' valleys of the monolayer. In this contribution, we study different sample preparation methods to maximize the stability of the chromium trihalide films. Using optical spectroscopy at different tempratures, we compare different geometries of the devices that use hexagonal boron nitride and thin graphite films to protect the ferromagnetic films from the ambient and protect the TMD monolayers from the effects of charge fluctuations that are known to broaden the photoluminescence spectra.

P072 **Th 19:00 - 21:00**

Lightweight high-performance Cu/Carbon Nanotube composites as future electrical conductors substituting Cu

Rajyashree Sundaram[1], Guohai Chen[1], Takeo Yamada[1], Don Futaba[1], Kenji Hata[1], Atsuko Sekiguchi[1]

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We present Cu-matrix carbon nanotube composites (Cu/CNT) as lighter electrically conducting promising Cu-substitutes. Lighter alternatives to Cu wiring in vehicles are vital for improved fuel-efficiency and CO_2 emission-cuts. In electric vehicles with higher amounts of Cu than regular automobiles, weight-reduction is essential to increase travel range per charge. In microelectronics, interconnects more stable than Cu are desired to keep up with rapidly miniaturizing devices of growing complexity and power consumption.

Our Cu/CNT (macrowires and microstructures) are at least 2/3rd as light as Cu with electrical conductivities 1-3 × 10^5 S/cm (17-50% of Cu) and strengths ~300 MPa similar to commercial Cu wires. The conductivity values are more temperature-stable than Cu with temperature coefficient of resistivity (TCR) as low as 4.4 × 10^4 /K (~10% Cu-TCR). The low TCR renders Cu/CNT a more reliable conductor for high-temperature operation e.g., in motor windings. Further, Cu/CNT current carrying capacities (CCC) surpass Cu and coefficients of thermal expansion (CTEs, 4-7 ppm/K) show lower mismatch with Si-CTE (3 ppm/K) than Cu-CTE (17 ppm/K). These CTE and CCC attributes make Cu/CNT better microelectronics interconnects than Cu with reduced delamination and current-failure.

P074 **Th 19:00 - 21:00**

Chains of iron nanoparticles decorated on single-walled carbon nanotubes: toward the design of advanced electrodes for electrochemical energy devices

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Tunable synthesis of electrocatalytically active nanostructures forming an electrically conductive network with a high surface area is of high interest for a wide variety of applications in, for instance, electrochemical energy devices and catalysis. Here, we present a novel approach to fabricate chains of magnetic Fe nanoparticles supported on single-walled carbon nanotubes (Fe/SWNT nanochains) using a one-step floating catalyst chemical vapor deposition synthesis process. The iron nanochains are interlinked and encapsulated in graphitic carbon layers protecting them against degradation. The SWNTs bridge between the Fe chains, forming a flexible, conductive and highly integrated network. The synthesized Fe/SWNT nanochains can be directly and continuously synthesized as ready-to-use 3D multifunctional electrodes.

We have shown that Fe/SWNT nanochains efficiently catalyze the production of hydrogen gas from water splitting with comparable performance to that of platinum especially at high currents. We have also observed that the Fe/SWNT nanochains have promising performance in other electrochemical energy devices. This work provides novel strategies and opens new doors to design multifunctional nanomaterials for various energy-related electrochemical devices.

P076 **Th 19:00 - 21:00**

High frequency-high response rate- large stroke electrochemically driven pure carbon nanotube artificial muscle yarns

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Carbon nanotube fibers assembled by millions of carbon nanotubes(CNTs), feature light weight, high strength, high electrical conductivity, high thermal conductivity, flexible structure (can be knotted and braided), and surface modifiability, which can act as artificial muscles. Artificial muscles convert various forms of energy (e.g. heat, chemistry, magnet, light, etc.) into mechanical energy. Herein, we report artificial muscle fibers prepared by the coiled carbon nanotube yarns. When electrochemically driven with the organic electrolytes, the single ply CNT yarns demonstrate excellent driving performance with 32.8% contraction strain, which is more than twice as reported previously (16.5%). The electrochemical drive response rate is slow and the response rate is independent of frequency according to our experimental results, we use multiple plies to provide response speed and drive performance. Previous reports on the mechanism of electrochemical driving are still shallow. Herein, we detailedly study the effects of different conditions on driving performance, including different ion sizes, different ion mobility, and ion concentration distribution in the yarns.

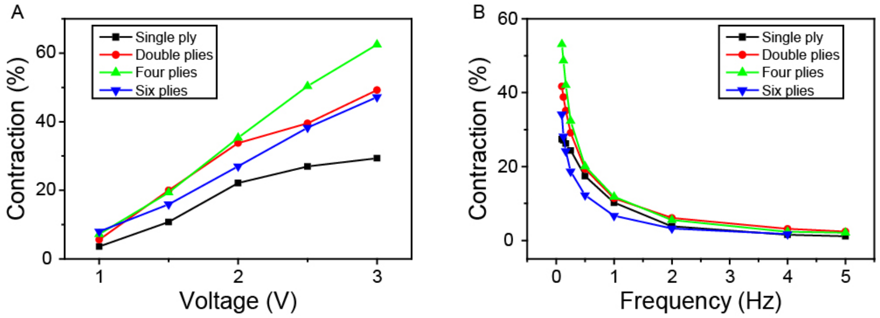

Figure A. Contraction as a function of applied 0.1 Hz square-wave potential for different plies CNT yarn muscle; Figure B. Contraction versus frequency for square-wave excitation of diffenent plies CNT yarn muscle by applying an voltage of 2V.

P078 **Th 19:00 - 21:00**

Hybridizing Fullerenes and Two-Dimensional Nanomaterials

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Fullerene has a definite zero-dimensional (0D) closed-cage molecular structure composed of sp^2-hybridized carbon atoms merely, enabling it as important building blocks useful for constructing supramolecular assemblies and micro/nano functional materials.[1] Upon hybridization 2D nanomaterials with fullerenes noncovalently or covalently, the physical/chemical properties of 2D nanomaterials can be tailored and in most cases improved, significantly extending their functionalities and applications.[2] Recently, we succeeded in synthesizing several novel fullerene-2D nanomaterial hybrids via both covalent and noncovalently approaches, including graphene,[3] g-C_3N_4,[4] black phosphorus,[5] and MoS_2,[6] and achieved enhanced photo/electrocatalytic activities.

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P080 **Th 19:00 - 21:00**

Carbon nanotube based Pt catalysts for selective oxidation of biomass-derived polyols

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Selective oxidation of biomass-derived polyols is one of the most important pathways for the effective utilization of biomass energy.1 Particularly, rational design of heterogeneous catalysts plays key roles in the exploration of green and efficient catalysis technology. Due to the unique electronic structures and surface chemistry properties, carbon nanotubes (CNTs) have been explored as a promising support for metal catalysts.2 We focused on the challenge that the Pt catalysts are in low conversion and poor selectivity for the glycerol oxidation reaction in base-free medium.3 First, the surface-functionalization means of CNTs have been optimized to improve the catalytic activity of supported Pt nanoparticles. Second, metal oxides (e.g. CeO_2, TiO_2) have been loaded on CNTs to form the composite supports for Pt catalysts.4 Addition of metal oxides changed the electronic structure of Pt and thus improved their catalytic activity. Defects introduced by metal oxides in these ternary catalysts can further improve the catalytic activity. Third, different organic molecules have been used as “ligand” to coordinate with Pt of Pt/CNTs or ternary catalysts, which would produce steric effect to regulate the selectivity of catalysts without affecting their activity.

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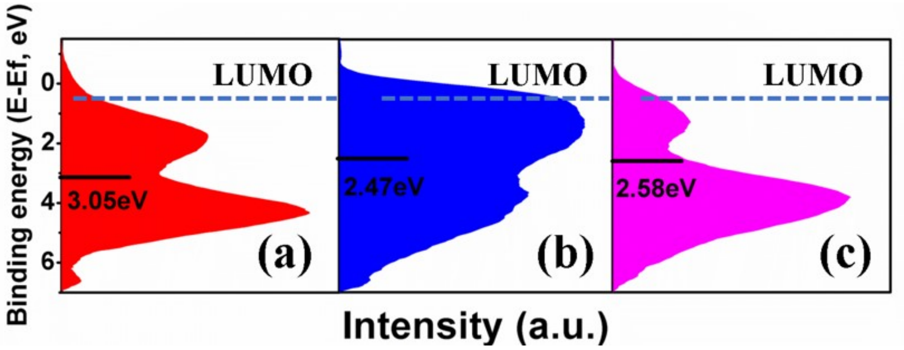

Fig. 1. Valence band photoemission spectra of Pt/CeO_2(a), Pt/CNT(b) and Pt/CeO_2-CNT(c). The black bar indicates the calculated d-band center. The imaginary line indicates the calculated LUMO value of glyceric acid.

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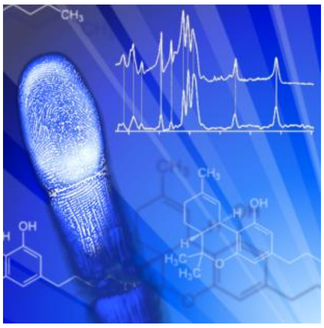
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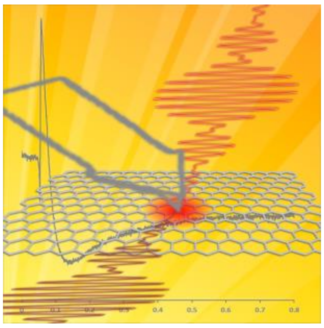

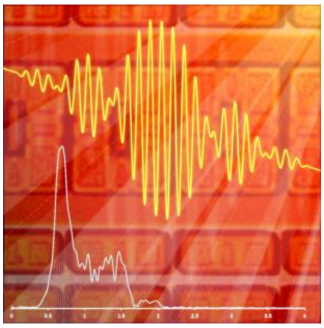

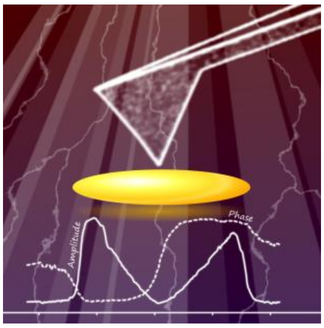
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Plenary program Franconia Hall

Session Pl9 Chair: Yutaka Ohno

08:30 - 09:15	K5	**Christophe Voisin** (École Normale Supérieure) *Carbon Nano-Structures as Quantum-Light Sources*
09:15 - 09:40	I15	**Suguru Noda** (Waseda University) *Production and Functionalization of Carbon Nanotubes for Electrochemical Energy Storage Devices*
09:40 - 10:05	C11	**Daniel A. Heller** (Memorial Sloan Kettering Cancer Center) *Carbon Nanotube Photoluminescence Solvatochromism in Biomedicine*

Coffee break CCW Lobby

Session Pl10 Chair: Daniel A. Heller

10:35 - 11:00	C12	**Yoshiyuki Miyamoto** (AIST) *Nanotubes as Laser-Field Enhancer Useful for Water Decomposition: a TDDFT Study*
11:00 - 11:25	I16	**Yutaka Ohno** (Nagoya University) *Carbon Nanotube-Based Stretchable Devices for Wearable Electronics*
11:25 - 11:50	C13	**Carola Meyer** (Universität Osnabrück) *Monitoring Singlet Transitions in Individual Molecules*

Closing Session Chair: Tobias Hertel

11:50 - 12:15		**Annick Loiseau, Shigeo Maruyama** *Closing Remarks*

Farewell

Abstracts Friday

Plenary Venue K5 (keynote)

Franconia Hall **Fr 08:30 - 09:15**

Carbon nano-structures as quantum-light sources

Christophe Voisin[1]

[1] *Physics Laboratory of Ecole Normale Supérieure, Paris*

Single-photon sources are a key building block for secured quantum telecommunications. In view of integration in long range telecommunication networks near-infrared emission, room temperature operation and electrical injection are the current challenges for single-photon generation.

Carbon nano-structures and especially carbon nanotubes have strong assets in this perspective. They were shown to be excellent single-photon emitters [1, 2]. In addition, their emission wavelength can be chosen over a wide range. Nevertheless, the reported brightness is consistently small and the spectral purity is not well controlled.

These key properties can be drastically improved by coupling the nanostructure to a small volume, high-finesse optical cavity through the so-called Purcell effect [3]. In fact, light-matter interaction at the scale of a single emitter can be strongly modified when the electromagnetic field in confined to volumes of the order of l3, which is the realm of cavity quantum electrodynamics. Originating from atomic physics, this field has become technologically relevant when solid state emitters (quantum wells, quantum dots…) were first coupled to integrated micro-cavities. Here, we used an original tunable cavity design using a scanning optical fiber in order to tackle the spatial and spectral mode matching issues. We show that the emission rate of the nanotube can be enhanced by a factor 60 leading to an effective luminescence quantum yield of about 40% and a coupling factor close to 100% [4].

In addition, our original designs brings a wide tuning range for the single-photon source. This new feature is very attractive for multiplexing approaches or for indistinguishability engineering from remote nano-sources for quantum computing.

References:
X. He et al., Nature Materials, 17, 663 (2018)
S. Zhao et al., Nature Com. 9, 3470 (2018)
A. Jeantet et al., Phys. Rev. Lett. 116, 247402 (2016)
A. Jeantet, et al., Nano Lett. 17, 4184 (2017)

Plenary Venue I15 (invited)

Franconia Hall **Fr 09:15 - 09:40**

Production and Functionalization of Carbon Nanotubes for Electrochemical Energy Storage Devices

Suguru Noda[1,2]

[1]*Department of Applied Chemistry, Waseda University, Tokyo 169-8555, Japan*
[2]*WRISE, Waseda University, Tokyo 169-8555, Japan*

Self-supporting, sponge-like paper of carbon nanotubes (CNTs) can be a new platform for high energy/power density batteries. Presently, battery electrodes are built on metallic foils having only two faces and large mass with the aid of polymeric binders and conductive fillers. CNT paper can replace all these components. Furthermore, it captures nanomaterials at high loading, activates insulative materials, and moderates volumetric change of active materials.

We have developed semi-continuous fluidized bed chemical vapor deposition method [1], which yields submillimeter-long few-wall CNTs with carbon purity >99 wt% and metal impurity <0.1 wt% [2]. By capturing capacitive particles (99 wt%) with CNTs (1 wt%), a lithium ion full cell with $LiCoO_2$-CNT cathode and graphite-CNT anode is demonstrated (Figure 1b) [2]. This platform is also effective to create electrodes of the emerging active materials such as Si anode [3] and S cathode [4] with practically high gravimetric, areal, and volumetric loadings.

[1] D.Y. Kim, et al., Carbon 49, 1972 (2011).
[2] Z. Chen, et al., Carbon 80, 339 (2014).
[3] K. Hasegawa and S. Noda, J. Power Sources 321, 155 (2016).
[4] T. Kowase, et al., J. Power Sources 363, 450 (2017).
[5] K. Hori, et al., J. Phys. Chem. C 123, 3951 (2019).

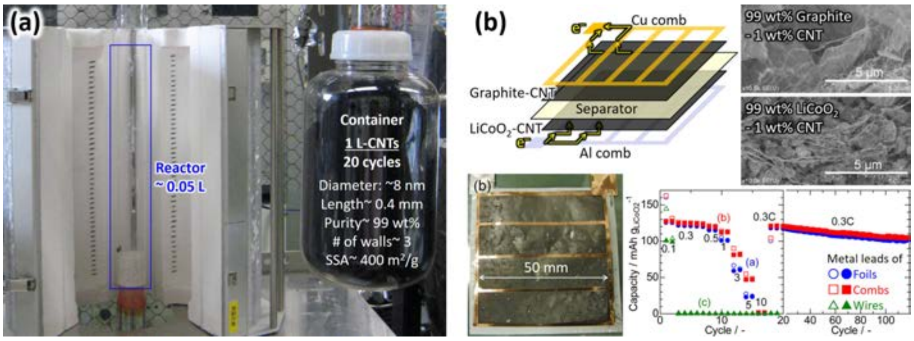

Figure 1. (a) Semi-continuous production of submillimeter-long few-wall CNTs by fluidized bed [1]. (b) Lithium ion full cell made of $LiCoO_2$-CNT cathode and graphite-CNT anode [3].

Plenary Venue C11 (contributed)

Franconia Hall **Fr 09:40 - 10:05**

Carbon Nanotube Photoluminescence Solvatochromism in Biomedicine

Daniel Heller[1,2]

[1]*Memorial Sloan Kettering Cancer Center, New York, NY 10065*
[2]*Weill Cornell Medicine, Cornell University, New York, NY 10065*

Modulation of the carbon nanotube photoluminescence band position has implications for applications such as sensing and imaging. We developed methods to modulate nanotube solvatochromic behavior to improve sensor responses, and we developed tools to observe solvatochromism within live cells and, recently, live animals. We found that nanotube solvatochromism extends to variations of local electrostatic charge, induced by adsorption/desorption of polyelectrolytes on the nanotube surface, such as proteins and nucleic acids. We also found that dielectric and charge-mediated solvatochromism can be compounded to exacerbate the response. Upon triggered desorption of a polyelectrolyte, amphiphilic molecules can adsorb to the recently-uncovered nanotube surface. The adsorption displaces water to result in hypsochromic shifting, which can be additive, as polyelectrolyte desorption will also cause a hypsochromic shift. We found that the amphiphile may be a surfactant but, recently, we found that proteins can result in a similar response, facilitating the detection of viruses. Carbon nanotube solvatochromism-based sensors allow measurements of biomarkers, drugs, and metabolites, facilitating improvements in disease detection, drug development, and biomedical research.

Plenary Venue C12 (contributed)

Franconia Hall **Fr 10:35 - 11:00**

Nanotubes as laser-field enhancer useful for water decomposition: A TDDFT study

Yoshiyuki Miyamoto[1], Hong Zhang[2], Xinlu Cheng[3], Angel Rubio[4,5,6]

[1]*CD-FMat, AIST, Japan*
[2]*College of Physical Science and Technology, Sichuan University, China*
[3]*Institute of Atomic and Molecular Physics, Sichuan University, China*
[4]*Nano-Bio Spectroscopy Group and ETSF, Universidad del Pais Vasco, Spain*
[5]*Max Plank Institute for the Structure and Dynamics of Matter, Germany*
[6]*Center for Computational Quantum Physics, Flatiron Institute, USA*

By performing the real-time TDDFT calculations [1,2] coupled with classical molecular dynamics, we studied laser-field induced water decomposition near the carbon nanotubes. Short and intense laser field can provide high photon flux [3] which is useful for high yield of photo-chemical reaction such as water decomposition harvesting hydrogen fuel. In order to reduce laser power some material that enhances laser field intensity is useful. In case of short laser pulse with full-width-of-half-maximum 10 fs, the presence of (8,0) nanotube is found to significantly reduce threshold laser power needed for water decomposition. When laser wavelength is 400 nm, the factor of the power-reduction is less than one eighth. [4] Since carbon nanotube is durable upon laser shot[5], we expect repeat of laser shining for cyclic water decomposition. We discuss physics of laser field enhancement which can be polarization and curvature effect of carbon nanotube.

References
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[2] O. Sugino and Y. Miyamoto, Phys. Rev. B59, 2579 (1999)
[3] D. Strickland and G. Mourou, Opt. Commun. 56, 219 (1985)
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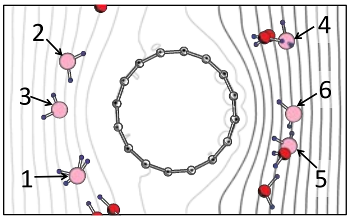

Potential profile around (8,0) nanotube at a moment of laser irradiation. Local field enhancement around water molecules from number 1-6 occurs that helps laser decomposition of water in lower power.

Plenary Venue I16 (invited)

Franconia Hall **Fr 11:25 - 11:50**

Carbon nanotube-based stretchable devices for wearable electronics

Yutaka Ohno[1]

[1]*Nagoya University, Nagoya 464-8601, Japan*

Wearable electronics are expected to revolutionize medical care and health promotion technologies. Carbon nanotube-based electron devices such as transistors and sensors are considered as key building blocks to realize flexible/stretchable electronics with excellent wearability and performance because of the high-carrier mobility, mechanical flexibility, and biocompatibility. In the presentation, after reviewing recent progresses of carbon nanotube-based electron devices, our recent works on flexible/stretchable transistors, integrated circuits, and biosensors will be introduced. A concept to design carbon nanotube-based analog integrated circuits, which are indispensable for sensor devices, will be presented, with a demonstration of the first carbon nanotube-based differential amplifiers on a flexible plastic film. Energy harvesting technologies are one of important power sources of wearable devices. CNT-based transparent and stretchable triboelectric energy harvesters, utilizing the contact electrification and electrostatic induction, will also be presented.

Plenary Venue C13 (contributed)

Franconia Hall **Fr 11:00 - 11:25**

Monitoring Singlet Transitions in Individual Molecules

Carola Meyer[1,4,5], Claire Besson[2,4,5], Philipp Stegmann[3], Michael Schnee[4,5], Zeila Zanolli[6], Asmus Vierck[7], Robert Frielinghaus[4,5], Paul Kögerler[8,4,5], Janina Maultzsch[9], Claus M. Schneider[4,5], Alfred Hucht[3], Jürgen König[3]

[1] *Fachbereich Physik, Universität Osnabrück, D-49069 Osnabrück, Germany*
[2] *Department of Chemistry, The George Washington University, Washington DC, USA*
[3] *Theoretische Physik, Universität Duisburg-Essen and CENIDE, Duisburg, Germany*
[4] *Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich, Jülich, Germany*
[5] *Jülich Aachen Research Alliance (JARA)–FIT, Jülich, Germany*
[6] *Catalan Institute of Nanoscience and Nanotechnology (ICN2), Bellaterra, Barcelona, Spain*
[7] *Institut für Festkörperphysik, Technische Universität Berlin, Berlin, Germany*
[8] *Institute of Inorganic Chemistry, RWTH Aachen University, Aachen, Germany*
[9] *Department of Physics, Friedrich-Alexander University Erlangen-Nürnberg, Erlangen, Germany*

Antiferromagnetic spintronics is an emerging field that holds great promise for technologies such as magnetic random access memories, neuromorphic computing and THz information technologies, because antiferromagnets (AFMs) do not produce and are insensitive toward magnetic stray fields. Here, we show how concepts of antiferromagnetic spintronics can be applied to individual molecules. This is by no means trivial since currently used methods to measure molecular spin states rely on the detection of a local magnetic moment.

We show that the switching between different $S = 0$ eigenstates of molecular complexes grafted covalently to carbon nanotube (CNT) quantum dots leads to a random telegraph signal (RTS) in the current through the devices (Figure 1).

The complexes contain either four MII (M=Co, Mn) ions as spin-carrying species in a tetragonal core. Analysing the statistics of the RTSs, we find that while CoII complexes switch independently between states, the same complexes with MnII ions exhibit a coherent superposition between the states of all molecules attached to the quantum dot. We attribute this difference to the fact that in contrast to MnII ions, CoII ions are prone to spin-orbit coupling, which is a known major source of decoherence.

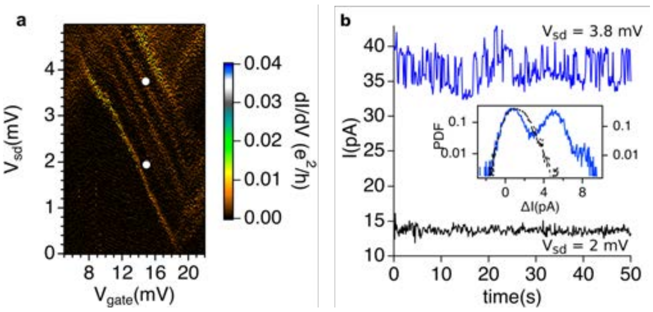

Figure 1: a Part of the stability diagram of a Co4- functionalized CNT quantum dot. b Parts of the time traces of the current taken at the positions indicated by white dots in a). The inset shows the histograms of the current traces.

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