THE 23RD INTERNATIONAL CONFERENCE

on the

SCIENCE & APPLICATIONS OF NANOTUBES

and Low-Dimensional Materials

4-9 JUNE 2023

Arcachon near Bordeaux, France

ABSTRACT BOOK

WELCOME

We are thrilled to welcome you in the charming seaside resort of Arcachon near Bordeaux and its unique environment, the Arcachon bay. We are confident that you will enjoy the venue and the local cuisine, and we have made every effort to ensure a productive and enjoyable experience at NT'23.

You are an integral part of the adventure and we are counting on you to deliver your best speeches and show world-class results on your posters, both during the plenary sessions and the seven symposia. As was the case at NT'19 and NT'22, symposia are embedded in the main conference program, with plenary sessions taking place in the mornings whereas afternoons will be dedicated to parallel symposia. Three long time slots of 3 hours have been reserved for poster sessions with food and drinks to ensure attendance and promote lively and fruitful discussions. While the schedule is full of exciting and informative events, we have also provided some free time for coffee breaks and lunches, allowing you to have informal talks with these far away colleagues and friends that you greet at NT. We apologize in advance that we cannot push the walls for more space. Nonetheless, we believe that the Arcachon Congress Center is a delightful venue and the perfect location for NT'23.

We hope you will very much enjoy NT'23. This should be the best reward for the efforts we have put into preparing it.

The organizers

Étienne Gaufrès
Alain Pénicaud
Laurent Cognet
Philippe Poulin

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~ BIO

13th Symposium on Carbon Nanomaterials, Biology, Medicine and Toxicology

Chair	**Dr Dan Heller,** Sloan Kettering Institute, USA
Co-Chairs	**Dr Laurent Cognet,** CNRS – University of Bordeaux, France
	Prof. Makita Landry, Berkeley University, USA

~ COMPUTATION AND THEORY

15th Symposium on Computational Challenges in Nanotubes, 2D Materials, and Their Macroscopic Assemblies

Chair	**Prof. Christophe Bichara**, CNRS, France
Co-Chairs	**Prof. Feng Ding**, Ulsan National Institute of Science and Technology & IBS, South Korea
	Prof. Jean-Christophe Charlier, Université catholique de Louvain in Belgium

~ ELECTRONICS

Symposium on structure, properties, applications – Electronics and Metrology

Chair	**Prof. Lian Mao Peng**, Peking University, China
Co-Chairs	**Dr Laëtitia Marty**, CNRS, University of Grenoble, France
	Prof. Yutaka Ohno, Nagoya University, Japan
	Prof. Michael Arnold, University of Wisconsin-Madison, US

~ ENERGY

5th Symposium on Materials for Energy and Sustainability

Chair	**Prof. Huiming Cheng**, IMR/Tsinghua University, China
Co-Chairs	**Prof. Philippe Poncharal,** University of Lyon, France
	Prof. Yury Gogotsi, Drexel University, US

SYMPOSIA ORGANISATION

SYNTHESIS

4th Symposium on Synthesis, Purification, Functionalization, and Manufacturing of Carbon Nanotubes and Low-Dimensional Materials

Chair	**Prof. Yan Li**, Peking University, China
Co-Chairs	**Prof. Catherine Journet**, University of Lyon, France
	Prof. Ming Zheng, NIST, USA

MACROMATERIALS

Symposium on thin films, fibers, 3D materials and their properties

Chair	**Prof. Esko Kauppinen,** Aalto University, Finland
Co-Chairs	**Prof. Adam Boies**, Trinity College and University of Cambridge, UK
	Prof. Suguru Noda, Waseda University, Japan
	Dr Philippe Poulin, CNRS – University of Bordeaux, France

FUNDAMENTAL PROPERTIES

Symposium on fundamental, structural and optical properties of 1D and 2D materials and their heterostructures

Chair	**Prof. Alexey Chernikov**, Univerdity of Dresden, Germany
Co-Chairs	**Dr Nicolas Izard,** CNRS – University of Montpellier, France
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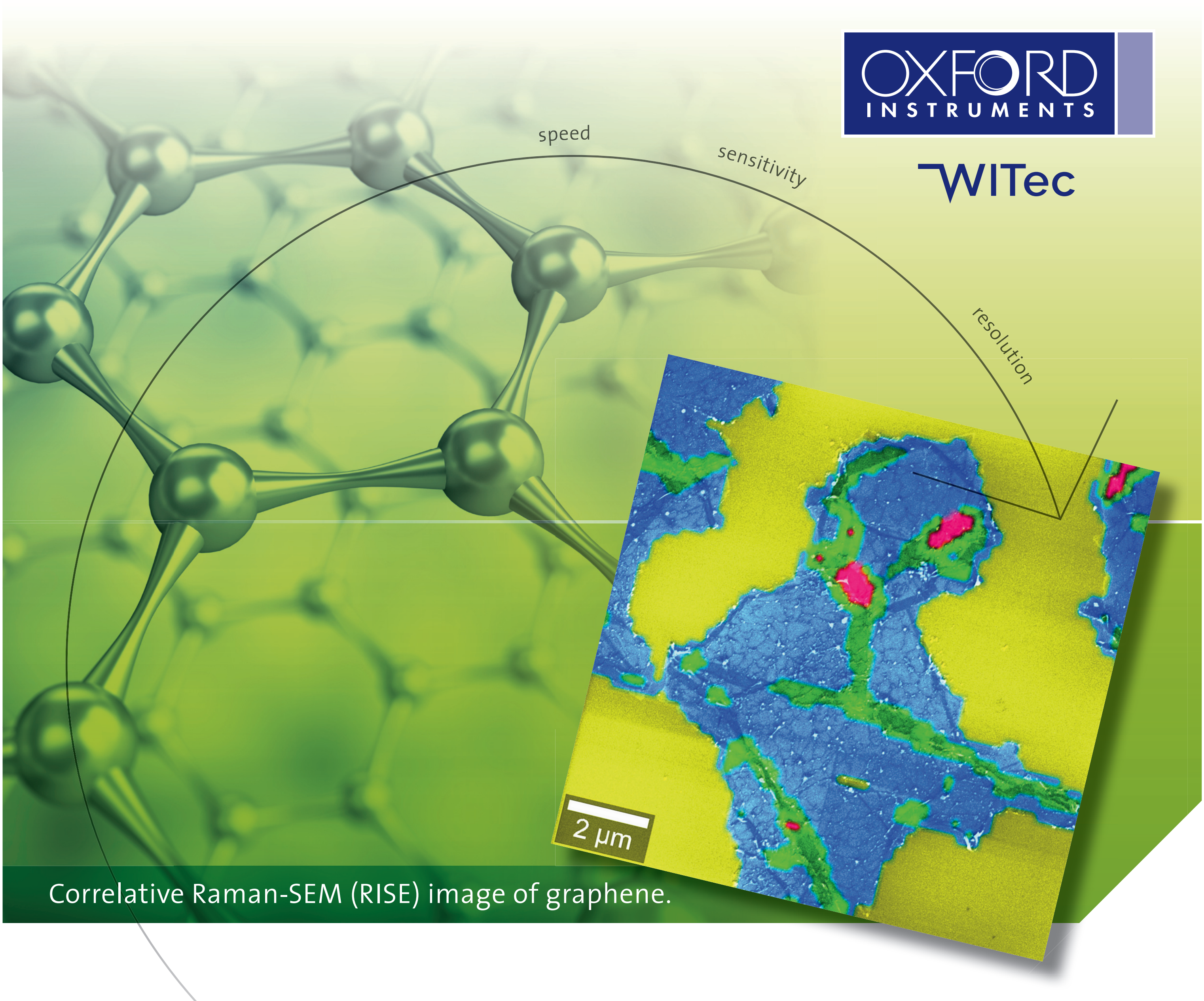

speed
sensitivity
resolution
2 µm

SOCIÉTÉ FRANCOPHONE D'ETUDE DES CARBONES

Francophone Carbon Association

Created in 1961

Preliminary Announcement

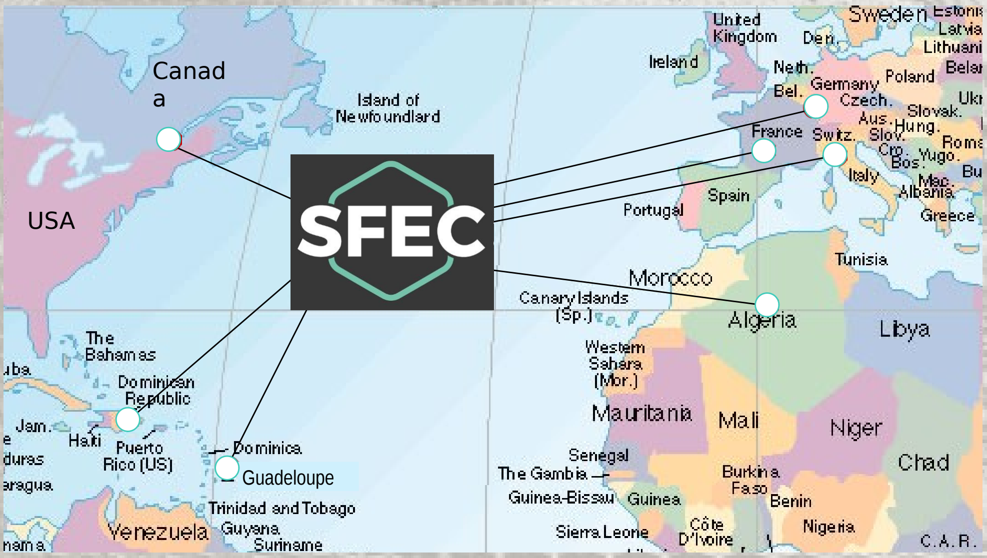
CARBON-2025

The Annual meeting of Carbon Scientists from around the World

June 29th – July 4th, 2025

Le Grand Large, Convention Center

SFEC Société Francophone d'Etude des Carbones



Goals

- Increasing knowledge about carbon materials of any kind: natural and synthetic, graphene- and diamond-based, from nano to macro
- Promoting interactions between academic research and industrial R&D
- Educating and training young scientists (Master and PhD students, postdocs) with oral and poster presentations and networking

Actions

- Annual congress
- International events
- Support to international Conferences, Workshops, and Schools
- Young Scientist Award (annual)
- Best PhD Student talk Award (sponsored by Micromeritics)
- Interactions with other national Carbon Societies within the European Carbon Association
- Interactions with other continental Carbon Groups (ACS, AACG, LACF)*

Management

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Scientific Council (G30)

34 members

Every scientist able to understand French welcome

To inquire about membership, ask the SFEC representative present at this event, or write to

alain.penicaud@crpp.cnrs.fr

***American Carbon Association, Association of Asian Carbon Groups, Latin American Carbon Federation**

SFEC Société Francophone d'Etude des Carbones ***is a member of the European Carbon Association***

TABLE OF CONTENT

WIFI AT PALAIS DES CONGRÈS

Welcome to Palais des Congrès - Arcachon

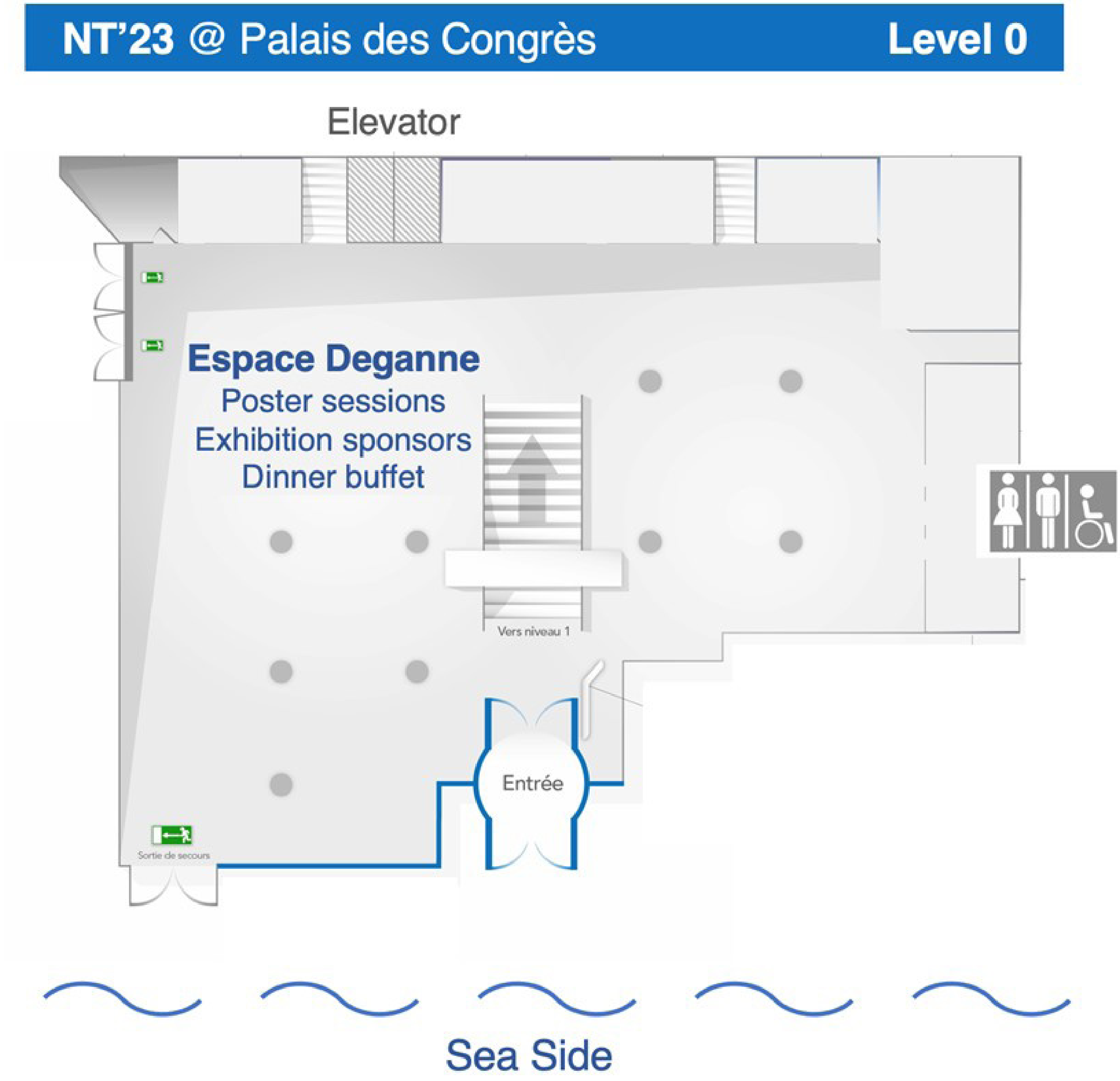
Just connect to
WiFi_Bassin_Arcachon

No password

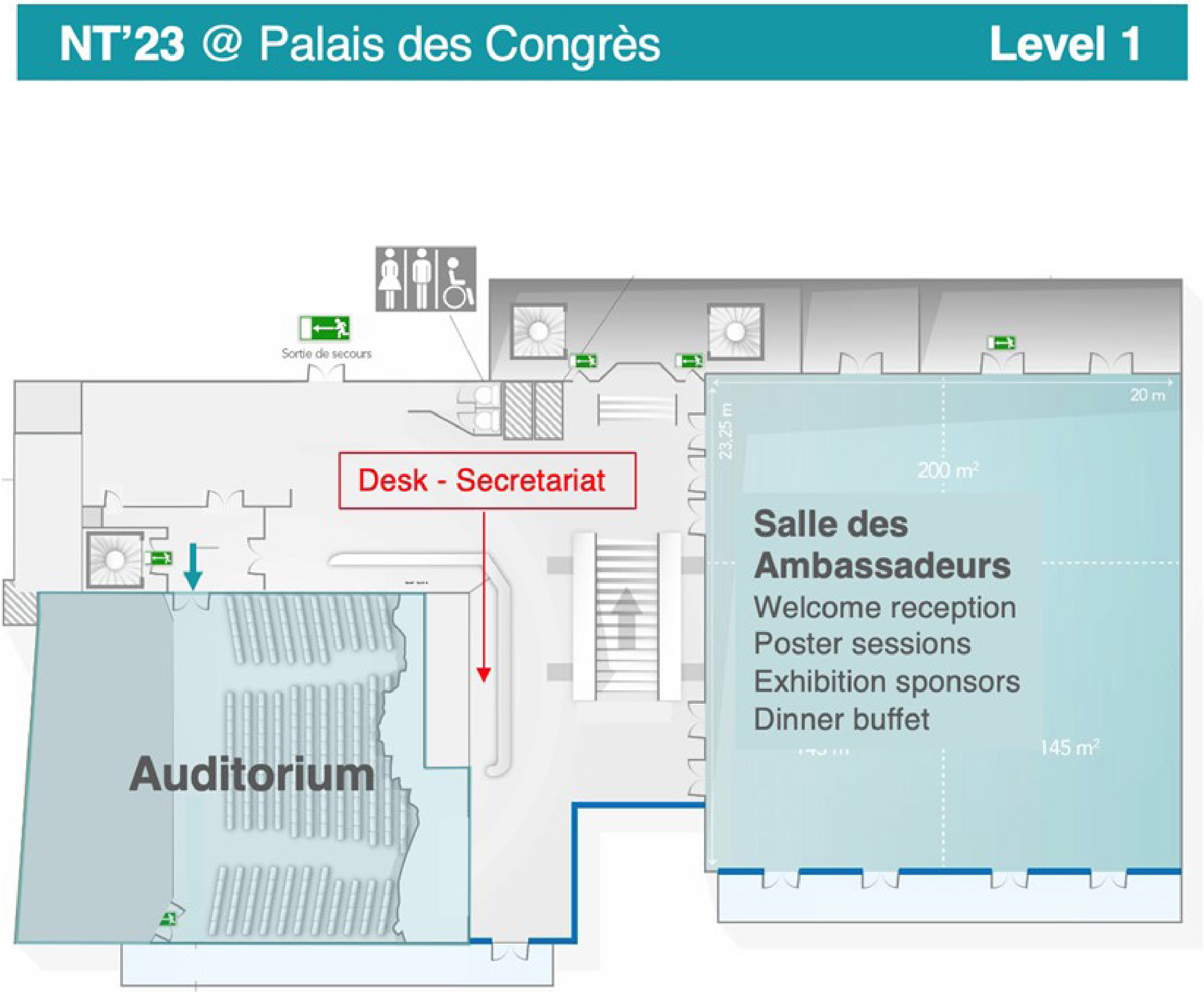
WHERE AND WHEN TO GO

EVENT		LOCATION	
Tutorials	Sun	Auditorium	Level 1, 2
Welcome	Sun	Salle des Ambassadeurs	Level 1
Plenary Sessions	Mo - Fri	Auditorium	Level 1, 2
Poster sessions & Exhibition Sponsor	Mo, Tu, Th	Espace Deganne Salle des Ambassadeurs	Level 0 Level 1
Symposium Bio	Mo, Tu	Salon VIP	Level 3
Symposium Computation & Theory	Tu, Th	Salle Ville d'Hiver	Level 3
Symposium Electronics	Mo, Th	Salle Dune du Pilat	Level 3
Symposium Energy	Mo Th	Salle Ville d'Hiver Salon VIP	Level 3 Level 3
Symposium Fundamental	Mo, Tu, Th	Auditorium	Level 1, 2
Symposium Macromaterials	Tu Th	Salle Dune du Pilat Salle du Moulleau	Level 3 Level 2
Symposium Synthesis	Mo, Tu	Salle du Moulleau	Level 2

FIND YOUR WAY IN THE PALAIS DES CONGRÈS

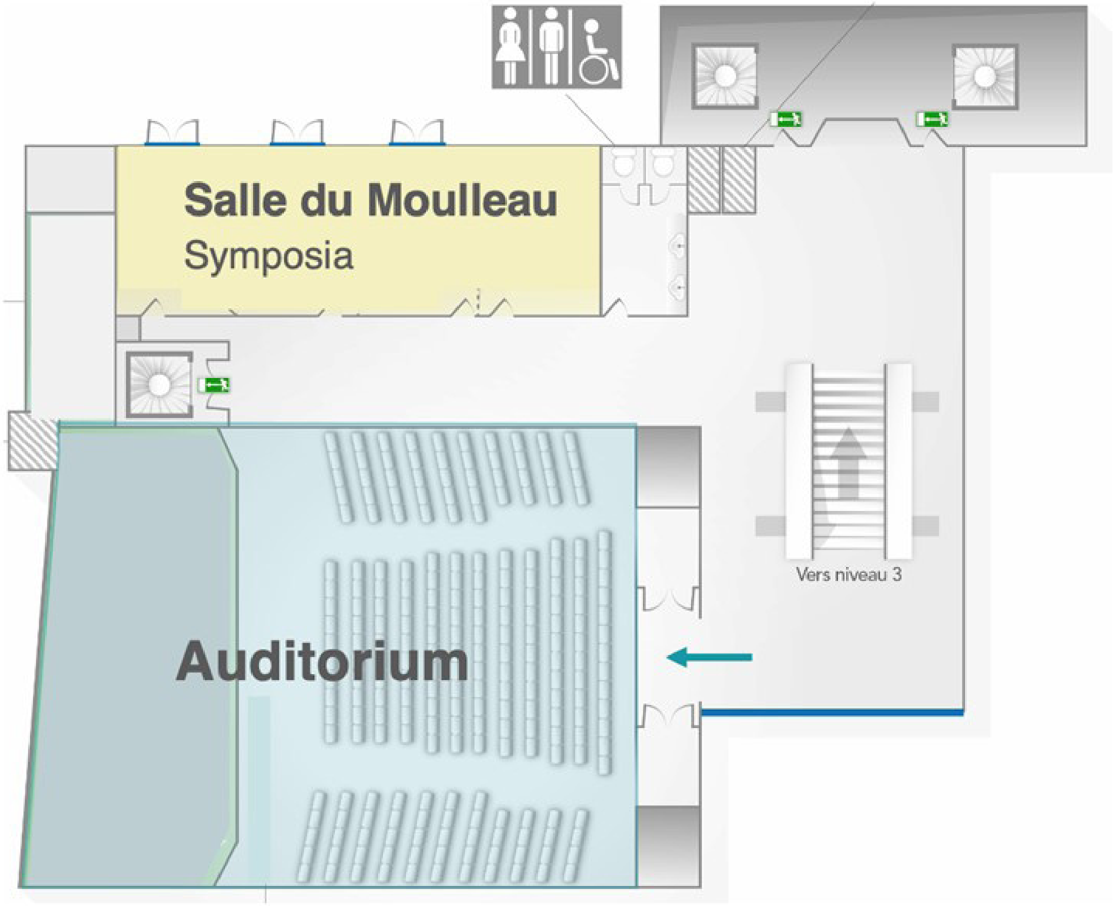


FIND YOUR WAY IN THE PALAIS DES CONGRÈS

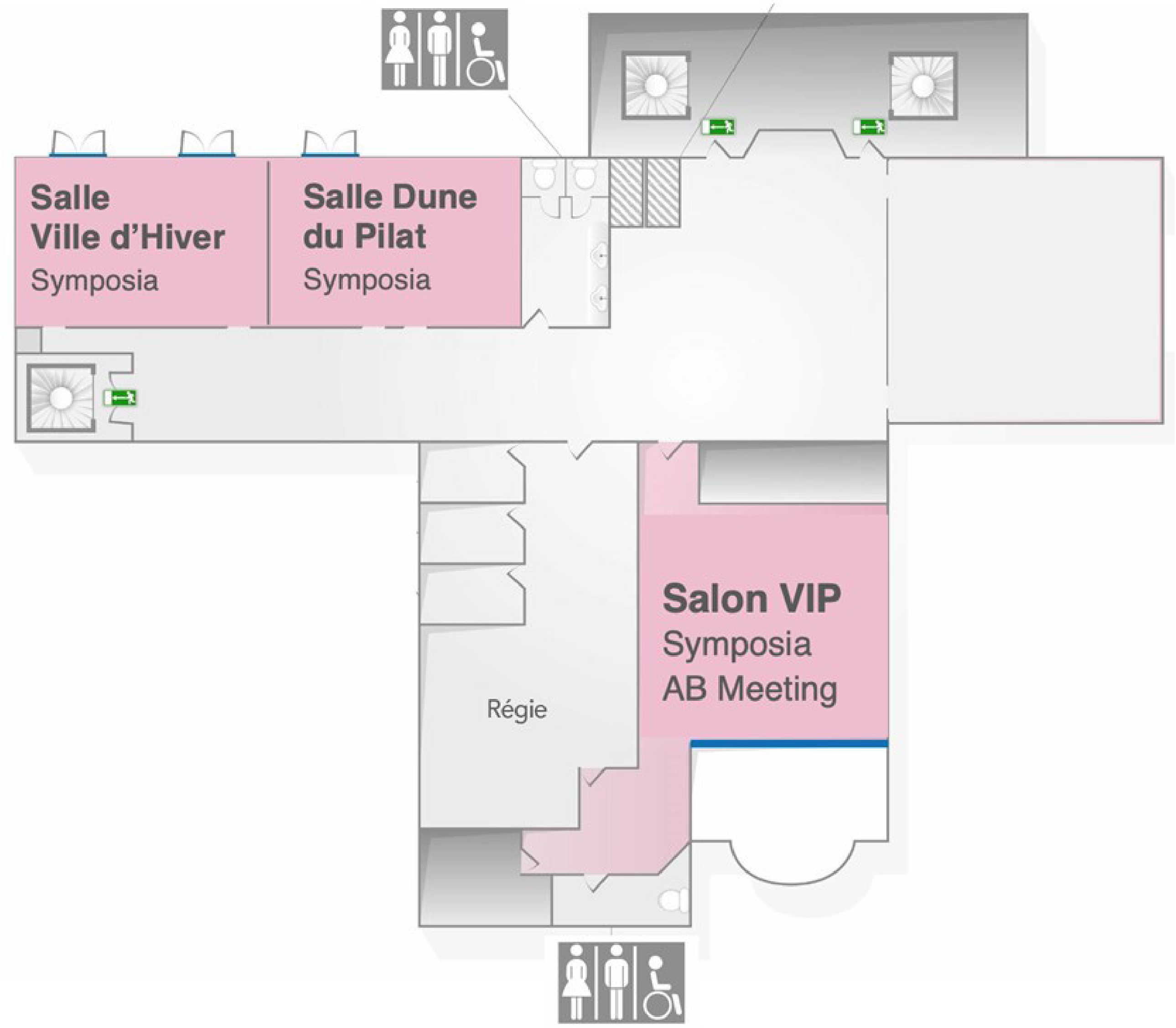


FIND YOUR WAY IN THE PALAIS DES CONGRÈS

NT'23 @ Palais des Congrès Level 2



NT'23 @ Palais des Congrès Level 3



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PROGRAM AT A GLANCE

Sunday 4		**Monday 5**		**Tuesday 6**		**Wednesday 7**		**Thursday 8**		**Friday 9**	
		8h25	**Opening**			**8h25**	**Practical info**				
		8h30	**K1** Ming Zheng	**8h30**	**K2** Young Hee Lee	**8h30**	**K3** Richard Martel	**8h40**	**K4** Katalin Kamaras	**8h30**	**K5** Matteo Pasquali
		9h15	**I1** Yasumitsu Miyata	**9h15**	**I4** Kazu Suenaga	**9h15**	**I6** Marcos Pimenta	**9h25**	**C12** Lei Shi	**9h15**	**I10** Markita Landry
		9h45	**C1** Emmanuel Picheau	**9h45**	**C4** Mathias Kuehne	**9h45**	**C8** Tao Wei	**9h45**	**C13** Christophe Voisin	**9h45**	**C16** Pascal Boulanger
		10h05	Coffee break	**10h05**	Coffee break	**10h05**	Coffee break	**10h05**	Coffee break	**10h05**	Coffee break
10h30	Desk opening	**10h45**	**I2** Antonio Setaro	**10h45**	**I5** Lian-Mao Peng	**10h45**	**I7** Silvia Giordani	**10h45**	**I8** L. Bocquet replaced by Nikita Kavokine	**10h45**	**I11** Geyou Ao
		11h15	**C2** Ana Cadena	**11h15**	**C5** Valery Luchnikov	**11h15**	**C9** Shigeo Maruyama	**11h15**	**C14** Vincent Jourdain	**11h15**	**C17** Yan Li
		11h35	**C3** Daniel Heller	**11h35**	**C6** François Lapointe	**11h35**	**C10** Domitille Baux	**11h35**	**C15** Benji Maruyama	**11h35**	**C18** Rufan Zhang
		11h55	**I3** Su-Yuan Xie	**11h55**	**C7** Jeff Blackburn	**11h55**	**C11** Sofie Cambré	**11h55**	**I9** Fei Wei	**11h55**	
		12h25	Lunch	**12h15**	Lunch	**12h15**	Lunch	**12h15**	Lunch		

PROGRAM AT A GLANCE

Sunday 4	Monday 5	Tuesday 6	Wednesday 7	Thursday 8	Friday 9
14h00 **Tutorial 1** Ardemis Boghossian	**14h30** Symposia	**14h30** Symposia	**14h30** **Excursion**	**14h30** Symposia	
15h15 **Tutorial 2** Chris Ewels					
16h30 Coffee break	**16h10** Coffee break	**16h10** Coffee break		**16h10** Coffee break	
17h00 **Tutorial 3** Damien Voiry **ends 18h15**	**16h50** Symposia **ends 18h10**	**16h50** Symposia **ends 18h10**		**16h50** Symposia **ends 18h10**	
	18h30 Poster sessions Exhibition sponsors Buffet dinner **ends 21h30**	**18h30** Poster sessions Exhibition sponsors Buffet dinner **ends 21h30**	**17h00** Free time	**18h30** Poster sessions Exhibition sponsors Buffet dinner **ends 21h30**	
19h30 **Welcome reception**			**19h00** **Conference Banquet**		

~ MONDAY, 5

	Bio	Fundamental	Energy	Electronics	Synthesis
	Salon VIP	**Auditorium**	**Salle Ville d'Hiver**	**Salle Dune du Pilat**	**Salle du Moulleau**
14h30	**OS01** Sebastian Kruss	**OS02** Thomas Pichler	**OS03** Patrice Simon	**OS04** Aaron Franklin	**OS05** Zhongfan Liu
15h10	**IS01** Abraham Beyene	**IS03** Alexander Hoegele	**IS07** Sang Ouk Kim	**CS12** Zhao Jianwen	**IS12** Adam Boies
15h30	**CS01** Simon Settele	**IS04** Laurent Alvarez	**IS08** Liming Dai	**IS09** Weifeng Wu	**IS13** Stephane Campidelli
15h50	**CS02** Hugh Mohan	**CS06** Yaxin Jiang	**CS09** Chen Xuecheng	**IS10** Youfan Hu	**IS14** Feng Yang
16h10	Coffee break	Coffee break	Coffee break	Coffee break	Coffee break
16h50	**CS03** Somen Nandi	**IS05** Xavier Marie	**CS10** Tomotaro Mae	**IS11** Kuniharu Takei	**CS16** Placidius Amama
17h10	**IS02** Toshiya Okazaki	**IS06** Thomas Szcopek	**CS11** Ming Xu	**CS13** Said Pashayev	**CS 17** Stephen Purcell
17h30	**CS04** Sara Behjati	**CS07** Klaus Eckstein	**Round Table**	**CS14** Ya Feng	**CS18** Yusuke Nakanishi
17h50	**CS05** Kazuhiko Matsumoto	**CS08** Christian Kramberger		**CS15** Ilan Boulet	**CS19** Feng Zhang (cancelled)

~ TUESDAY, 6

	Bio	Fundamental	Computation & Theory	Macromaterials	Synthesis
	Salon VIP	**Auditorium**	**Salle Ville d'Hiver**	**Salle Dune du Pilat**	**Salle du Moulleau**
14h30	**IS15** Delphine Bouilly	**OS06** Jana Zaumseil	**OS07** Alister Page	**OS09** Qingwen Li	**IS24** Jin Zhang
14h50	**CS20** Anton Naumov				**IS25** Jianying Ouyan
15h10	**CS21** Quentin Grésil	**IS17** Yannick Chassagneux	**IS19** James Elliot	**CS32** Yue Qi (cancelled)	**IS26** Zdenek Sofer
15h30	**CS22** Luc Chavignon	**CS25** Erin Christensen	**CS30** Xiao Wang (cancelled)	**CS33** Anastasios Karakasidis	**IS27** Ryo Kitaura
15h50	**CS23** Linda Sistemich	**CS26** Eric Anderson	Emil Parth	**CS34** Shuhui Wang	**CS37** Han Li
16h10	Coffee break	Coffee break	Coffee break	Coffee break	Coffee break
16h50	**IS16** Cecilia Menard-Moyon	**CS27** Igor Bondarev	**OS08** Zhuhua Zhang	**IS22** Oren Regev	**CS38** Song Qiu
17h10	**CS24** Lin Zhu	**IS18** Yuichiro Kato		**IS23** Aldo Zarbin	**CS39** Rufan Zhang
17h30	**Round Table**	**CS28** Michael Arnold	**IS21** Mina Maruyama	**CS35** David Tilve-Martinez	**Round Table**
17h50		**CS29** Charlotte Berrezueta	**CS31** Alberto Guandalini	**CS36** Kazufumi Kobashi	

~ THURSDAY, 8

	Energy	Fundamental	Computation & Theory	Electronics	Macromaterials
	Salon VIP	**Auditorium**	**Salle Ville d'Hiver**	**Salle Dune du Pilat**	**Salle du Moulleau**
14h30	**OS10** Michael Strano	**IS30** Jean-Sebastien Lauret	**OS11** Vincent Meunier	**OS12** Gilad Zeevi	**IS38** Il Jeon
14h50		**IS31** Toshiya Okazaki			**IS39** Yutaka Ohno
15h10	**IS28** Fei Wei	**CS43** Finn Sebastian	**IS33** Wei Ji	**CS50** ChenChen Liu	**CS55** Jin Zhong
15h30	**IS29** Alessandro Siria	**CS44** Dimitri Golberg	**IS34** Hakim Amara	**CS51** Nathaniel Safron	**CS56** Rajath Alexander
15h50	**CS40** Hayashi Yasuhiko	**CS45** Jean-Baptiste Marceau	**CS47** Daniel Vadseth	**IS36** Kenji Hata	**CS57** Yanwu Zhu
16h10	Coffee break	Coffee break	Coffee break	Coffee break	Coffee break
16h50	**CS41** To be announced	**IS32** Salomé Forel	**IS35** Daniel Hedman	**CS52** Mengyu Zhao	**IS40** Juan Vilatela
17h10	**CS42** Chen Chen	**CS46** Yang Gao (cancelled)	**CS48** Daniel Förster	**IS37** Maria-Luisa della Rocca	**IS41** Milo Shaffer
17h30	**Round Table**	**Round Table**	**CS49** Philip Kloza	**CS53** Andreas Hüttel	**CS58** Lee Donju
17h50			**Round Table**	**CS54** Yang Wei	**CS59** John Bulmer

WEDNESDAY AFTERNOON EXCURSIONS

~ GENERAL RECOMMENDATION

Take a raincoat, light walking shoes, sunglasses, sunscreen, hat, water bottle.

~ PILAT SAND DUNE

14h15: Departure by bus from the entrance of the Casino, behind the Palais des Congrès

~ BOAT TOUR

14h00: Departure by walk from the entrance of the Palais des Congrès

~ OYSTERS FARM

14h15: Departure by bus from the entrance of the Palais des Congrès

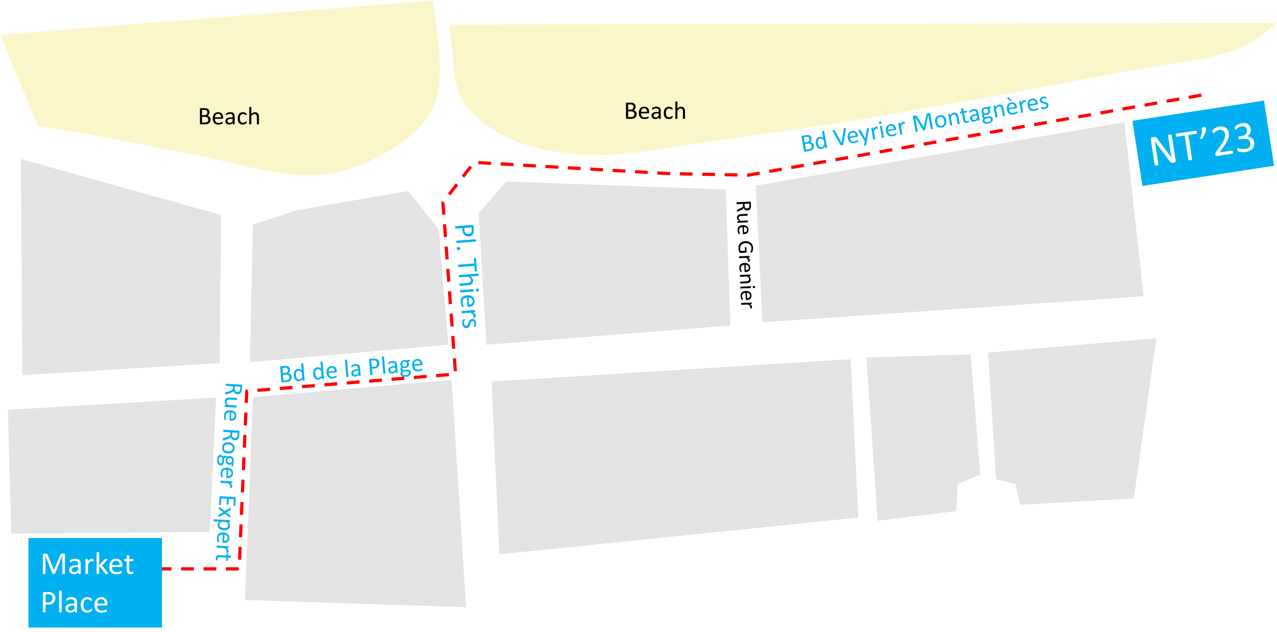
WEDNESDAY NIGHT

~ CONFERENCE BANQUET

Degustation of local French food in the old market place of Arcachon. At 8 mins by walk from the Palais des Congrès.

Where: Arcachon Market (see map)
Pl. des Marquises, 33120 Arcachon

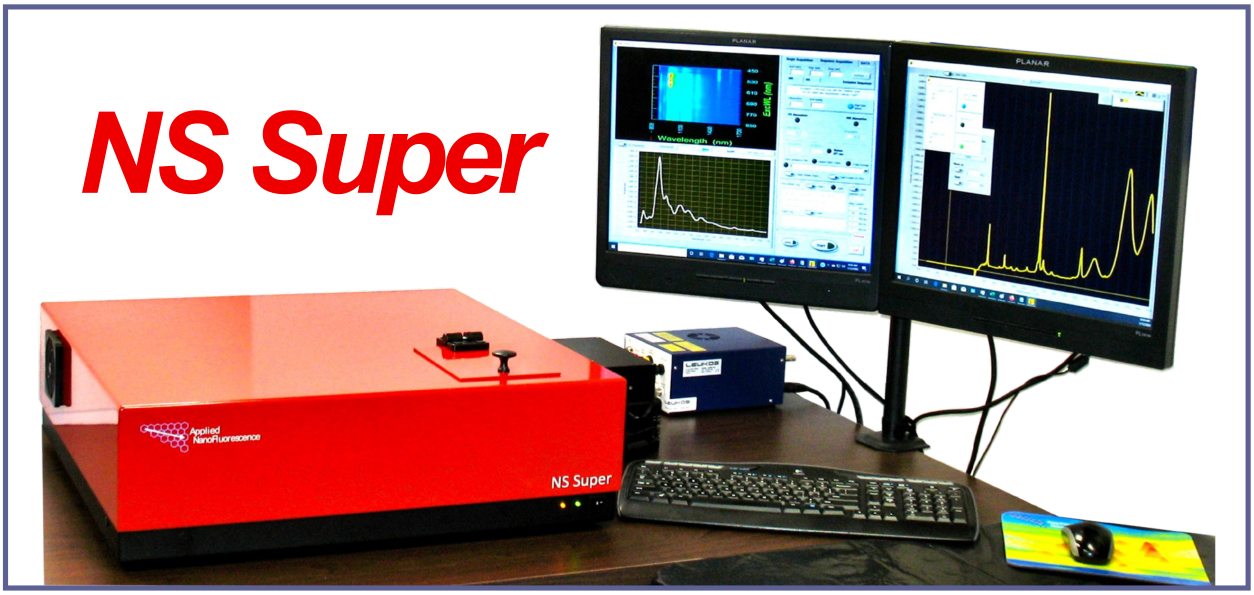
When: Wednesday at 19h00



MAP OF ARCACHON

Applied
NanoFluorescence

NS Super



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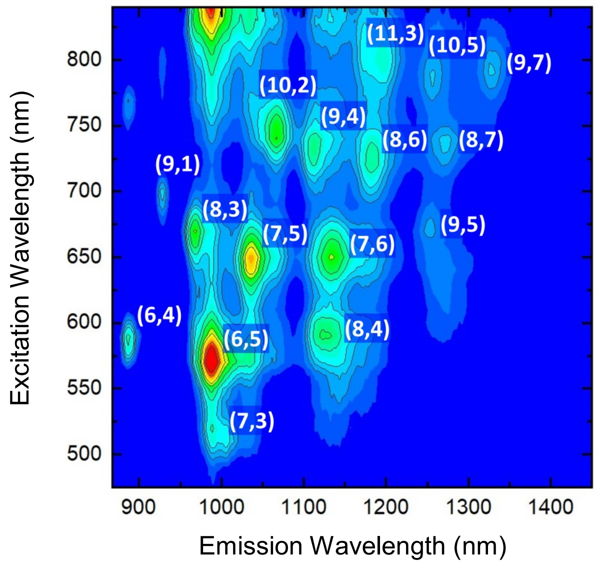

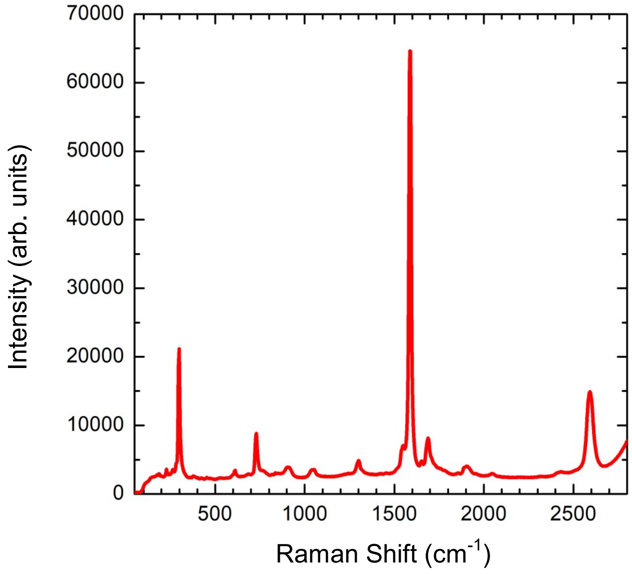

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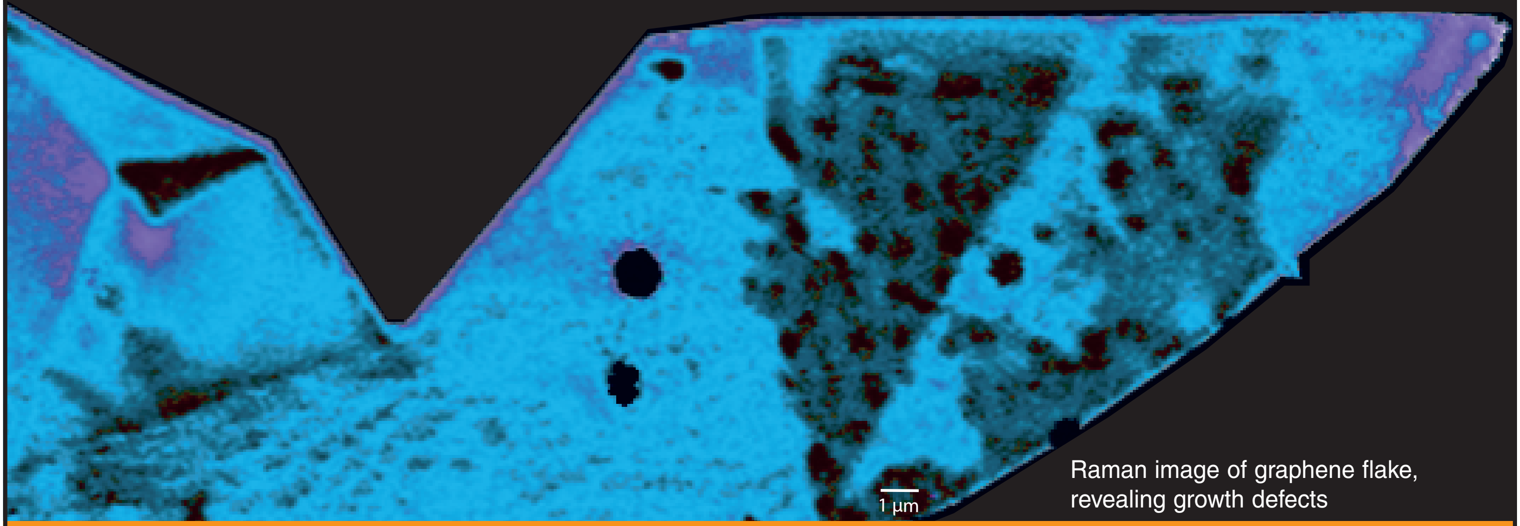
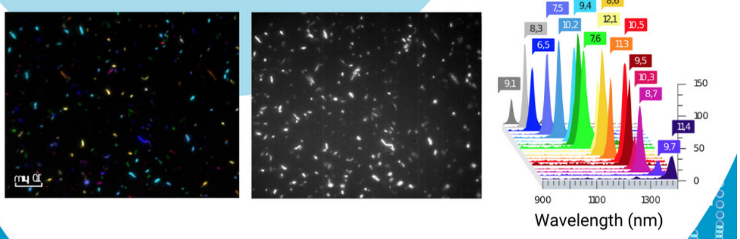
ABSTRACTS


1 µm


900
1100
1300
Wavelength (nm)
0
50
100
150

T1

DEVELOPMENT OF OPTICAL NANOTUBE SENSORS BY ENGINEERING BIOLOGICAL WRAPPINGS

A. A. Boghossian [1*]

[1]Ecole Polytechnique Fédérale de Lausanne (EPFL), 1015 Lausanne (Switzerland)
**email: ardemis.boghossian@epfl.ch*

Single-walled carbon nanotubes (SWCNTs) emit near-infrared fluorescence that is ideal for optical sensing applications. These fluorescence emissions can optically penetrate biological and synthetic materials that are otherwise opaque to visible light. This penetrability is ideal for deep-tissue and opaque packaging applications. The SWCNT fluorescence is also indefinitely photostable, enabling long-term and continuous optical measurements. Importantly, these emissions respond to changes in the SWCNT environment. This sensitivity serves as a promising basis for the optical detection of analytes. However, in the absence of appropriate functionalization, SWCNTs can interact and respond non-selectively to off-target analytes and undesired changes in the environment. Current endeavors therefore focus on controlling these fluorescence responses through SWCNT surface functionalization.

In this tutorial, we will discuss the state-of-the-art approaches for engineering SWCNT fluorescence through surface functionalization. The tutorial will focus on recent advancements in DNA and protein-based strategies. It will review advances in the experimental and computational fronts and conclude with an outlook on emerging efforts in this growing field.

T2

ATOMIC-SCALE MODELLING OF CARBON NANOTUBES FOR EXPERIMENTALISTS

C. Ewels *

T3

INTERCALATION-BASED EXFOLIATION OF LAYERED MATERIALS

D. Voiry [1*]

[1]*Institut Européen des Membranes (IEM, CNRS UMR5635, UM, ENSCM), Montpellier (France)*
**email: damien.voiry@umontpellier.fr*

2D materials have gained widespread attention in optoelectronics and energy storage, but their potential applications extend far beyond those fields[1]. Due to their unique properties and versatile composition, 2D materials are increasingly being explored for environmental applications. In particular, their two-dimensional aspect and atomic thickness make them well-suited for developing innovative technologies. The use of exfoliated 2D materials relies essentially on the preparation of individual nanosheets with controlled thickness and defect density.

In this context, the intercalation-based exfoliation of layered materials is a broadly applicable strategy for the scalable production of atomically thin (from mono- to few-layer) sheets, including graphene, black phosphorus, hexagonal boron nitride and transition metal dichalcogenides[1]. This strategy typically involves the intercalation of foreign species (ions or small molecules) into the interlayer spaces of layered materials, followed by a mild exfoliation process (spontaneously or via bath sonication, stirring or manual shaking). In this tutorial, I will review several intercalation-based exfoliation methods and highlight the factors that influence the quality of exfoliated nanosheets. I will also introduce the phase-transition phenomena involved in intercalation-based exfoliation, which may induce the resultant nanosheets to differ electronically and structurally from their bulk counterparts.

References

[1] Bhimanapati, R. *et al.* Recent Advances in Two-Dimensional Materials beyond Graphene, **ACS Nano**, 9, 12, 11509–11539

[2] Yang, R. *et al.* Synthesis of atomically thin sheets by the intercalation-based exfoliation of layered materials. **Nature Synthesis**, 2, 101–118 (2023)

K1

DNA-GUIDED FUNCTIONALIZATION OF CARBON NANOTUBES

M. Zheng [1*]

[1]*National Institute of Standards and Technology - Gaithersburg (United States)*
**email: ming.zheng@nist.gov*

Controlling carbon nanotube structure, functionalization, and placement at atomic precision is a fundamental challenge. DNA-guided manipulation of carbon nanotubes may offer a path to overcome the challenge. In this talk, I will first report current status of DNA-based carbon nanotube sorting. I will then present our work on DNA-controlled functionalization of single-chirality carbon nanotubes, using the photochemical Guanine oxidation reaction first reported by the Weisman group (ACS Nano, 2019, 13, 8222). By employing resonance Raman and fluorescence spectroscopy, we are able to reveal strong sequence-dependent modification of carbon nanotubes. We have also used cryo-EM to characterize the reaction product. By DNA screening we identify a sequence C3GC7GC3 whose reaction with an (8,3) enantiomer yields minimum disorder-induced Raman mode intensities and photoluminescence Stokes shift, suggesting ordered defect array formation. Single-particle cryo-EM shows that the C3GC7GC3 functionalized (8,3) has an ordered helical structure with a 6.5Å periodicity. Reaction mechanism analysis suggests that the helical periodicity arises from an array of G-modified carbon-carbon bonds separated by a fixed distance along an armchair helical line. Our findings may be used to remodel nanotube lattices for novel electronic properties.

References

Lin et al. “DNA-guided lattice remodeling of carbon nanotubes” Science 2022, v.377, pp.535-539

K2

RECENT PROGRESSES IN VAN DER WAALS LAYERED MAGNETIC SEMICONDUCTORS

Y.H. Lee [1*]

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Ferromagneticsm in van der Waals two-dimensional (2D) materials has been reported recently. Intrinsic CrI3 and CrGeTe3 semiconductors reveal ferromagnetism but the Tc is still low below 60K. In contrast, monolayer VSe2 is ferromagnetic metal with Tc above room temperature but incapable of controlling its carrier density. Moreover, the long-range ferromagnetic order in doped diluted chalcogenide semiconductors has not been demonstrated at room temperature. The key research target is to realize the long-range order ferromagnetism, Tc over room temperature, and semiconductor with gate tunability. In this talk, we introduce magnetic dopant, for example, vanadium in semiconducting WSe2 and manifest Tc at room temperature and gate tunability at low doping concentration. We further explore different doping concentrations including highly degenerate regime and demonstrate unconventional magnetic order by random telegraph spin noises via interlayer coupling and strange metal.

K3

MID-IR OPTICAL EFFECTS IN GRAPHENE AND NANOTUBES WITH CHEMICAL GRAFTS AND DOPING

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Surface plasmons are electromagnetic waves in materials coupled to oscillating electrons, which can be engineered to form antennas capable of guiding and concentrating light below the diffraction limit. The plasmons of nanocarbon materials are in the mid-infrared and can be tailored by the material's shape, conductance, and doping, but it is also tinted by electron-phonon interactions forming resonance loops and interference phenomena. This talk will present the general properties of Mid-IR plasmons in nanocarbons in the context of electron-phonon interactions and Fano anti-resonances. Experiments performed in the last years will be first reviewed to gain a better understanding of the mid-IR response in graphene and nanotube films. The Fano antiresonances in nanocarbons (graphene, single-walled, and double-walled nanotubes) is ascribed to electron-phonon (e-ph) interactions enabled by surface chemistry, disorder, and doping [1-3]. We will then discuss strategies for promoting these optical effects in the Mid-IR spectra of the graphene and nanotubes. The role of redox doping [4] and the modulation of the anti-resonances in the plasmonic response after chemical grafting will be discussed to gain insight into the e-ph interaction mechanism. Better control on the growth of graphene and on the covalent chemistry of nanocarbons using e.g. sulfur atoms will also be discussed as new tools for tailoring the optical properties of thin films. Through examples, I will describe how a promotion of e-ph interactions can be used to track chemical processes at interfaces, amplify MIR signals, and serve as modulators of THz waves [5].
Note that part of this work was done in collaboration with T. Hertel and his group (U. Würzburg). This talk is dedicated to Phaedon Avouris and his achievements on this topic and on nanocarbon research.

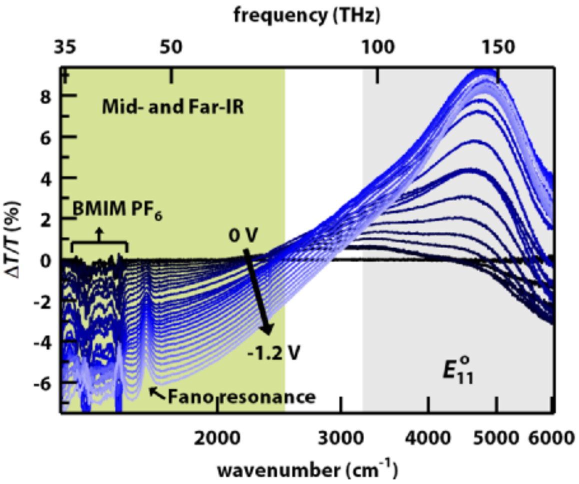

Figure abstract. Wavelength-dependent transmittance difference with applied potential of a double-wall carbon nanotubes (5 nm) thin film [Ref. 5].

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K4

SMALL ORGANIC MOLECULES IN NANOTUBES - ENCAPSULATION, CHARACTERIZATION AND REACTIONS

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The long tubular cavities of nanotubes can naturally act as encapsulation spaces for small molecules and thus form nanocontainers or nanoreactors [1]. In this talk, I will discuss various methods of encapsulation and subsequent chemical reactions resulting in metallic clusters [2], polymers [3,4], nanoribbons [5,6] or inner nanotubes [7]. The size of the tube limits the molecular dimensions and determines the reaction pathways by geometric constraints. Encapsulation can be performed from vapor phase by sublimation, from various solutions by nanoextraction and from liquid phase. In all cases, the elimination of side products, mainly adsorbed molecules on the outer surface of the tubes, is crucial [3]. The two most often used types of nanotubes consist of carbon and boron nitride, respectively. Because of the weaker secondary interaction of organic molecules with boron nitride than carbon, encapsulated molecules are much more easily removed from boron nitride nanotubes [7]. Besides classical characterization methods, mostly Raman spectroscopy and photoluminescence, high-resolution transmission electron microscopy [3, 5-7] as well as near-field spectroscopy and microscopy (infrared [2,4] and Raman [5]) can be employed to detect the constituents of the hybrid systems and follow the processes happening on the nanoscale.

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K5

M. Pasquali [*]

I01

1D TRANSITION METAL CHALCOGENIDES: GROWTH, STRUCTURES, AND PROPERTIES

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Transition metal chalcogenides (TMCs) are attractive materials with a wide variety of nanostructures and properties. In particular, recent advances in growth techniques have enabled the fabrication of various 1D forms of TMCs. In this talk, we report on our recent progress in the fabrication and characterizations of such TMC-based 1D nanostructures including nanotubes, nanoscrolls, nanowires, nanoribbons, and 1D interfaces (Figure 1). For example, the edges of layered transition metal dichalcogenides (TMDCs) can be used to grow TMDC nanoribbons with controlled edge structure by chemical vapor deposition (CVD) [1]. This process also creates in-plane heterostructures with 1D interfaces that exhibit various functions such as chiral or wavelength-tunable electroluminescence [2,3], directional exciton-energy transport [4], and band-to-band tunneling [5]. Isolated boron nitride (BN) nanotubes have enabled the templated synthesis of single-wall TMDC nanotubes [6]. In addition to TMDCs, we have recently achieved the wafer-scale growth of bundles of atomically-thin W_6Te_6 wires by salt-assisted CVD [7]. The W_6Te_6 bundles can be tailored into thin, nanoribbon-like structure, where a 2D carrier gas is formed [8]. Such ribbon-shaped bundles have been further used for a conversion to layered nanoribbons of WS_2, WSe_2 and WTe_2 [9] and for synthesis of metal-intercalated ternary TMC [10]. These TMC-based 1D nanostructures would provide opportunities for exploring low-dimensional physics and novel device applications.

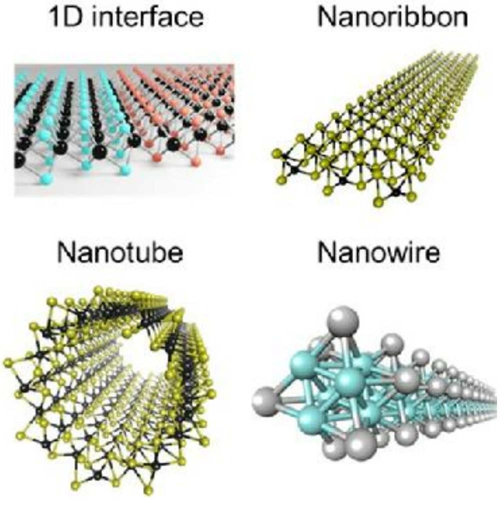

Figure 1. Structure models of TMC-based 1D nanostructures.

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I02

TAILORING THE PROPERTIES OF SINGLE-WALLED CARBON NANOTUBES: THE EFFECT OF FUNCTIONALIZATION

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Single-walled carbon nanotubes are all-carbon nanostructured one-dimensional systems with outstanding mechanical, electrical, and optical properties. For targeted applications it is desirable to fine-tune their properties. Among the different strategies, a wide set of physico-chemical functionalization treatments has been developed over the years. Here we will focus on the developments achieved through a noncovalent functionalization technique we developed some years ago [1] to bridge a triazine derivative onto the nanotubes' sidewalls without affecting the pi-conjugation of the nanotubes nor causing any structural defects while preserving the nanotube emissive features. The triazine derivative can be exploited as platform to immobilize virtually any molecular or nanostructured systems of interest in the immediate proximity of the tubes. On the same time, the integration of this functional platform also affects the density of charges within the nanotubes, offering a fine-tuned control the position of the Fermi level within the functionalized tubes. We will show how this lets us modulate the photoluminescence of the tubes, switching their emission on and off through the attachment of the switchable spiropyran/merocyanine system [2]. We also will focus on a class of ad hoc synthesized charge-transfer agents that either donate or withdraw electrons depending on the arrangements of their building units [3] and how their decoration affects the properties of the tubes.

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I03

S.Y. Xie *

I04

ELECTRON MICROSCOPY AND SPECTROSCOPY OF LOW-DIMENSIONAL HYBRID MATERIALS

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Electron microscopy and spectroscopy are widely used to characterize various low-dimensional materials. Identifying the atomic structures and/or measurements of local optical properties are of great importance in designing nanoscale devices based on hybrid nanostructures. Electron energy-loss spectroscopy (EELS) has been widely used for elemental identification in transmission electron microscopes (TEM) by using core-level excitations. Recent developments of monochromators after the e-beam guns have enabled us to access optical and vibrational information from the valence EELS ranges of nanometric materials. Here we show our latest studies to develop the possibilities of EELS applied for low-dimensional hybrid materials. Examples for atomic defects in in-plane hybrid TMDCs[1], monolayer structures of metal chlorides intercalated in bi-layer graphene[2, 3], surface adatoms for catalysis[4], one-dimensional hetero-nanotubes[5], isotopically heterogeneous graphene[6], and the other new forms of 1D/2D hybrid materials [7] will be shown.

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I05

YTTRIUM-INDUCED PHASE-TRANSITION TECHNOLOGY FOR FORMING PERFECT OHMIC CONTACTS IN TWO-DIMENSIONAL ELECTRONICS

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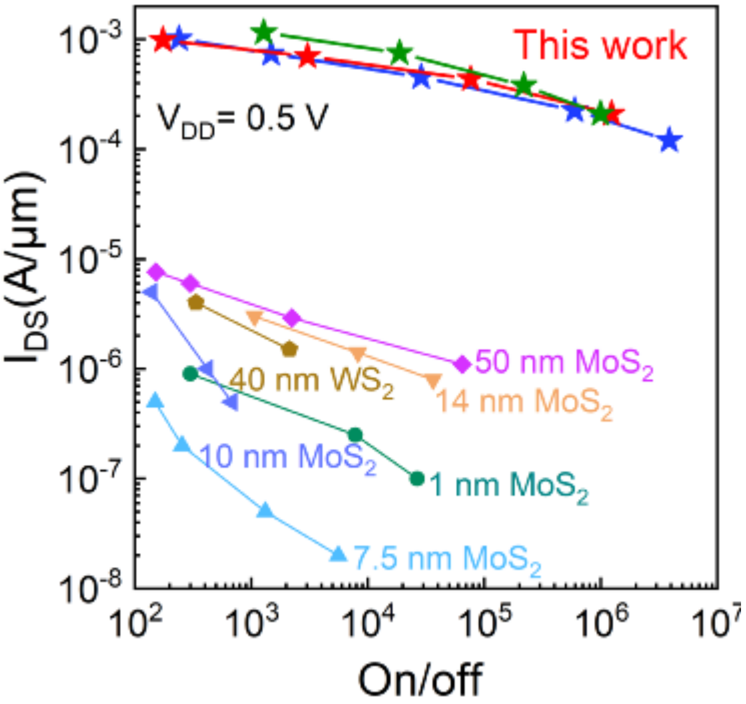
The van der Waals (vdW) strategy is promising for overcoming the Fermi pinning challenge in two-dimensional (2D) transistors. However, the lack of advanced-node lithography-compatible methods hinders wafer-scale integrated manufacturing of vdW contacts. An yttrium-doping-induced phase-transition technology is developed for making perfect ohmic contacts with two-dimensional semiconductors. In particular InSe FET is scaled down to 10 nm in channel length and 0.5 V on supply voltage [1], showing a record high transconductance of 6 millisiemens per micrometer and a room-temperature ballistic ratio in the saturation region of 83 percent, surpassing those of any reported silicon FETs; and can effectively suppress short-channel effects with a low subthreshold swing of 75 millivolts per decade and drain-induced barrier lowering of 22 millivolts per volt. Furthermore, low contact resistance of 62 ohm micrometers is reliably extracted in 10-nm ballistic InSe FETs, leading to a smaller intrinsic delay and much lower energy-delay product than the predicted silicon limit.



Comparison of ballistic 2D InSe FETs and other short-channel 2D FETs.

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I06

ELECTRON-PHONON INTERACTIONS IN TWISTED AND ANISOTROPIC 2D MATERIALS STUDIED BY RESONANCE AND POLARIZED RAMAN SPECTROSCOPY

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In this seminar I will discuss the use of Raman spectroscopy to study phonons and electron-phonon interactions in 2D materials. I will start reviewing the Raman spectra of graphene, showing that measurements performed by changing the energy of the incident photon provide information about the electronic structure of the material. I will then focus on the resonance Raman effect in twisted bilayer graphene (TBG), presenting experimental results performed in TBG samples with different twisting angles that allow the distinction of intralayer and interlayer electron-phonon (el-ph) interactions [1], and theoretical calculations of the double-resonance (DR) Raman intensity in graphene by imposing the momentum conservation rules for these two el-ph processes [2]. I will then present angle-resolved polarized Raman measurements in triclinic ReSe2 and show that the Raman tensor elements for the different phonons are given by complex numbers due to the resonance effect. I will show that the wavevector dependence of the electron–phonon interaction is essential for explaining the distinct results observed for each phonon mode [3].

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I07

CARBON NANO-ONIONS FOR BIOMEDICAL APPLICATIONS

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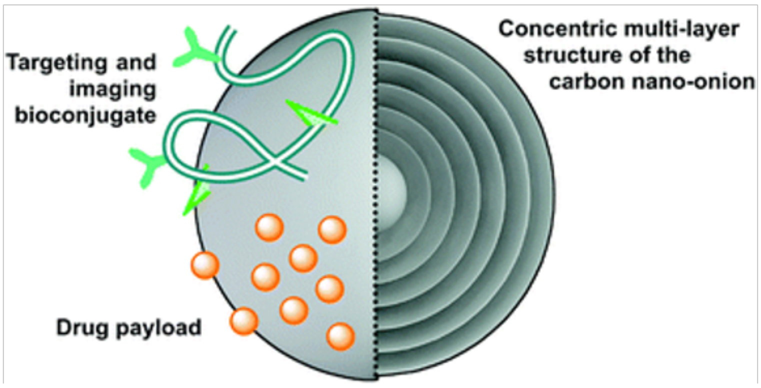
In this presentation, carbon nano-onions (CNOs) will be discussed as a potential vesicle for nanocarrier-type drug delivery systems.1 CNOs, or multi-layer fullerenes, consist of multiple concentric layers of sp2 hybridized carbon and are emerging as platforms for biomedical applications because of their ability to be internalized by cells and low toxicity.2

In my research group we have developed methodology for the synthesis of pure, monodispersed CNOs and various chemical functionalization strategies for the introduction of different functionalities (receptor targeting unit and imaging unit) onto the surface of the CNOs. The modified CNOs display high brightness and photostability in aqueous solutions and are selectively taken up by different cancer cell lines without significant cytotoxicity. Supramolecular functionalization with biocompatible polymers is an effective strategy to develop engineered drug carriers for targeted delivery applications. We reported the use of a hyaluronic acid-phospholipid (HA-DMPE) conjugate to target CD44 overexpressing cancer cells, while enhancing solubility of the nanoconstruct. Non-covalently functionalized CNOs with HA-DMPE show excellent in vitro cell viability in human breast carcinoma cells overexpressing CD44 and are uptaken to a greater extent compared to human ovarian carcinoma cells with an undetectable amount of CD44. In addition, they possess high in vivo biocompatibility in zebrafish during the different stages of development suggesting a high degree of biosafety of this class of nanomaterials.3

We recently synthesized Boron/nitrogen co-doped CNOs 4 and examined their interactions with biological systems. Our study on the toxicological profiles of BN-CNOs and oxidized BN-CNOs in vitro in both healthy and cancer cell lines, as well as in vivo on the embryonic stages of zebrafish (Danio rerio) demonstrate that these new class of carbon nanoparticles have high cyto-biocompatibility and a high biosafety. 5 Non covalent functionalization of BN-CNOs with HA-DMPE gave dispersions with long term aqueous stability. 6

Our results encourage further development as targeted diagnostics or therapeutics nanocarriers.



Figure

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I08

WATER FLOWS IN 1D AND 2D NANOCHANNELS, FROM CARBON MEMORIES TO QUANTUM FRICTION

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The emerging field of nanofluidics explores the molecular mechanics of fluids. This world of infinitesimal fluidics is the frontier where the continuum of fluid dynamics meets the atomic nature of matter, or even its quantum nature. Nature fully exploits the fluidic oddities at the nanoscale and it is capable of breath-taking technological feats using a fluidic circuitry made of multiple biological channels, such as ionic pumps, proton engines, ultra-selective pores, stimulable channels, ... A major challenge at stake is to harness the strange properties of fluid transport at nanoscale to reproduce or mimick some of these functionalities?

In this talk, I will discuss various experimental and theoretical results that we obtained recently in my team on the transport of water and ions in ultra-confinement, both in 1D nanotubes and 2D channels obtained by van der Waals assembly. I will in particular discuss the water-carbon couple, which highlights a variety of exotic transport properties. I will focus on two such phenomena: the emergence of memory in quasi–two-dimensional water channels and the development of elementary ion-based computing, with basic forms of Hebbian learning [1]; and the nearly frictionless flows of carbon nanotubes and its quantum roots [2,3].

I will conclude by briefly discussing how such nanoscale emerging phenomena can be exploited to develop technological innovations for water and energy.

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I09

CONTROLLABLE PREPARATION OF ULTRALONG CARBON NANOTUBES AND THE DEVELOPMENT OF EXTREME PROPERTIES

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Carbon nanotubes with superior properties are expected to be critical materials in many cutting-edge applications, including aerospace, military equipments and mobile communication etc. Crucial advances have been made in the controllable preparation and properties development of carbon nanotubes, as it has been reported that the tensile strength of defect-free carbon nanotubes and carbon nanotube bundles can approach the theoretical limit. However, the large-scale controllable preparation of carbon nanotubes with macro-length and the cross-scale transfer of excellent properties have not been well solved, which seriously limited its practical applications. Based on this research status, the report will introduces the latest progress of the research group in the controllable preparation and extreme performance development of ultra-long carbon nanotubes, including the evolutionary growth mechanism of carbon nanotubes, the large-scale controllable preparation of ultra-long carbon nanotubes, and the cross-scale precise assembly and extreme performance development of carbon nanotubes. The prospects and challenges of the further development of carbon nanotubes will also be discussed.

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I10

IMAGING NEUROMODULATORS WITH CARBON NANOTUBES

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Neurons communicate through neurotransmitter signals that either terminate at the postsynaptic process ("wired transmission") or diffuse beyond the synaptic cleft to modulate the activity of larger neuronal networks ("volume transmission"). Molecules such as dopamine, serotonin, and neuropeptides such as oxytocin belong to the latter class of neurotransmitters and have been the pharmacological targets of antidepressants and antipsychotics for decades. Owing to the central role of neuromodulators over a range of behaviors and psychiatric disorders, real-time imaging of the signal's spatial propagation would constitute a valuable advance in neurochemical imaging. To this end, we present a library of nanoscale near-infrared fluorescent nanosensors for dopamine (Beyene et al. Science Advances 2019; Yang et al. Nature Protocols 2021), serotonin (Jeong et al. Science Advances 2019), and oxytocin, where the nanosensors are developed from polymers pinned to the surface of single wall carbon nanotubes (SWNT). We characterize our findings in the context of their utility for high spatial and temporal neuromodulator imaging in the brain, describe nanosensor exciton behavior from a molecular dynamics (MD) perspective, and validate nanosensor for use to elucidate neuromodulator signaling variability with disease or pharmacological perturbations at a synaptic scale.

We next use this dopamine imaging nanosensor to study dopamine signaling deficits in Huntington's Disease (HD), where dysregulation of dopamine transmission plays a key role in multiple neurodegenerative diseases. While several treatments for physical and psychiatric HD symptoms target dopaminergic neuromodulation, little is known about the relationship between dopamine and the principal cause of HD, production of mutant huntingtin protein. Specifically, knowledge of what drives decreased dopamine release at motor symptom onset is uncertain and could be driven by decreasing dopamine release site numbers, decreasing dopamine quantal release per site, or a combination of the two. By imaging dopamine activity in the striatum of R6/2 HD model mice, we find that late-disease decreases in evoked dopamine release are primarily driven by decreases in the number of dopamine release sites as opposed to net decreases in dopamine release per release site. We discuss how to use these findings as optimal therapeutic intervention timepoints for siRNA-based HD therapies, discuss how dopaminergic projections are affected by mutant huntingtin, and whether specific targeting of these loci is important for developing gene-therapy efforts.

I11

CARBON NANOTUBES FOR PROFILING CARBOHYDRATE-PROTEIN RECOGNITION

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The recognition interactions between cell surface carbohydrates and carbohydrate-binding proteins (CBPs) play a vital role in a multitude of cellular activities, such as immune responses and infections. Our laboratory develops glyconanomaterials, such as carbohydrate-decorated single-wall carbon nanotubes (SWCNTs), for detecting specific carbohydrate-protein interactions and understanding their underlying mechanisms, that are crucial for discovering therapeutic and diagnostic mechanisms. We created noncovalent complexes of SWCNTs and glycopolymers, which are polymers with carbohydrate pendant groups and have been used extensively to mimic the functions of naturally occurring glycoconjugates. These glycopolymer-wrapped SWCNTs showed distinct nanostructure-induced interactions between the internal sugar group of glycopolymers and a specific CBP, as compared to the currently known interaction behavior of CBPs with the terminal glycan of oligosaccharides. Additionally, we demonstrated the role of water in creating fluorescent quantum defects on SWCNTs as a step toward the covalent functionalization of bright SWCNTs with carbohydrates via bioorthogonal click chemistry in aqueous environment. These glyconanomaterials can potentially lead to the creation of versatile optical sensors for detecting carbohydrate-protein interactions with enhanced specificity and sensitivity.

C01
INTENSE RAMAN D BAND WITHOUT DISORDER IN FLATTENED CARBON NANOTUBES

E. Picheau [1,*], A. Impellizzeri [2], D. Rybkovskiy [3], M. Bayle [2], J.Y. Mevellec [2], F. Hof [1], H. Saadaoui [1], L. Noé [4], A. Cefas Torres Dias [4], J.L. Duvail [2], M. Monthioux [4], B. Humbert [2], P. Puech [4], C. Ewels [2], A. Pénicaud [1]

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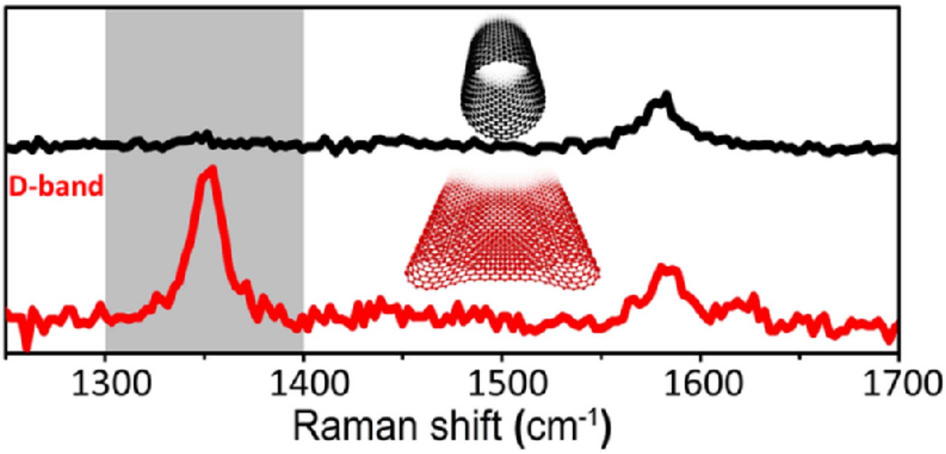
Above a critical diameter, single or few-walled carbon nanotubes (CNTs) spontaneously collapse as flattened carbon nanotubes (FCNTs). FCNTs can be consider as few layer graphene nanoribbons (GNRs), with continuity at the edges forming two lateral cavities. FCNTs overcome the as-yet unsolved difficulty to obtain scalable GNRs with atomically smooth edges, critical for electronics.[1] FCNTs can be obtain in solution by reported methods,[2,3] and has been deposited on a surface. A close correlation between atomic force microscopy and Raman spectroscopy allowed to measure Raman spectra of isolated self-collapsed FCNTs. Strikingly, the collapse provokes the appearance of an intense and narrow D band (see figure 1), independent of the presence of topological defects. It arise solely as a signature of folding, as shown by experimental and theoretical evidences.[4] This conclusion should have wide repercussions for the field of graphene and related materials regarding defect quantification and serve as a basis to revisit materials comprising structural distortion where poor carbon organization was concluded on Raman basis. Our finding also emphasizes cultural differences in understanding of a defect between chemists and physicists, a possible source of confusion for researchers working in nanotechnologies.



Raman spectra CCNT/FCNT. Raman spectra of a cylindrical (black, top) and of a collapsed (red, bottom) carbon nanotube

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C02

GRAPHENE NANORIBBONS IN CARBON AND BORON NITRIDE NANOTUBES FROM 1,2,4-TRICHLOROBENZENE

A. Cadena [1,*], B. Botka [2], Á. Pekker [2], C.D. Tschannen [3], C. Lombardo [3], L. Novotny [3], A.N. Khlobystov [4], E. Dodony [5], Z. Fogarassy [5], B. Pécz [5], K. Kamarás [6]

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Synthesis of graphene nanoribbons from small molecules encapsulated in nanotubes has many advantages: uniform width, clean edges, and easily removable, volatile side products. We present the synthesis of graphene nanoribbons from the liquid precursor 1,2,4-trichlorobenzene. The first step is the encapsulation, which takes place by immersing the open nanotubes in the liquid. The removal of the precursor molecules adsorbed on the outer surface can be achieved by simply letting them evaporate. This procedure is followed by a thermal reaction resulting in nanoribbons with width determined by the nanotube diameter and length up to 100 nm. The formation of nanoribbons was proven by transmission electron microscopy and macroscopic and tip-enhanced Raman scattering. [1]

The above synthesis can be performed also in boron nitride nanotubes where the nanoribbon formation has not been as successful so far as inside carbon nanotubes. The significance of producing graphene nanoribbons using boron nitride nanotubes lies in the transparent nature of these tubes which, contrary to carbon nanotubes, allows obtaining information of the reaction products in a wide optical range. In this case, the reaction products were analyzed with Raman scattering, transmission electron microscopy and wide-range optical spectroscopy. [2]

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C03

CARBON NANOTUBE QUANTUM WELL DEFECT EMISSION FOR MACHINE LEARNING-GUIDED DIAGNOSTICS

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We employ the photoluminescence of single-walled carbon nanotube (SWCNTs), and covalent sp3 quantum well defects (aka organic color centers, OCCs) on SWCNTs, to develop new diagnostic methods for cancer and other diseases. Serum biomarker measurements are widely used for diagnosis, but these markers largely provide low sensitivity and specificity. We developed a method using defect-modified SWCNTs to identify a “disease fingerprint” through the collection of large data sets of molecular binding interactions to an array of quantum defect-modified carbon nanotubes. We found that a library of OCCs exhibited differentiated spectral variation in response to an ensemble of molecular binding events in patient serum. Via machine learning algorithms, we built a prediction model of nanosensor responses that reliably identified ovarian cancer substantially better than the established, FDA-approved biomarker, CA125. We have expanded this approach to other indications without known biomarkers, providing a general method to identify diseases.

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C04

EVIDENCE AND ANALYSIS OF DISCONTINUOUS THERMODYNAMIC PROPERTIES UNDER EXTREME ONE DIMENSIONAL CONFINEMENT

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Recent interest in one-dimensionally confined fluids, where confinement approaches molecular dimensions, has demonstrated exceptionally high fluxes from slip flow and large distortions of fluid phase boundaries [1,2]. The Center for Enhanced Nanofluidic Transport (CENT) was recently formed as an intellectual hub for studying extreme fluid confinement in what we label Single Digit Nanopores (SDNs). To this end, in this work, we note that predicting such phenomena for a given conduit dimension has been confounded by a dearth of fundamental thermodynamic measurements and analysis as a function of confinement diameter and wall composition. To this end, we develop a platform based on Raman spectroscopy and ultra-long carbon nanotubes with diameters less than 3 nm suspended over electron microscopy windows to identify and study new types of vibrational coupling to the CNT environment. Electron diffraction assigned Double Walled Carbon Nanotubes (DWNT) suspended across with 20 µm slit on 1,500 µm transmission electron microscopy (TEM) windows are used to probe in vacuum an enormous 10 to 15% Radial Breathing Mode (RBM) downshift shift with increasing temperature that is both reversible and robust over dozens of cycles. A new analysis based on a harmonic oscillator model is able to assign the hyperbolic trajectory to a reversible increase in damping, generating a shift that is the reverse of prior expectations. The environmental source of the coupling is assigned to graphitic ribbons shown by TEM to decorate the surface up to an axial coverage of 60%. A linear, strain-dependent coupling of the ribbon fragments driven by thermal expansion of the supporting nanotube describes the distinctive cusp that appears throughout the 91 temperature scans of 3 distinct DWNTs. We find that each connection of the fragments with the DWNT surface keeps the ratio of spring to damping frequencies constant, producing a remarkable saturation of the RBM frequency in the low-tension limit. The high fidelity of the oscillatory model shows that the RBM has negligible intrinsic temperature dependence and that evidence for impurity-induced damping as a confounding variable is commonly present in experiments previously thought to be on pristine systems. Overall, these findings significantly increase our understanding of the environmental coupling of 1D nano-mechanical systems, providing the basis for new technological applications and improved spectral analysis.

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C05

HEXAGONAL ARRAYS OF CARBON MICROPYRAMIDS FORMED BY SELF-ASSEMBLY OF SOOT NANOPARTICLES ON THE SURFACE OF RESISTIVELY HEATED CARBON FILAMENTS IN LOW-OXYGEN ATMOSPHERE

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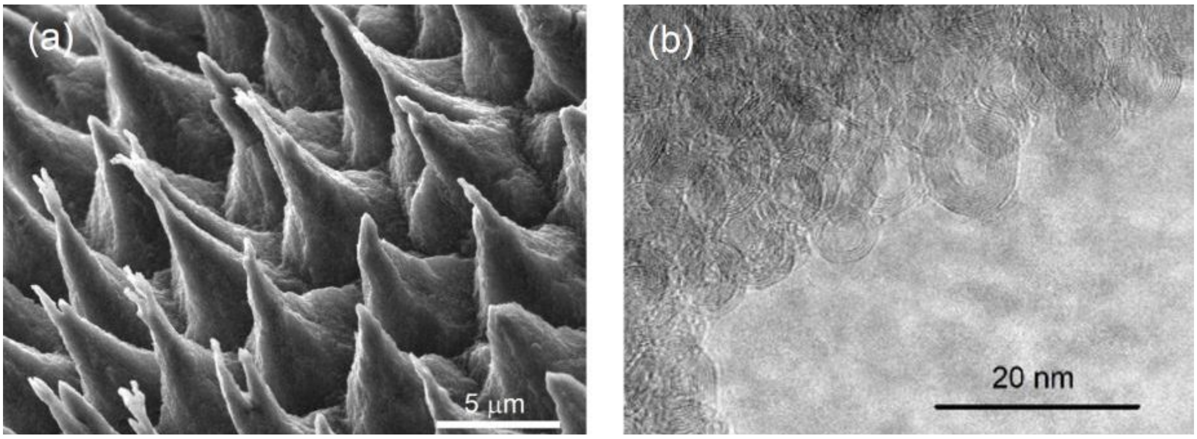
Almost regular hexagonal arrays of microscopic pyramids consisting of soot nanoparticles are formed on the surface of graphitized filaments of chitosan, which are resistively heated to ∼1800−2400 °C under an Ar atmosphere containing trace amounts of oxygen (∼300 ppm) [1]. At higher temperatures (T >2200)°C, approximately) the soot particles are represented mainly by multi-shell carbon nano-onions. The height and width of the pyramids are strongly dependent on the temperature of the resistive heating, diminishing from 5 to 10 µm at T ≈ 1800°C to ∼1 µm at 2300−2400 °C. The pyramids always point normally to the surface of the filaments. As appeared, the pyramids are soft and can be easily destroyed by touching them, but can be hardened by heating under an oxygen-free atmosphere. The thermophoretic force generated by a strong temperature gradient near the tubes may be the cause of the structure formation. The regular mutual arrangement and the sharp extremities of the micropyramids allow considering them as prospective microstructures for advanced applications. We have demonstrated that the individual carbon micropyramids emit a tunneling current upon application of a local electrical field. This indicates the principal possibility to create field emitter arrays on the base of the micropyramid ensembles. The pyramids arrays may be also investigated for the creation of superhydrophobic and bactericidal coatings, as well as ultra-black materials.



The self-assembled soot micropyramids. (a) An array of micropyramids self-assembled at 2000°C and relative oxygen concentration 300 p.p.m. (b) Soot nanoparticles (carbon nano-onions) which form the micropyramids.

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C06

CHALLENGES AND STRATEGIES IN SENSING CHEMICALS WITH CARBON NANOTUBE THIN-FILM ELECTRONIC DEVICES

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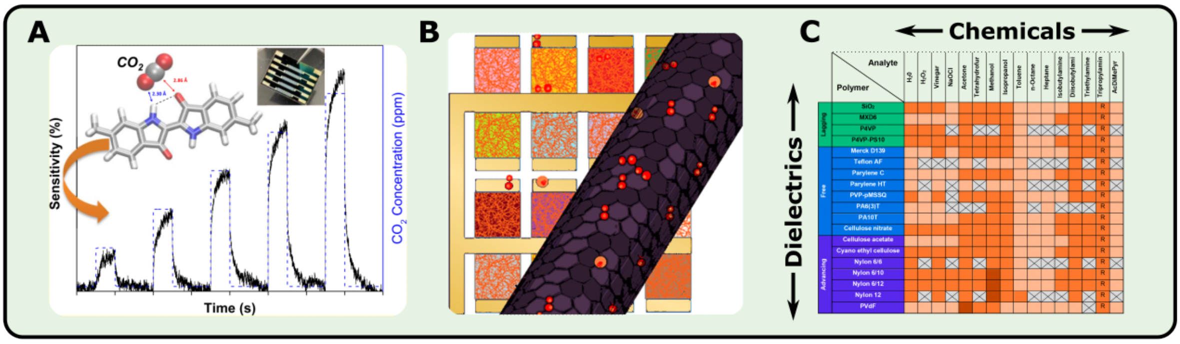
Semiconducting single-walled carbon nanotubes (sc-SWCNTs) are attractive for chemical detection with electronic devices [1] due to their special characteristics: since they are structured with a one-atom-thick wall in a quasi-1D form factor, sc-SWCNTs are particularly sensitive to electrostatics in their environment. Furthermore, their bandgap of about 1 eV is much larger than the thermal energy at room temperature, and at the same time it is in a suitable range for electronic applications. Their density of state also exhibits van Hove singularities that cause strong modulation of their conductivity and optical properties with charge carrier injection. The biggest challenge in chemical detection with sc-SWCNT thin-film electronic devices is their lack of selectivity and several approaches have been devised to impart specificity. [1] In this talk we will present different chemical detection strategies with enriched sc-SWCNTs using electronic transduction and discuss their advantages and disadvantages. We will demonstrate detection of ammonia at concentrations below 1 ppm using sc-SWCNTs wrapped with a decomposable polymer in a chemiresistor configuration. [2] Selective detection of CO_2 with chemiresistors was obtained by developing a SWCNT-wrapping indigo-fluorene-based copolymer with specific interactions for carbonyls. [3] Finally, we will present a strategy for differentiating the response of sensing elements to a variety of volatile analytes by modifying the nature of the gate's polymer dielectric in a three-electrode, bottom-gate chemitransistor configuration. [4] This methodology paves the way for the implementation of sc-SWCNT-based chemitransistors in a printed cross-reactive sensor array.



A) Selective CO2 sensing using an indigo-fluorene-based copolymer used in wrapping and enriching sc-SWCNTs. B) Cartoon representation of a sc-SWCNT network FET sensor array. C) A matrix displaying the compound response (difference in mobility and shift in threshold voltage) for an array of sc-SWCNT network FET transistors with various polymer gate dielectrics exposed to a series of volatile compounds.

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C07

SOLAR ENERGY HARVESTING IN SEMICONDUCTING SWCNT-BASED HETEROJUNCTIONS

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Quantum-confined semiconductors provide highly tunable optical and electrical properties for a wide variety of emerging 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. In this talk, I will discuss the use of a variety of rationally designed heterojunctions between s-SWCNTs and organic and inorganic semiconductors to harvest visible/near-infrared photons and convert these excitations into long-lived charge-separated states and electrical current. Type-II heterojunctions between s-SWCNTs and monolayer transition metal dichalcogenides (TMDCs) enable rapid exciton dissociation and microsecond charge-separated state lifetimes.1-3 I will discuss new results that consider how charge separation efficiency and rate depend on interfacial band alignment, as well as the degree of bound charge transfer character of the resulting charge-separated state. I will also discuss new results demonstrating that graded bandgap energy funnel architectures that mimic photosynthetic energy transfer pathways can enable energy harvesting p-n junctions formed solely from s-SWCNT thin films.4 Finally, I will discuss new results on Type-II heterojunctions formed between s-SWCNTs and novel molecular perylene diimide (PDI) based electron acceptors.5 Taken together, these studies provide fundamental insights into the links between ground-state thermodynamics and excited-state dynamics for model nanoscale heterojunctions used to harvest solar energy and produce long-lived charge-separated states.

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C08

SPATIALLY RESOLVED MOLECULAR ENGINEERING OF GRAPHENE

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Exploring the tailored physical/chemical properties is at the forefront of graphene research.[1] The emerging development of covalent molecular engineering represents a rather promising tactic for this purpose carrying several unique advantages. In this line, we have developed two scenarios, including reduction-mediated lithography and laser writing, for spatially resolved covalent 2D-patterning of graphene, affording a variety of well-structured graphene architectures.[2-3] Furthermore, based on the combination of 2D-patterning techniques and post-functionalization approaches, more promising hierarchically ordered multifunctional graphene architectures were facilely constructed. We further demonstrated that the chemical information of these built 2D-systems can be finely manipulated by establishing complete write/read/erase circles.

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C09

SUPER MACKAY CLUSTER $FE_{42}CO_{13}$ FOR CHIRALITY SELECTIVE GROWTH OF SINGLE-WALLED CARBON NANOTUBES

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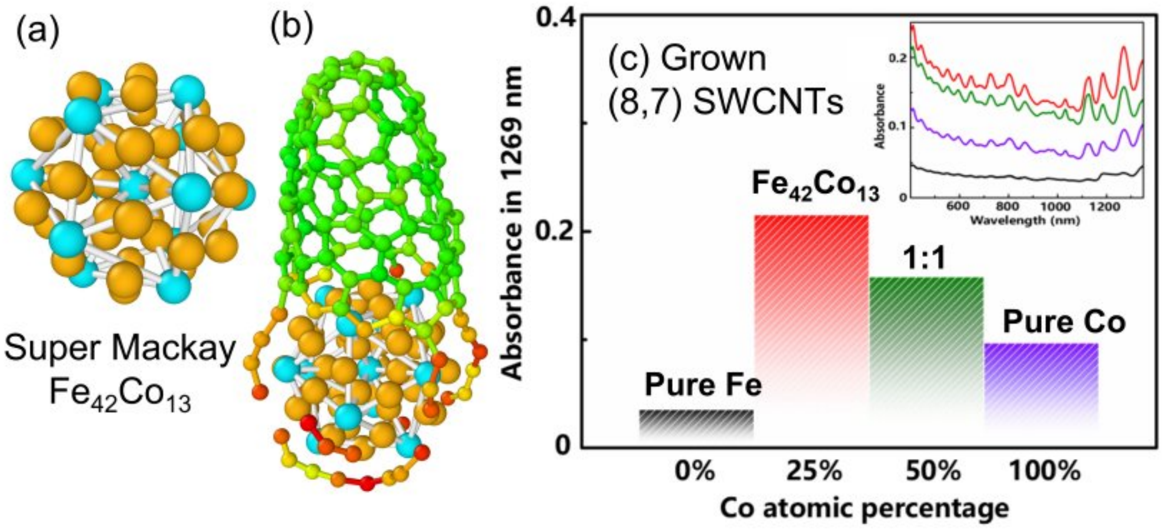
We propose a super Mackay cluster $Fe_{42}Co_{13}$ for the selective chirality growth of single-walled carbon nanotubes. The double icosahedral structure, the so-called Mackay structure, is well known by theoretical works[1,2]. However, the Mackay structure is meta-stable in our molecular dynamics simulation (MD). The most stable structure in MD simulation is shown in Fig. 1(a); internal core $Fe_{12}Co$ is rotated 15 degrees from the Mackay structure. If we let this cluster vibrate at high temperatures, we can observe the mode-crossing rotation of the inner core. From MD simulations, we found the extremely high melting point of $Fe_{42}Co_{13}$ cluster, 1800K. We believe the extremely high melting point originates from this unique mode-crossing vibration. By preliminary MD simulation of carbon nanotube growth, we found the fully solid behavior of this catalyst up to 1800K, as in Fig. 1(b). The chirality of SWCNT of the simulated nanotube will be discussed. As we can guarantee the fully solid catalysts in the usual CVD condition, we try to grow chirality-specific SWCNTs based on this super Mackay cluster. The preliminary result based on ACCVD [3] is shown in Fig. 1(c). The $Fe_{42}Co_{13}$ alloy ratio gives a higher growth efficiency than pure Co, pure Fe, and a 1:1 mixture.



Super Mackay structure and growth of SWCNTs. (a) super Mackay structure of Fe42Co13. Co atoms are in cyan and Fe atoms are in orange. (b) Molecular dynamics simulation of growth. (c) CVD growth of SWCNTs by zeolite-supported bimetallic alloy at 850 C. The absorption corresponds to (8,7) nanotubes.

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C10

OPTICAL PROPERTIES OF METALLIC CARBON NANOTUBES: BEYOND THE STANDARD SEMI-EMPIRICAL MODEL FOR PLASMONIC PREDICTIONS

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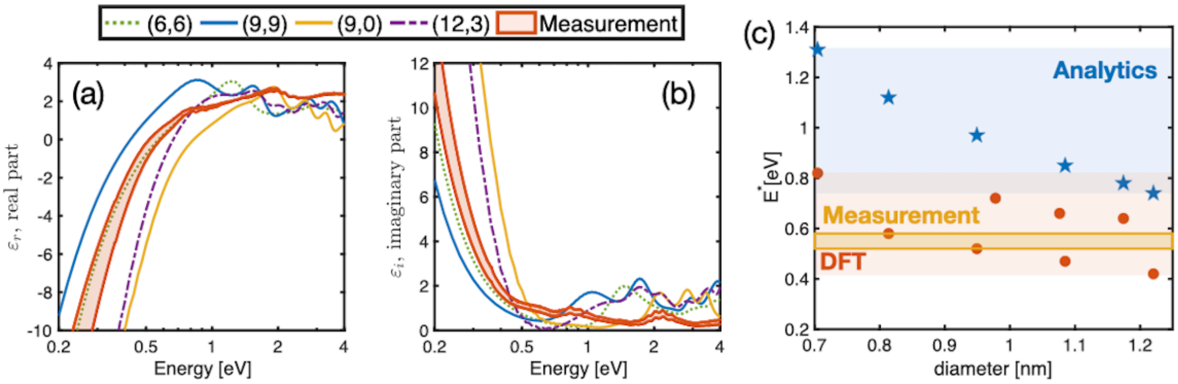
In recent years, plasmonics has become a rapidly growing area of research with the potential to bring advancements in various fields such as sensing[1] and highly integrated photonic devices[2]. In an effort of miniaturization, metallic Single-Wall Carbon NanoTubes (m-SWCNT) could be envisioned as the smallest metallic wire, a building block for plasmonic devices at the nanoscale. In order to engineer such practical nanotube-based optical devices, the knowledge of m-SWCNT complex dielectric constant is fundamental. However, experimental measurements are mostly limited to unsorted samples[3] or focused only on a narrow frequency range[4]. Furthermore, most theoretical calculations have focused on the optical properties of semiconducting SWCNT or missed the intraband-transitions contribution of m-SWCNT. An analytical model, known as the surface conductivity model[5], has also been developed but has not been confronted with experiments. Therefore, we investigate the intraband-transitions contribution to the optical properties of metallic carbon nanotubes both experimentally and theoretically[6]. The experimental dielectric constant for m-SWCNT samples is derived from reflectance measurements through electromagnetic modeling and Kramers-Kronig relations (figure a-b). It is found in remarkable agreement with the predictions from ab initio calculations but demonstrates a failure of the standard semi-empirical model[5] (figure c), widely used in various fields of physics especially for predicting the optical properties of many 2D materials. We report new theoretical predictions for the plasma frequency of m-SWCNT unambiguously validated by experimental observations.



m-SWCNT experimental complex dielectric constant (a) real and (b) imaginary part compared with DFT calculations. (c) Cut-off energy as a function of the diameter from analytics (blue stars), DFT (red dots), and measurement (yellow area).

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C11

CHIRALITY-DEPENDENCE OF TRIPLET EXCITONS IN (6,5) AND (7,5) SWCNTS REVEALED BY OPTICALLY-DETECTED MAGNETIC RESONANCE

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The excitonic structure of single-wall carbon nanotubes (SWCNTs) consists of multiple singlet (SE) and triplet excitons (TEs) of which only one SE is optically bright.[1] To stimulate future applications in nanophotonics, a deeper understanding of the role of TEs in the photophysics of SWCNTs is highly needed. Previously, an unambiguous proof of the existence of TEs in SWCNTs was provided by combining optical spectroscopy with a spin-sensitive technique, namely optically detected magnetic resonance (ODMR).[2,3] In this work, we report the detailed characterization of TEs in chirality-purified samples of (6,5) and (7,5) SWCNTs, either randomly oriented in a frozen solution or with in-plane preferential orientation in a film, by means of optically detected magnetic resonance (ODMR) spectroscopy. In both chiral structures, the nanotubes are shown to sustain three types of TEs. One TE exhibits axial symmetry with zero-field splitting (ZFS) parameters depending on SWCNT diameter, in good agreement with the tighter confinement expected in narrower-diameter nanotubes. The ZFS of this TE also depends on nanotube environment, pointing to slightly weaker confinement for surfactant-coated than for polymer-wrapped SWCNTs. A second TE type, with much smaller ZFS, does not show the same systematic trends with diameter and environment and has a less well-defined axial symmetry. This most likely corresponds to TEs trapped at defect sites at low temperature, as exemplified by comparing SWCNT samples from different origins and after different treatments. A third triplet has unresolved ZFS, implying it originates from weakly interacting spin pairs. Aside from the diameter dependence, ODMR thus provides insights in both the symmetry, confinement, and nature of TEs on semiconducting SWCNTs.[4]

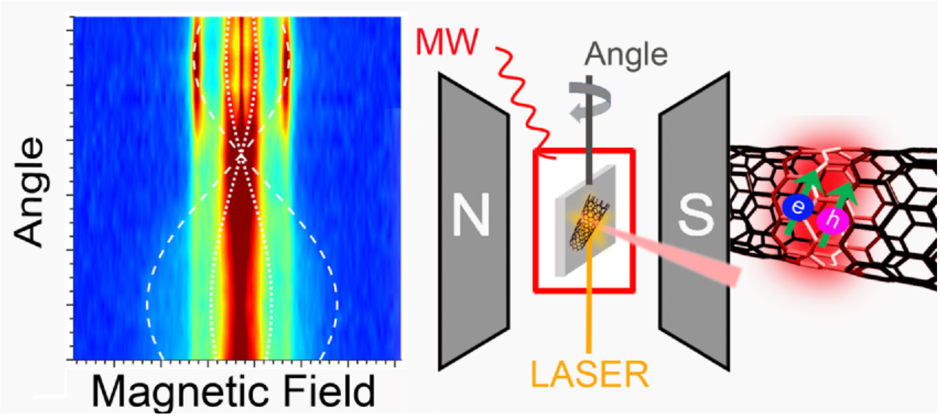

Figure 1. ODMR of triplet excitons in carbon nanotubes as a function of the angle of the magnetic field with the film plane.

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C12

THE EVOLUTION OF CONFINED PRECURSOR MOLECULES INSIDE CARBON NANOTUBES

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Unraveling the chemical reaction process still remains a challenge. The 1D nanospace of carbon nanotube is an ideal nanoreactor for synthesis of nonexistent or unusual materials, e.g., previously we have synthesized ultra-long linear carbon chains [1-4]. Thanks to the confinement of the carbon nanotube, the evolution (or reaction) of precursor molecules under high temperature or high pressure can be studied in detail now. Here, our recent results discovered that some precursor molecules with/without hexatomic rings can be converted into graphene nanoribbons [5-7], whereas some aromatic molecules can be transformed into linear carbon chains [8]. These unusual phenomena are beyond the conventional chemical reaction. In addition, many kinds of 1D elemental or compound chains can be obtained by using the same confined synthesis [9], which paves the way to create a library of novel 1D materials that do not exist or are yet to be explored.

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C13

COUPLED COLORED CENTERS GRAFTED ON A SINGLE WALL CARBON NANOTUBE FOR QUANTUM LIGHT GENERATION.

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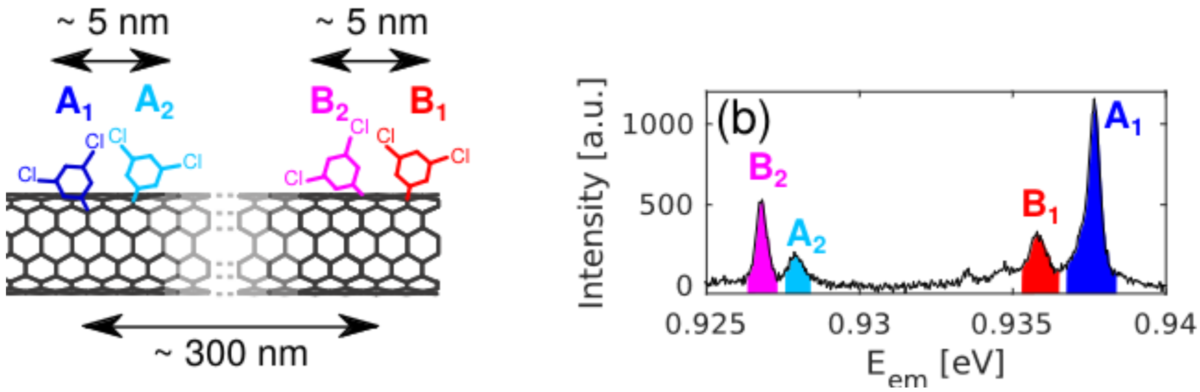
The development of covalent diazonium functionalization of carbon nanotubes brings unique opportunities in terms of original quantum sources of light, similar to colored centers in large gap semi-conductors. However, carbon nanotubes colored centers have unique assets, such as their versatile emission energy that can be tuned using the nanotube bandgap and the chemical nature of the grafted molecule. This opens avenues for original interplay between neighboring centers. In particular, it should be possible to create a linear ensemble of closely packed single-photon sources along the carbon nanotube backbone. The physical proximity of several dopants would make it possible to couple them to a resonant cavity mode and to induce original dynamics and light emission properties. Here, we investigate experimentally the case of a series of four quantum emitters attached to the same carbon nanotube within a few hundreds of nanometers. We explore their properties using excitation photoluminescence spectroscopy, polarization and super-localization measurements and time-resolved techniques such as correlation and photoluminescence decay measurements. We show that the ensemble of quantum emitters splits into two pairs with qualitatively different behaviors in terms of spectral diffusion and luminescence saturation, which we interpret as electronically coupled or uncoupled quantum emitters.



Ensemble of four quantum emitters grafted on the same single wall carbon nanotube.

C14

IN SITU STUDIES OF THE KINETICS OF GROWTH AND ETCHING OF INDIVIDUAL SWCNTS BY OPTICAL MICROSCOPY

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Understanding the kinetic selectivity of carbon nanotube growth at the scale of individual nanotubes is essential for the development of growth methods with high chiral selectivity. Here we report on the use of homodyne polarization microscopy [1,2] for high-throughput imaging of long individual carbon nanotubes under real growth conditions (at ambient pressure, on a substrate), and with sub-second time resolution. Our in situ observations on hundreds of individual nanotubes [3] reveal that about half of them grow at a constant rate all along their lifetime while the other half exhibits stochastic changes in growth rates, and switches between growth, pause and shrinkage. Statistical analysis shows that the growth rate of a given nanotube essentially varies between two values, with similar average ratio (~1.7) regardless of whether the rate change is accompanied by a change in chirality. These switches indicate that the nanotube edge or the catalyst nanoparticle fluctuates between different configurations during growth. In addition, we will report our recent investigations of the influence of the growth parameters (temperature, precursor and etchant concentrations) on the kinetics of growth and etching of individual SWCNTs using the same experimental approach [4].

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C15
THERMODYNAMIC UNDERSTANDING OF CARBON NANOTUBE CATALYST ACTIVITY

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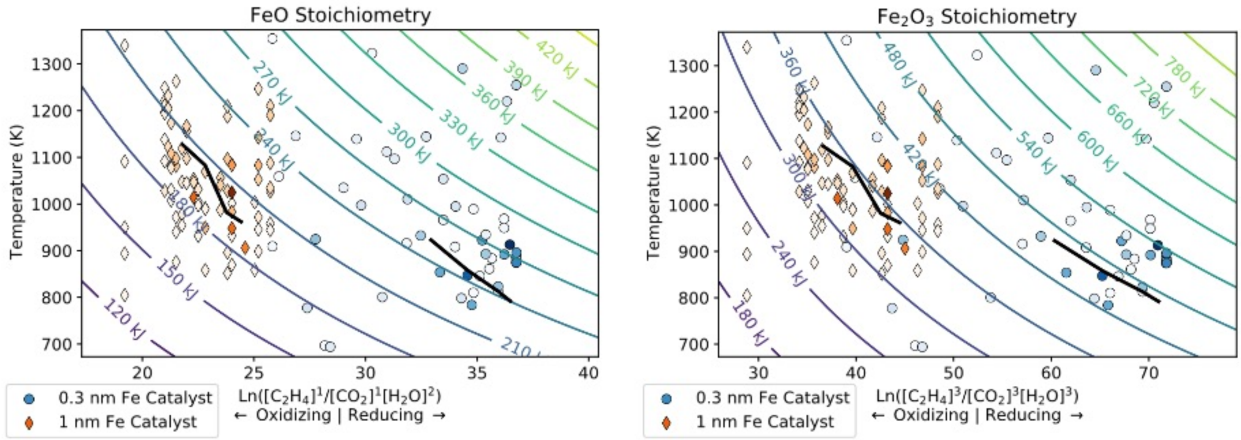
Understanding and controlling nanoparticle catalyst behavior as it relates to carbon nanotube (CNT) growth is key to scaling their production. In supported catalyst growth, the reduction of an oxidized metal catalyst enables growth, but the reduction also leads to catalyst deactivation via Ostwald ripening, agglomeration, and other effects. Here, using a machine learning planner based on a novel jump regression algorithm, we identified optimal conditions for CNT growth as a function of the driving force for catalyst reduction in a fraction of the time and cost of conventional experimental approaches. We found a discontinuous jump in yield corresponding to the phase transformation from oxidized to reduced metal catalyst. Indeed, we found that growth peaked at the oxidation/reduction boundary as we varied temperature and the reducing potential of the growth gases. We believe that by operating at the thermodynamic boundary between oxidized and reduced catalysts we optimize catalyst activity by inhibiting Ostwald ripening-induced deactivation, thereby keeping the catalyst particles smaller and more numerous. Our work identifies optimal thermodynamic conditions for the production of small diameter single-walled CNTs using iron catalyst, and establishes a rationale for a generalized understanding the behavior of other metal catalysts in CNT growth. We demonstrate the value of physics-aware machine learning-driven design of experiments to greatly accelerate materials science.



CNT Yield results versus thermodynamic reduction potentials for FeO (left) and Fe2O3 (right). The yield roughly follows Gibbs free energy of reduction contours, supporting the hypothesis that CNT yield optimal at the oxidation/reduction boundary. The thinner catalyst film (blue circles) became active at more reducing conditions than the thicker catalyst film (red diamonds), indicating that they are more difficult to reduce.

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C16

VERTICALLY ALIGNED CARBON NANOTUBES: LATEST ADVANCES IN SYNTHESIS AND APPLICATIONS

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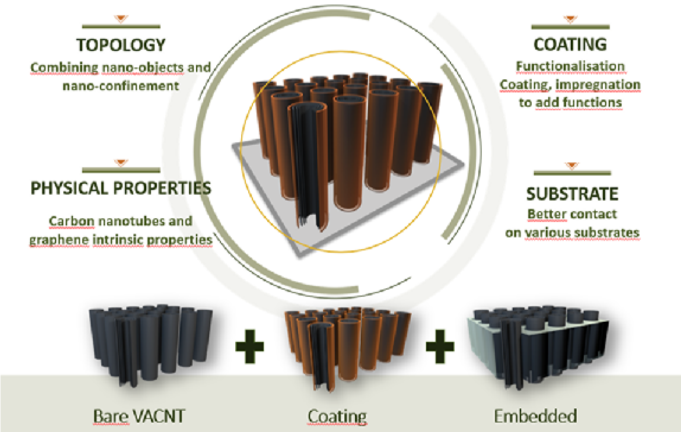
Amongst the great family of carbon nanotubes and graphene materials, Vertically Aligned Carbon NanoTubes (VACNT) received particular interest as they gather advantages of carbon nanotubes plus a specific structure that enhance final properties of any applications . VACNT array is a perfect Z-axis anisotropic structure for which electrical, thermal as well as mechanical properties of Carbon nanoTubes (CNT) are maintained and some other like tortuosity, diffusion, light absorption came from the structure itself. The main roadblock for VACNT was the scaling-up of the manufacturing process but recent progresses in the synthesis of VACNT completely changed VACNT arrays availability for industry and new research areas.This presentation will review the latest progress made considering VACNT synthesis, with a detailed approach on CVD processes (one step process with co-injection or 2 steps processes with catalyst predeposition, their advantages and drawbacks), catalysts materials as well as additives to the growth of VACNT. VACNT are grown from a substrate and a large review of the substrates will be given as well to highlight some applications like energy storage [1]. Recipes to grow VACNT will also be reviewed with the angle of having a lower CO2 footprint (lower temperature, green gas, waste and recycling) [2]. Some synthesis has limitations leading to thin VACNT arrays, some other can be unlimited leading to ultra-long VACNT considered as wires or yarns [3]. VACNT also benefit with all the advantages of post treatment such as functionalization, transfer and other processes to make "VACNT-composites" made from VACNT and a matrix. The presentation will review all these "engineering" processes, illustrated with most promising applications. We will highlight functionalization for energy applications, biocompatibility for biotechnologies [4], polymer matrices impregnation for composites applications as well as VACNT transfer on various secondary substrates to ease their use in new applications.



VACNT add functions to structures

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C17

COEFFECTS OF CATALYSTS AND CARBON-SUPPLY CONDITIONS ON SINGLE-WALLED CARBON NANOTUBE GROWTH

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Structure-controlled synthesis of single-walled carbon nanotubes (SWCNTs) is one of the most important research topics in the field. It is known that catalysts play a key role in the nucleation and growth of nanotubes in chemical vapor deposition. Therefore, the effect of catalysts on the selective growth of SWCNTs caused much attentions from the very beginning. Later, theoretical studies showed the importance of growth kinetics, which was echoed by some experimental evidences. Relying on the statistic study of structures of SWCNTs grown with different catalysts at different conditions and the in-situ study of SWCNTs on catalysts using high resolution electron microscope, we clarified the co-effects of catalysts and growth conditions on the selectivity of SWCNT growth. The structure-specified growth of SWCNTs can be achieved by manipulating the template effect of the catalysts together with the optimization of kinetic growth condition. We also found the different growth modes of SWCNTs on various catalysts.

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C18

CONTROLLED SYNTHESIS AND PROPERTIES OF ULTRALONG CARBON NANOTUBES

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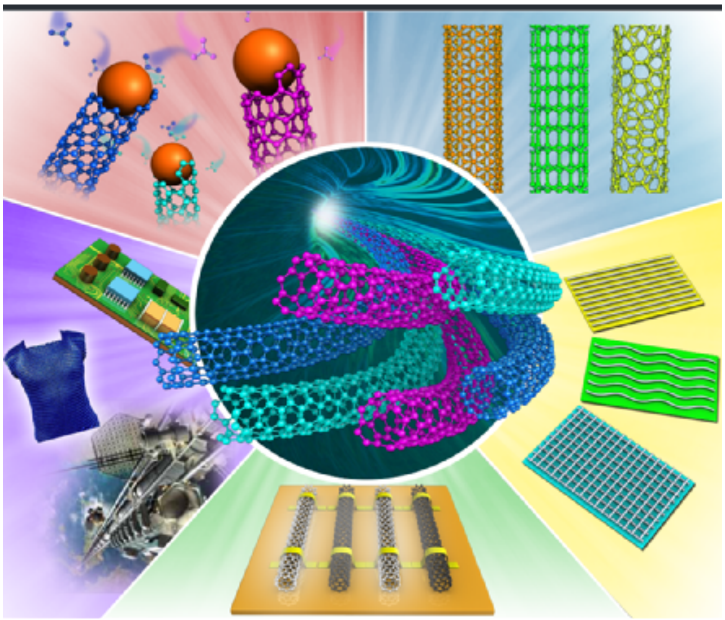
Carbon nanotubes (CNTs) have drawn intensive research interest in the past near 30 years due to their excellent properties and wide applications. Ultralong CNTs usually have perfect structures and lengths up to centimeters, even decimeters, showing extraordinary mechanical, electrical, and thermal properties. Ultralong CNTs are promising candidates for transparent displays, nanoelectronics, superstrong tethers, aeronautics and aerospace, etc. The controlled synthesis of ultralong CNTs with perfect structures is the key to fully exploit the extraordinary properties of CNTs. Over the past two decades, significant progress has been made in the study of ultralong CNTs, but there are also great challenges in controlled synthesis and mass production of ultralong CNTs, which limits their application.

In this talk, I will talk three aspects about ultralong CNTs.
(1) The growth mechanism of ultralong CNTs.
(2) The controlled synthesis of ultralong CNTs with ultrahigh yields.
(3) The structural coloration of CNT fibers and their properties.



Controlled Synthesis and Applications of Ultralong Carbon Nanotubes

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OS01

NEAR INFRARED IMAGING AND DETECTION OF PATHOGENS WITH MULTIPLEXED NANOSENSORS

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Infectious diseases are worldwide a major cause of morbidity and mortality. Fast and specific detection of pathogens is needed to combat these diseases. Additionally, pathogens affect plant health and have a huge impact on agriculture. Optimal methods to detect them would be non-invasive and without extensive sample-taking/processing. We developed a set of near infrared (NIR) fluorescent nanosensors and used them for remote fingerprinting of clinically important bacteria/viruses and to detect pathogen responses in plants [1,2,3]. The nanosensors are based on single-walled carbon nanotubes (SWCNTs) that fluoresce in the NIR optical tissue transparency window, which offers ultra-low background and high tissue penetration. To identify bacteria relevant for humans they were chemically tailored to detect released metabolites as well as specific virulence factors (lipopolysaccharides, siderophores, DNases, proteases) and integrated into functional hydrogel arrays with different sensors. These hydrogels are exposed to important bacteria (Staphylococcus aureus,Escherichia coli, …) and remote NIR imaging allows to identify and distinguish them. In another approach, we developed nanosensors that change their spectral signature in response to polyphenols, which are released by plants when they are exposed to insects and pathogens. Using these sensors we visualized the plant's chemical defense remotely in the NIR. Finally, we show the detection of corona virus proteins using aptamer modified SWCNTs. In summary, such nanosensors in combination with NIR imaging concepts demonstrate huge potential for precise monitoring of pathogens.

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OS02
RECENT PROGRESS IN UNDERSTANDING TAILORED CARBON NANOTUBES AND CONFINED CARBYNE HYBRID SYSTEMS

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Precise tailoring of the properties of carbon nanotubes yields to completely new properties. Especially tailoring 1D cylinders by encapsulating 1D chains yields new hybrid structures with novel properties. In this contribution I will present an overview of recent progress understanding the fundamental properties of these novel hybrid systems confining carbyne inside carbon nanotubes by using inelastic scattering as probe (resonance Raman and EELS). Stabilized by the encaging nanotubes allows high yield (stepwise) synthesis [1,2] and specific tailoring by doping and isotope engineering [3]. This enables tracing nano chemical reactions and unraveling their growth [4]. These systems also have the biggest resonance Raman cross section so far [5] which makes them particularly suitable for sensing application such as truly local contact free temperature sensors [1,6]. In addition, I will show first results on complementary nanospectroscopic EELS inside a TEM [7] allow to directly assign the structure & properties of individual carbyne@CNT hybrids. This shows the full potential to unravel functional CC@CNT as individual 1D quantum wires and as a perfect 1D reference system for new local EELS nanospectroscopy studies inside a TEM as completely new toolbox to directly monitor the influence of local structure on the vibronic structure, the electronic transport & optical properties.

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OS03

P. Simon *

OS04

NANOELECTRONICS FROM NANOMATERIALS: HOW WE ENABLE AND HINDER A PROMISING FUTURE

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When the first carbon nanotube (CNT) transistor was demonstrated in the late 90's, enthusiasm for a future of nanomaterial-based electronics grew at an outrageous pace. Within five years, researchers from nearly every discipline – from electrical engineering to chemistry – were working on advancing transistors from these semiconducting molecules of pure carbon. This research fervor opened even more broadly with the advent of two-dimensional semiconductors, such as the transition metal dichalcogenides (e.g., MoS_2) and their contrasting properties compared to CNTs, including large band gap and high effective mass. While the thousands of scientific papers published on nanomaterial-based transistors over the years provide evidence of the tremendous promise they can bring for future electronics, there are aspects of this disciplinarily diverse field that hinder progress. Important questions have emerged without consistent answers, such as: Does mobility matter for high-performance transistors? How much current is needed for certain applications? How are the current and corresponding operating voltage properly measured and reported? What are the foremost limitations to nanomaterial-based devices? In some ways, the inconsistent perspectives and reports from the research community have fueled an off/on interest in nanomaterials from industry. In this talk, I'll provide some historical perspective on what brought us to the present moment in nanomaterial-based transistors and suggest some ways that we can better enable their promising future. Through more consistent benchmarking and messaging, continued progress can be made, and we can reduce the hindrance that misinformation may generate. There's little doubt that a future of nanoelectronics from nanomaterials is a bright one, we just need to make sure we get there.

OS05
CVD GRAPHENE: GROWTH FRONTIERS & MASS PRODUCTION

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With 18 years history of graphene materials, there still exist lots of technical challenges towards graphene industry, including: 1) Low-cost mass production technology; 2) Batch peeling-transfer technology; 3) Transition from single-layer graphene component to macroscopic materials with retained intrinsic performances; 4) Dispersing technology into matrix materials; 5) Irreplaceable killer applications. Beijing Graphene Institute (BGI), established in 2018 and currently having over 330 employees, aims to solve these challenging issues by paying particular emphasis to mass production of high-quality CVD graphene materials and manufacturing equipment. BGI is devoted to providing the best graphene materials and related equipment to the market as well as the graphene-related R&D services to enterprises. The current R&D emphasis on CVD graphene materials at BGI is laid on three different directions: 1) high-quality graphene films and wafers for general purpose; 2) graphene-skinned materials (GSM); 3) purpose-oriented graphene materials focusing on thermal managements, optical communications and medical applications. The star products into market are A3-size graphene films with mm grain boundaries, 4- and 6- inch single crystal graphene wafers, superclean graphene films with best thermal and electrical performances, graphene-skinned glass & fibers, graphene-skinned aluminum oxide fibers, etc. The graphene-skinned glass fibers have been used for deicing applications with extremely high electrothermal conversion efficiency up to 94%. At BGI, we are also working for the customized graphene growth depending on the special needs and requests from customers. There is a great space in this area, which is particularly important before graphene films and wafers find their practical application market in next ten years.

OS06

AN OVERVIEW OF LUMINESCENCE FROM AND CHARGE TRANSPORT IN DENSE NETWORKS OF PRISTINE AND FUNCTIONALIZED SWCNTS

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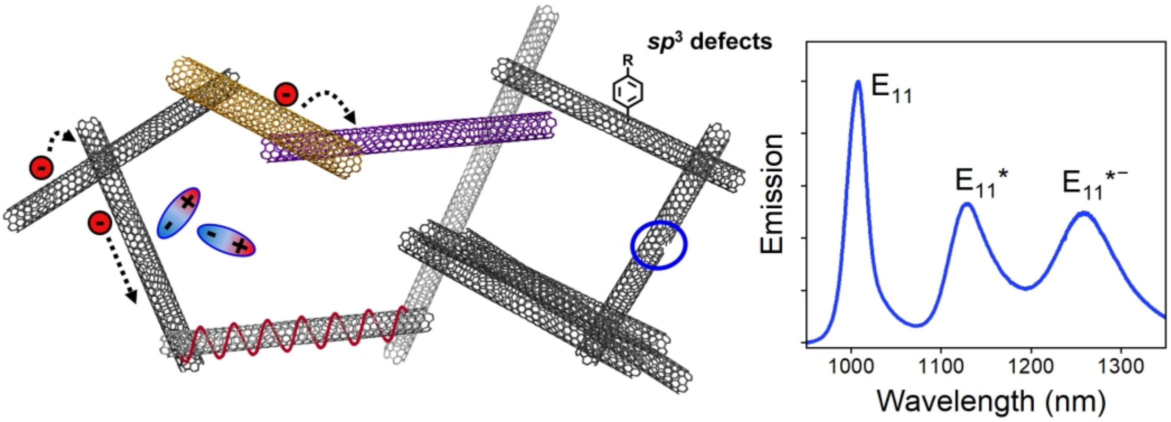
Advanced sorting methods have enabled the purification of large amounts of semiconducting and even monochiral single-walled carbon nanotubes (SWCNTs) that can be integrated in devices with outstanding properties. For example, field-effect transistors based on solution-processed random networks of sorted SWCNTs exhibit high charge carrier mobilities and on/off current ratios that are suitable for a wide range of electronic applications [1]. To further improve performance, it is important to understand the interplay of various parameters such as nanotube density, length, diameter distribution, n- and p-doping, intentional and unintentional defects and their impact on macroscopic charge transport properties [2]. Furthermore, the narrow near-infrared emission of SWCNTs in networks is sensitive to their dielectric environment, interactions with each other and with the substrate. It can be tuned by electrochemical and electrostatic doping leading to red-shifted trion emission [3] and by the controlled introduction of luminescent sp^3-defects [4]. These quantum defects with characteristically red-shifted emission and long photoluminescence lifetimes, enable higher quantum yields and even single-photon emission at room temperature. For chiral (6,5) SWCNTs, the type of defect emission (E_{11}* or E_{11}*$^-$) is governed by the precise binding configuration, which depends on the functionalization chemistry [5]. I will give an overview of the field in general with a focus on recent progress of understanding inter- and intra-nanotube charge transport in random networks of SWCNTs, their emission properties and the impact of sp^3 defects on both of them.



Schematic illustration of parameters affecting charge transport in a network of SWCNTs and impact of functionalization on luminescence spectra.

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OS07

WHAT CAN WE LEARN ABOUT CVD AND NANOMATERIAL GROWTH USING COMPUTATIONAL APPROACHES?

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Over the last few decades, catalytic chemical vapor deposition (CVD) has matured as a synthetic technique for producing many low-dimensional inorganic nanomaterials, such as carbon nanotubes, graphene, boron nitrides and transition metal dichalcogenides. van der Waals heterostructures comprising these 1D and 2D allotropes have also been recently developed. During this time, computational approaches have played a critical role in developing our understanding how these materials are structured, behave and grow. In this talk, I will summarise our own recent contributions to this field, and will discuss how molecular dynamics and quantum chemistry help us understand the chemistry of CVD nanomaterial growth [1,2], nucleation mechanisms of 1D and 2D inorganic nanomaterials [3] and heterostructure stability [4]. I will also discuss how machine learning and graph neural networks are emerging as powerful approaches for identifying improved heterogeneous catalytic interfaces for CVD nanomaterial growth [5].

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OS08
GROWTH OF 2D MATERIALS ON CURVED SURFACES

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Chemical growth of two-dimensional (2D) materials with controlled morphology is critical to bring their tantalizing properties into fruition. The growth usually occurs on a nonideal substrate, which involves either discrete curved features or continuous undulation, at a scale significantly larger than the materials thickness. Using a newly developed method based on the Metropolis algorithm and taking graphene as a prototype, we find that either isolated curved features or periodical undulations on substrates can cause lattice stress in 2D materials, which interacts with the growth chemistry and results in a variety of lattice defects in 2D materials. More specifically, as the feature's size increases by just nanometers, the lattice defects can vary from adatoms, dislocation pairs, and grain boundary scars to long-range grain boundaries, in contrast to previously reported defect-free modes of rigid colloidal crystals growing on spheres. On the other hand, 2D materials growing on periodically undulated substrates with nonzero Gaussian curvature of practical relevance follow three distinct modes: defect-free conformal, defect-free suspension and defective conformal modes. The curvature induced stress gradually lifts the materials from substrate and progressively turns the conformal mode into a suspension mode with increasing the undulation amplitude. Further enhancing the undulation can trigger Asaro–Tiller–Grinfield growth instability in the materials, manifested as discretely distributed topological defects due to strong stress concentration. We further rationalize the above results by model analyses and establish 'phase diagrams' for guiding the control of growth morphology and defects via substrate patterning.

OS09

TAILORING CARBON NANOTUBE FIBERS FOR WEARABLE SMART DEVICES

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Carbon nanotube fibers are ideal multifunctional electronic materials due to its unique combination of structural, mechanical, electrical and thermal properties, enabling them promising candidates for developing intelligent materials and devices in areas of sensing, actuating and computing fields etc.. In my talk, I will introduce our recent research progress in the strengthening, shaping and functionalization of CNT fibers for wearable smart devices. My talk includes three aspects: 1) Gas-phase spinning of high-performance CNT fibers and wet functionalization of CNT fibers with desirable morphology, strength and conductivity; 2)Fabrication of CNT fibers for artificial muscles with multifunctionalities and knittability. For instance, through the construction of a high-twist-pervaded structure, the CNT fiber produced a large reversible contraction of 62.4% under high load (10000 times the mass of the yarn muscle) and low driving voltages (<5 V). Interestingly, the fiber can be also fabricated as an artificial neuromuscular device by multilayered coaxial integration strategy, making it with adaptive actuation upon environmental change; 3) Fabrication of fiber-shaped self-powered sensing devices for smart textile. For instance, a fiber-shaped artificial optoelectronic synapse was constructed with double-twisted architecture consisting of high-density TiO2-x and MoS2 arrays. Such a simple structure can emulate both electrical and light-induced synaptic functions such as excitatory postsynaptic current, short/ long-term plasticity, and ‘‘learning-forgetting-relearning’’ behavior. As a proof-of-concept demonstration, multiple fiber devices were woven into commercial textiles to form optoelectronic synapse arrays for perception and memory of image information. Finally, I will show my viewpoints on the future development of CNT fibers and their promise in smart textiles and composites.

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OS10

EVIDENCE AND ANALYSIS OF DISCONTINUOUS THERMODYNAMIC PROPERTIES UNDER EXTREME ONE DIMENSIONAL CONFINEMENT – THE CENTER FOR ENHANCED NANOFLUIDIC TRANSPORT (CENT)

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Not all nanopores are created equal. By definition, all have characteristic diameters or conduit widths between approximately 1 and 100 nm. However, the narrowest of such pores, perhaps best called Single Digit Nanopores (SDNs), defined as those with less than 10 nm diameters, have only recently been accessible experimentally for precision transport measurements. To address the challenges of bridging the deficiencies of theory and experiment for fluids confined within the most extreme conduits, we have formed the Center for Enhanced Nanofluidic Transport (CENT). This talk will outline some of the major successes of this collaboration in understanding the thermodynamics and transport through SDN systems. In one recent advance, highlighted in this presentation, we develop a platform based on Raman spectroscopy and ultra-long carbon nanotubes with diameters less than 3 nm suspended over electron microscopy windows to identify and study new types of vibrational coupling to the CNT environment. Electron diffraction assigned Double Walled Carbon Nanotubes (DWNT) suspended across with 20 µm slit on 1,500 µm transmission electron microscopy (TEM) windows are used to probe in vacuum an enormous 10 to 15% Radial Breathing Mode (RBM) downshift shift with increasing temperature that is both reversible and robust over dozens of cycles. A new analysis based on a harmonic oscillator model is able to assign the hyperbolic trajectory to a reversible increase in damping, generating a shift that is the reverse of prior expectations. The environmental source of the coupling is assigned to graphitic ribbons shown by TEM to decorate the surface up to an axial coverage of 60%. A linear, strain-dependent coupling of the ribbon fragments driven by thermal expansion of the supporting nanotube describes the distinctive cusp that appears throughout the 91 temperature scans of 3 distinct DWNTs. We find that each connection of the fragments with the DWNT surface keeps the ratio of spring to damping frequencies constant, producing a remarkable saturation of the RBM frequency in the low-tension limit. The high fidelity of the oscillatory model shows that the RBM has negligible intrinsic temperature dependence and that evidence for impurity-induced damping as a confounding variable is commonly present in experiments previously thought to be on pristine systems. Overall, these findings significantly increase our understanding of the environmental coupling of 1D nano-mechanical systems, providing the basis for new technological applications and improved spectral analysis. This platform sets forth a new and reliable approach for studying the environmental coupling of the CNT to phases of interest for study, with future work demonstrating its utility for investigating fluids in single digit nanopores under extreme confinement. CENT is organized around critical gaps in our understanding of nanoscale hydrodynamics, molecular sieving, fluidic structure, and thermodynamics. These knowledge gaps are, in turn, an opportunity to discover and understand fundamentally new mechanisms of molecular and ionic transport that may inspire novel membranes for separations, new gas-permeable materials and energy storage devices.

OS11
CLASSIFICATION OF 2D CARBON ALLOTROPES

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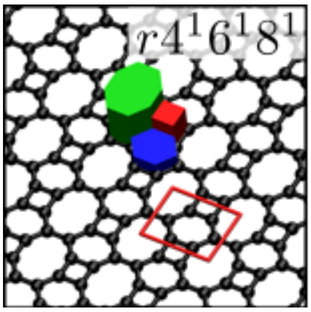
A unified taxonomy for sp^2 nanocarbon allotropes in two dimensions (2D) is proposed where structures are assigned a unique symbol associated with the geometry of each allotrope.[1] The naming scheme will be demonstrated for all the structures described in the literature and is further illustrated for a number of other topology-allowed carbon sp^2 systems. The symbol is easy to use and gives a direct access to geometrical features such as the number of polygons and their arrangement. It facilitates the classification of structures reported in the literature, where many such structures are found to have been assigned a name based on each author's somewhat arbitrary choice. The naming scheme can be applied to 1D systems and has the potential to be expanded to mixed sp^2-sp^3 carbon system as well as non-carbon nanostructures in 2D. In this talk, I will also present a search algorithm for 2D structures and show why not all structures obeying Euler criteria are acceptable solutions.



Example of the application of the proposed naming scheme where polygon counts and lattice symmetries are used.

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OS12

CARBON NANOTUBE TRANSISTORS PROGRESS TOWARDS INTEGRATED CIRCUITS AND HIGH-PERFORMANCE CMOS LOGIC

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This talk will present the latest advances in the field of high-performance carbon nanotube field effect transistors (CNFETs). CNFETs may extend the scaling of digital systems beyond the limits of traditional Si CMOS to deliver logic density, speed, and energy benefits. Additionally, the low temperature of CNFET fabrication enables new monolithic 3D architectures with high-speed and low-energy logic in the back-end-of-line, enabling ultra-dense 3D interconnectivity between logic and memory for large benefits in computing energy efficiency and throughput.

Many fundamental building blocks as well as complex digital logic systems have been demonstrated using CNFETs. Moreover, the CNFET technology started its transition from the academia into multiple commercial manufacturing facilities (at relaxed nodes), demonstrating process compatibility with existing fab manufacturing equipment and flows.

Over the last few years there have been major advances in the synthesis and sorting of single-walled carbon nanotubes (CNTs), along with improved miniaturization of CNFET components. These include solutions of highly enriched semiconducting CNTs enabling better control over the band gap, assembly of dense aligned CNTs, gate-stack, doping and low contact resistance for both p-type and n-type CNFETs. We will share our perspectives on the remaining challenges for the realization of high-performance highly-scaled CNFET CMOS systems.

Acknowledgments: This work is supported in part by the US Department of Defense, DARPA and the Stanford SystemX Alliance. Our work is performed in collaboration with the Corporate Research team at TSMC.

IS01

FLUORESCENCE MODULATION OF DNA FUNCTIONALIZED SINGLE WALL CARBON NANOTUBES BY CATECHOL-BEARING MOLECULES

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Single wall carbon nanotubes (SWCNTs) have several photophysical properties that make them attractive for imaging in biology. Small diameter (~1 nm) SWCNTs fluoresce in the near-infrared (NIR) region of the spectrum (900 – 1300 nm), which can facilitate imaging in optically challenging biological specimens. SWCNTs exhibit superior photostability and are considered to be non-photobleaching on time scales of interest to biological imaging. Furthermore, SWCNT fluorescence can be selectively sensitized to the local chemical environment, which has served as a basis for the synthesis and application of optical biosensors for a variety of biologically important molecules including metabolites, signaling molecules, proteins, and oligonucleotides. One class of optical biosensors that have been particularly successful in our research includes (GT)N oligonucleotide functionalized SWCNTs that exhibit exquisite fluorescence turn-on response to compounds that contain catechol-like motifs, including some of the most neurotransmitters in the brain. In this work, we offer new insights into the mechanism of molecular recognition and fluorescence modulation of this sensor class by catechol-like compounds. We carried out a fragment-based structure activity relationship to establish how the structural and electronic properties of these compounds correlated with their ability to modulate SWCNT-fluorescence. This helped us establish a spectrum of substrate functionalities that are detectable by this sensor class. Intriguingly, our experiments revealed that solution phase fluorescence turn-on events are critically influenced by factors that are not intrinsic to the analytes, such as solution pH. We will discuss the pH dependence of fluorescence turn-on events and establish structural and electronic correlates for these dependencies. As a results of these explorations, we have been able to achieve an improved understanding of sensor dynamics and sensing mechanism. We expect that the insights gleaned from this work will contribute to the body of knowledge that underpins SWCNT-based optical sensors. Finally, we will discuss new developments from our lab regarding the biological applications of this class of biosensors, including our continued efforts to leverage the flexibility of the nanosensor to study aspects of catecholamine neurochemistry that elude conventional methods of inquiry.

IS02

OXYGEN-DOPED CARBON NANOTUBES FOR NEAR-INFRARED IMAGING PROBES

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Single-walled carbon nanotubes (CNTs) emit fluorescence in the near-infrared (NIR) region, which is highly transparent for biomaterials. Because the fluorescence quantum yield of CNTs can be increased by modest chemical functionalization, bio-imaging applications of functionalized CNTs are especially interesting. In this presentation, we report the synthesis of epoxide-type oxygen-doped CNTs (Ep-CNTs) and their application as near-infrared fluorescent probes. Treated (6, 5) nanotubes show photoluminescence at ~1280 nm, which corresponds to the most transparent regions for biomaterials. Immunoassays and fluorescence vascular angiography of mice are demonstrated by using the Ep-CNTs as infrared fluorescent labels and imaging agents, respectively. From a practical point of view, the biodistribution of the Ep-CNT imaging probe after administration to mice is also investigated.

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IS03

EXCITONS IN MOIRÉ HETEROSTRUCTURES

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Van der Waals crystals of two-dimensional semiconducting transition metal dichalcogenides have evolved as an increasingly significant material platform in condensed matter research. With access to a variety of single-crystal monolayers, a wide range of van der Waals heterostructures can be assembled into rationally designed vertical stacks with emergent flat bands of correlated electrons and tailored optical properties of strongly bound excitons. In my talk, I will present our recent insight into the roles of layer constituents, atomic registry and twist angle for the formation of excitons with distinct spin-valley degrees of freedom and layer character in MoSe2-WS2 heterobilayers with canonical moiré superlattices [1] and MoSe2-WSe2 heterostacks subject to mesoscopic lattice reconstruction [2,3].

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IS04
TUNING OF OPTO-ELECTRONIC PROPERTIES INTO SINGLE-WALLED CARBON NANOTUBES BY CHROMOPHORE ENCAPSULATION

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Chromophore are encapsulated into host single-walled carbon nanotubes to create hybrid nano-systems with tunable optical and electronic properties. The interplay between the confined molecules and the host nanotube is a key factor[1,2].

From Raman spectroscopy and G-band shift measurements, a significant charge transfer from the confined dye to the nanotube is evidenced. A photo-activated electron transfer is also inferred for small diameter (~9 Å) semiconducting and metallic tubes.[3] The key parameters that govern the charge transfer are the nanotube diameter and the electron donor or acceptor character of the molecules. The resonance Raman intensities of the confined molecules are strongly affected by applying an external pressure.[4]

Furthermore, photoluminescence intensities of nanotubes are either significantly enhanced or quenched depending on the electron donor or acceptor character of the molecules.[5] Indeed, the electron (hole) transfer up (down)-shifts the Fermi level of the nanotubes, modulating the radiative de-excitation efficiency.

Therefore, molecule confinement into nanotubes is an interesting strategy for the engineering of new opto-electronic devices.

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IS05

CONTROL OF THE EXCITON AND SPIN/VALLEY PROPERTIES IN ATOMICALLY THIN TRANSITION METAL DICHALCOGENIDES

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In this talk I will first recall briefly the general properties of 2D excitons in Transition Metal Dichalcogenides (TMD) monolayers : giant binding energy, oscillator strength, exchange interactions, spin/valley locking ...[1].

Encapsulation of TMD monolayers in hexagonal boron nitride (hBN) yields narrow optical transitions approaching the homogeneous exciton linewidth [2,3]. We have demonstrated that the exciton radiative rate in these van der Waals heterostructures can be tailored by a simple change of the hBN encapsulation layer thickness as a consequence of the Purcell effect [4].

We also measured the exciton fine structure by magneto-photoluminescence spectroscopy in magnetic fields up to 30 T [5,6]. I will show that the bright-dark exciton splitting can be tuned by a few meV, as a result of a significant Lamb shift of the optically active exciton which arises from emission and absorption of virtual photons triggered by the vacuum fluctuations of the electromagnetic field [7] .

Finally I will present recent experimental results on spin/valley pumping of resident electrons in WSe2 and WS2 monolayers [8]. Using a spatially-resolved optical pump-probe experiment, we measure the lateral transport of spin/valley polarized electrons over very long distances (tens of micrometers) [9]. These results highlight the key role played by the spin-valley locking effect in TMD monolayers on the pumping efficiency and the polarized electron transport.

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IS06

ATOMIC SCALE CHEMICAL ORDERING IN FRANCKEITE—A NATURAL VAN DER WAALS SUPERLATTICE

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Francheite is a naturally occurring sulfosalt mineral with a van der Waals superlattice structure, found in Bolivia and first described by Stelzner[1]. This van der Waals heterostructure is composed of alternating incommensurate 2D layers, namely the H-layer (PbS) and Q-layer (SnS_2). Franckeite has attracted attention recently due to its semiconducting properties and the possibility for exfoliation of flakes[2,3]. An extensive review on preceding characterization is given in the work of Makovicky[4], including a detailed description of the atomic site modulation caused by the incommensurate structure.

Here we present several new experimental observations of franckeite, including atomic structure measurement using state-of-the-art high-angle annular dark-field (HAADF) scanning transmission electron microscopy (STEM) and atom probe tomography (APT). With atomic-number image contrast in HAADF STEM (Fig1) direct information about both the geometric structure and its chemistry is provided, including several new chemical ordering effects. Notably, these chemical ordering effects have yet to be taken into account in electronic structure calculations of franckeite. We also present further physical characterization of exfoliated franckeite, including the measurement of optical absorption edge by optical reflectometry, Raman spectroscopy, spatially resolved X-ray photoemission spectroscopy, and measurement of room temperature Seebeck coefficient.

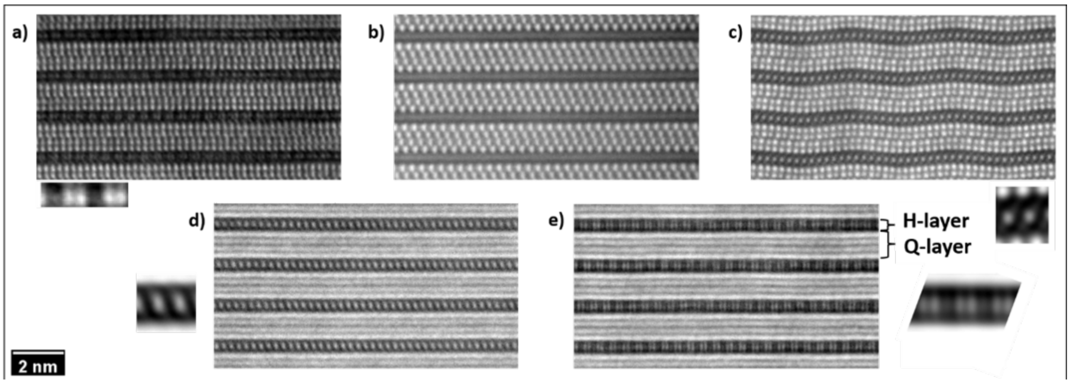

Figure 1. HAADF STEM images a) along and c) perpendicular to modulation direction, with projected atom columns in both H-layer and Q-layer. b) Resolving atom columns only in the four atomic layer thick Q-layer. d) and e) Resolving atom columns only in the H-layer. Scale bar the same for all images (bottom left). Insets show template averaged images of the projected H-layer (scale bar does not apply). HAADF-STEM images of franckeite: atomically resolved Q-layer, H-layer and van der Waals gaps are distinguishable. (a) In the [100] viewing direction, the displacive modulation is visible. (b) In [010], the modulation is averaged along the projection leading to a blurring of the atomic columns when the sample thickness is in the order of, or larger than, the modulation wavelength.

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IS07
CHEMICALLY MODIFIED GRAPHENE FOR ARTIFICAL MUSCLE FIBERS & SINGLE ATOM CATALYST

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Graphene Oxide Liquid Crystal (GOLC) is an intriguing 2D carbon based soft material, which exhibits nematic type colloidal discotic liquid crystallinity with the orientational ordering of graphene oxide flakes in good solvents, including water. Since our first discovery of GOLC in aqueous dispersion at 2009, this interesting mesophase has been utilized over world-wide for many different application fields, such as 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, including highly oriented 1D fibers, 2D films and 3D nanoporous structures. In particular, human muscle inspired graphene based nanocomposite fiber actuators will be highlighted along with its interesting demonstration for biomimetic behaviors. Besides, relevant research works associated to the nanoscale assembly and chemical modification of various low dimensional materials, including 2D TMDs and MXene, will be presented particularly aiming at energy and environmental applications. In the last part of presentation, our first discovery of single atom catalyst will be introduced also, including other relevant research efforts exploiting the customized heteroelement doping of graphene based structures.

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IS08

CARBON-BASED METAL-FREE ELECTROCATALYSIS FOR CLEAN ENERGY AND ENVIRONMENTAL REMEDIATION

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Since our discovery of the first carbon-based metal-free electrocatalyst (C-MFEC, i.e., N-doped carbon nanotubes) for oxygen reduction in fuel cells in 2009, the field of C-MFEC has grown enormously. C-MFECs, as alternatives to noble metal-based electrocatalysts, have been widely demonstrated for efficient oxygen reduction, oxygen evolution, hydrogen evolution, carbon dioxide reduction, nitrogen reduction, and many other electrocatalytic reactions. Recent worldwide research effort has shown great potential for applications of C-MFECs in fuel cells for clean energy conversion, metal-air batteries for energy storage, water splitting for hydrogen fuel generation, and other electrochemical processes for value-added chemical production. Further research and development of C-MFECs could revolutionize clean energy and environmental remediation technologies. In this talk, I will summarize some of our work on the development of C-MFECs for clean energy and environmental remediation, along with an overview on recent advances, current challenges, and future perspectives in this exciting field.

IS09
CARBON NANOTUBE PHOTODETECTORS FOR HIGH-SPEED OPTICAL COMMUNICATIONS

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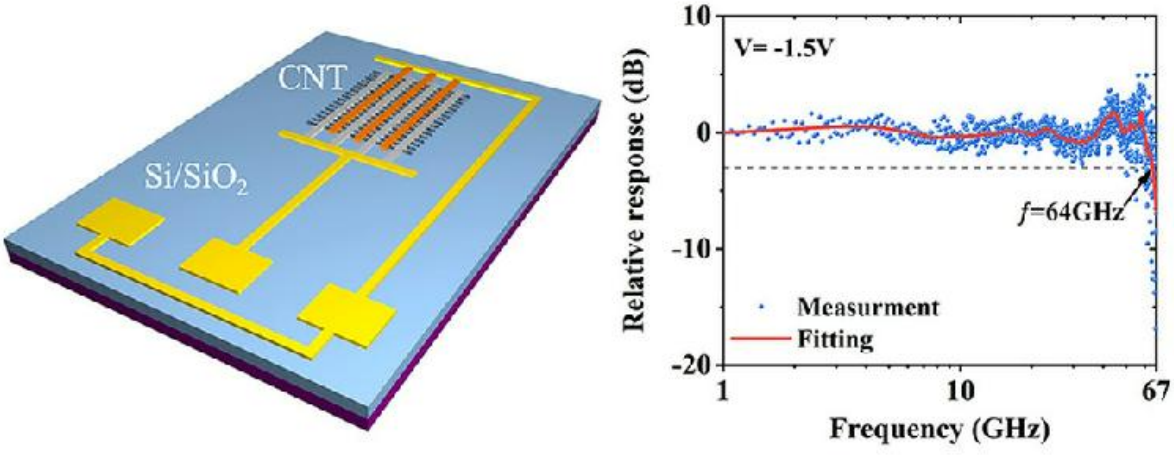
The future interconnect links in intra- and inter-chip require the photodetector with high bandwidth, ultra-wide waveband, compact footprint, low-cost, and compatible integration process with silicon complementary metal-oxide-semiconductor (CMOS) technology. Here, we demonstrate a CMOS-compatible carbon nanotube (CNT) photodetector that exhibits high responsivity, high bandwidth and broad spectral operation over all optical telecommunication band based on high-purity CNT arrays asymmetrically contacted by palladium and hafnium electrodes. The ultrafast CNT photodetector on silicon substrate with the active area of 100 μm^2 has a high responsivity of 1.5 A/W and bandwidth of 22.1 GHz at 1.55 μm wavelength. It shows clear open eye diagrams with 40 Gbit/s non-return-to-zero (NRZ) on-off-keying (OOK) signals and the bit error rate (BER) is about 5.2×10^{-3} under 100 Gbit/s Nyquist-shaped OOK data transmission with digital signal processing (DSP), which can address the demand for high-speed optical interconnects in and between data centers. For CNT photodetector, the bandwidth is closely related to device capacitance. Therefore, we first improve the bandwidth of the CNT photodetector by scaling down the device area to reduce device capacitance. The CNT photodetector exhibits a bandwidth of 64 GHz by scaling down the active area to 20 μm^2 and the device capacitance is decreased to 33 fF. In addition, we further fabricate the photodetector on quartz substrate in order to reduce parasitic capacitance between device and substrate. The CNT photodetector on quartz substrate has a smaller capacitance of 12 fF and exhibits a setup-limited 3 dB bandwidth over 67 GHz even at zero bias at 1.55 μm. Our work indicates that CNT photodetector has great potential for future high-speed optical communication at 1.55 μm band with high performance and low cost. As the CNT photodetectors are fabricated by doping-free process, it also provides a cost-effective solution to integrate CNT photonic devices with CNT-based CMOS integrated circuits, paving a way for future CNT-based high-speed optical interconnects and optoelectronic integrated circuits (OEICs).



Bandwidth of the ultrafast CNT photodetector. Structure and bandwidth of the ultrafast CNT Photodetector

IS10

CARBON NANOTUBE BASED FLEXIBLE INTEGRATED FLASH MEMORY ARRAY FOR PHYSIOLOGICAL INFORMATION STORAGE

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In general, there is a conflict between low program/erase voltages and a long retention capability in flash memories. Here, by using a stacked heterogeneous structure that combines different dielectrics with different relative dielectric constants and different thicknesses, flash memories based on CNT thin film on an ultrathin substrate have been demonstrated with a long retention time (projected to be approximately 10^8 s), low program/erase voltages (±2 V), and good endurance (projected to be over 10^6 cycles), simultaneously. An integrated flexible flash memory array of 24 bit by 16 bit has been further constructed and integrated with flexible sensors and sensor interface circuits to realize physiological information acquisition, processing, and storage from the human body surface .

References

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IS11
NANOMATERIAL-BASED FLEXIBLE SENSOR SYSTEM

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Human interaction is of great interests for a next class of human society to realize convenient, comfortable, and safe life. One of the approaches is a flexible sensor system with a feedback function, which is human friendly when it contacts to human due to mechanically flexible and soft body. In fact, multiple flexible sensor systems have been reported by using different types of flexible and/or stretchable materials. The challenge for the practical application is to integrate sensors onto such flexible films without sacrificing mechanical softness and flexibility. For this challenge, several approaches to embed or attach the flexible and/or stretchable sensors have been reported from some groups including our group [1,2]. In this talk, multimodal flexible sensors as an electronic skin (e-skin) for IoT applications including wearable devices are discussed as our approaches to integrate the sensor and feedback functions [3,4]. After introducing some flexible and printed sensors using nanomaterials such as graphene and carbon nanotubes, machine learning technique to analyze the datasets obtained from the flexible sensors are discussed briefly.

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IS12
CARBON NANOTUBE SELF-ASSEMBLY

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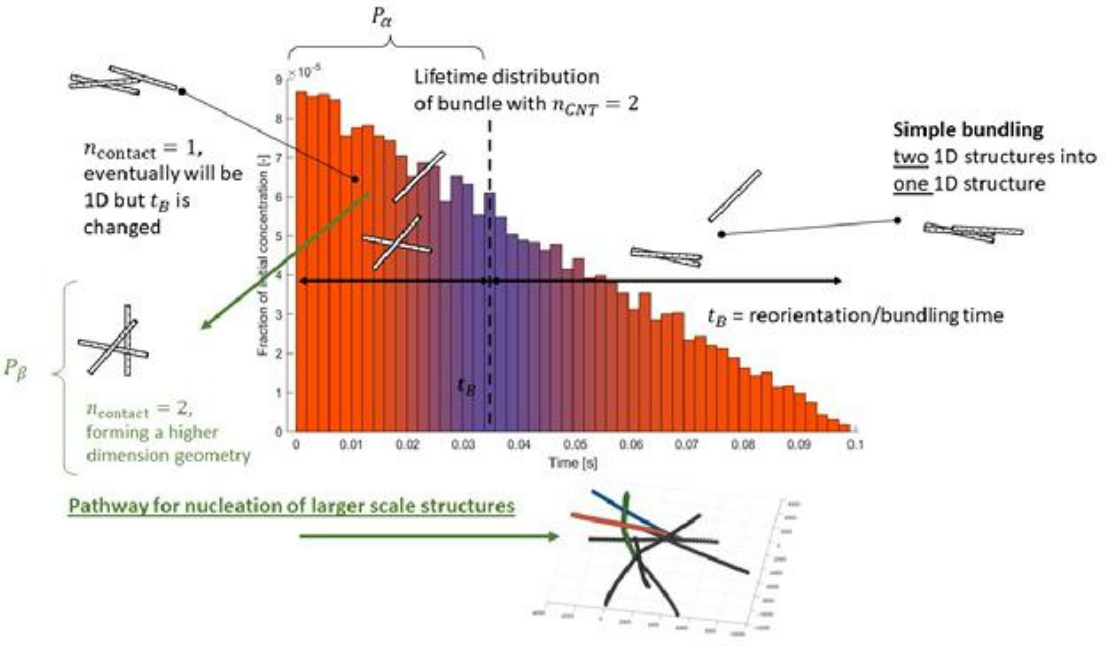
This presentation presents the development of methods to measure and understand the self-assembly of carbon nanotubes (CNTs) into bundles, aerogels and larger materials produced from a floating catalyst CVD process. CNTs individually exhibit exceptional physical properties, surpassing state-of-the-art bulk materials, but are used commercially primarily as additives rather than as a standalone macroscopic product. This limited use of bulk CNT materials is a result of the inability to harness the remarkable nanoscale properties of individual CNTs into macroscopic materials. CNT self-assembly for the purposes of large-scale synthesis has enables a pathway for large-scale materials production. Here, we report the development of a new framework for modelling the onset of CNT self-assembly by identifying the nucleation of 3D structures that are distinct from 1-D bundles of agglomerating and “coalescing” CNTs. This work employs meso-scale models to predict 1) the gas-phase collisions of CNTs, 2) the lowering of surface energy via bundling, 3) the nucleation of a 3D cluster and 4) the expansion of the cluster to a large-scale aerogel. The work is supported by new experimental measurements of the catalyst particle density and CNT growth rates. These new measurements show that the FC-CVD production of CNTs results in among the fastest growth rates ever measured for CNT production, whether substrate, fluidized bed or floating catalyst based. The presentation will also include expansion of the use of electric fields to align CNTs for better properties of as-produced materials prior to post treatment methods.



CNT Aerogel. Figure 1: Probability schematic of timescale between successive bundling collisions and pathway for nucleation of larger-scale structures.

IS13

SYNTHESIS AND PROPERTIES OF “BOTTOM-UP” GRAPHENE QUANTUM DOTS (GQDS)

D. Medina-Lopez [1], T. Liu [2], L. Rondin [2], D. Beljonne [3], J.S. Lauret [2], S. Campidelli [1,*]

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Despite its outstanding electronic, optical and mechanical properties, the use of graphene for real-world applications is severely limited because of its semi-metallic character. It is well known that when a material is reduced to nanoscale dimensions, the electronic confinement induces original size-dependent properties. For the last decade, a great attention has been paid to the size reduction of graphene using conventional “top-down” approaches (lithography and etching, thermal treatments and oxidation of bulk materials) to fabricate graphene quantum dots (GQDs)[1] or graphene nanoribbons (GNRs).[2] However, the “top-down” approaches do not allow a sufficient control of the structure of the material and of the oxidation state of the edges, which drastically affect the properties. In order to truly control, with the required level of precision, the morphology and the composition of the materials and of its edges, the bottom-up approach is the relevant way to proceed.[3,4] Here, I’ll present the “bottom-up” synthesis of graphene quantum dots and the first investigation of the photoluminescence (PL) properties of at the single molecular-scale. The GQDs exhibited emission of single photons at room temperature with high brightness and purity.[5-7] Beyond this first demonstration, our interest deals with the study of the structure-property relationship in GQDs and how the size, the symmetry of the particles will permit to tune the emission properties and finally be able to perform reverse engineering to design GQD with tailor-made properties.[8]

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IS14

HOST-GUEST ASSEMBLY OF SINGLE-WALLED CARBON NANOTUBES WITH WELL-DEFINED METAL CLUSTERS

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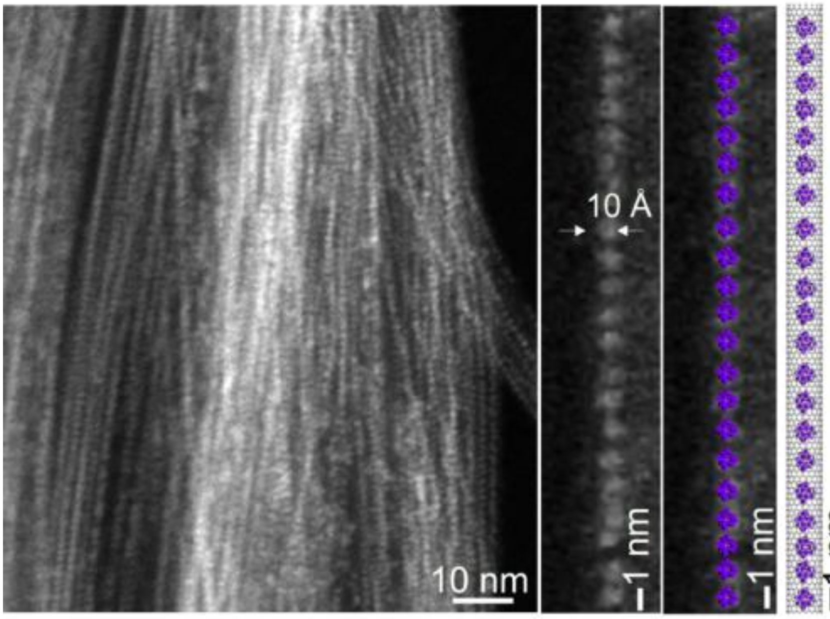
Manipulating the strong van der Waals intertube interactions between the single-walled carbon nanotubes (SWCNT) bundles and modulating the electronic properties of their surface are key steps for harnessing the extraordinary properties of SWCNTs[1]. The inner surface of SWCNTs has a more suitable curvature, larger contacting area than the outer-surface, which is particularly attractive in host-guest chemistry triggered by electron transfer. There exists a perfect size match between SWCNT cavity and polyoxometalate clusters. The redox polyoxometalates encapsulated in SWCNT cavities could adjust the electronic state of nanotubes via electron transfer. Here we reported a strategy of host-guest molecular interaction between SWCNTs and inner redox polyoxometalate clusters with designed size (Figure 1), thus selectively separated SWCNTs with semiconducting[2], metallic, and single-chirality[3]. The polyoxometalates with designable size and redox property enable the flexible regulation of interaction between the nanotubes and the clusters, thus tuning the structure of sorted SWCNTs. Besides, the metal nanoclusters with well-defined structures also enabled the flexible modulation the surface electronic structure of SWCNTs, which facilitated the heterogeneous catalysis by the localized electronic effect.



Encapsulation of polyoxometalate clusters in SWCNTs.

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IS15

SURFACE FUNCTIONALIZATION OF GRAPHENE FIELD-EFFECT TRANSISTORS FOR BIOANALYTICAL APPLICATIONS

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Graphene, with its atomically-thin 2D dimensionality, presents a remarkably high electrical conductance which is also particularly sensitive to small changes in the distribution of charged species near its surface. Taking advantage of this property, graphene field-effect transistors (GFETs) are increasingly used as bioanalytical nanosensors, *i.e.* for the detection or quantitation of various types of biologically-relevant molecular analytes, such as nucleic acids, proteins, ions or small molecules. By analyzing data from published literature on GFET bioanalytical sensors, we have recently shown that reported detection metrics vary enormously between studies, and argued that this variance is mainly driven by disparities in the bio-recognition interface [1]. Indeed, the selectivity of GFET sensors must be engineered, typically by functionalizing the graphene surface with biological molecules having a specific affinity for the chosen analyte (*e.g.*, antibodies to capture the corresponding antigen, or single-stranded DNA to capture its complementary sequence). Yet, the coverage, orientation, stability, and interactions between immobilized probes, blocking species and captured analytes are often not well known or controlled. In this presentation, I will discuss our current efforts to understand and regulate the surface functionalization of graphene field-effect transistors. Using electrical measurements, Raman spectroscopy and theoretical simulations, our group has investigated graphene functionalization via non-covalent chemistry, using pyrene derivatives, and covalent chemistry, using aryldiazonium reagents [2], as well as its further biofunctionalization with DNA strands and proteins [3]. I will describe our recent developments in controlling these different functionalization routes, and compare their use for bioanalytical purposes.

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IS16
THERAPEUTIC APPLICATIONS OF GRAPHENE OXIDE CONJUGATES

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The relatively low-cost production of graphene oxide (GO) and its dispersibility in various solvents, including water, combined with its tunable surface chemistry, make GO an attractive building block to design multifunctional materials. There are many applications for which it is fundamental to preserve the intrinsic properties of GO, for example in the biomedical field. As a consequence, the derivatization of GO to impart novel properties has to be well controlled and the characterization of the functionalized samples thoroughly done and unambiguous. Despite the great progress in the functionalization of GO, its chemistry is not always well controlled and not fully understood.[1,2] In this context, I will explain some strategies for the controlled functionalization of GO through the selective derivatization of the epoxides and hydroxyl groups without alteration of its properties. I will also present different approaches for the derivatization of GO with bioactive molecules and the potential of the conjugates as nanocarriers for targeted cancer phototherapies and targeted therapy of B-cell-mediated autoimmune diseases.[3-5]

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IS17

TELECOM SINGLE PHOTON SOURCE FROM A FIBERED CAVITY COUPLED GRAFTED CARBON NANOTUBE

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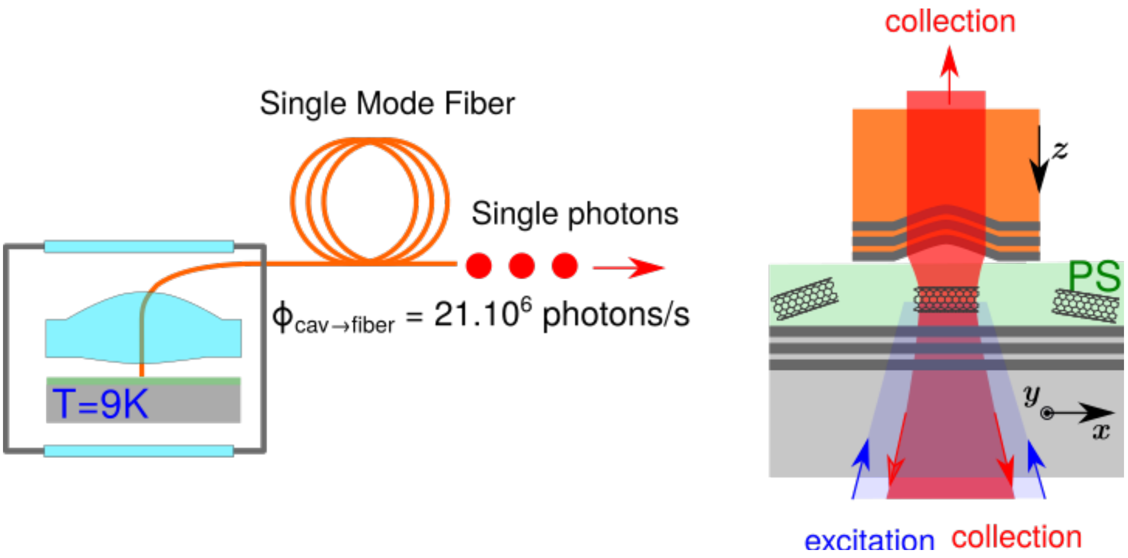
In the quest for secured quantum telecommunications, single-photon sources are a key building block. To fully exploit the transmission windows of the existing fiber network, wavelengths in the range of 1.3 to 1.6 µm are highly desirable. While in the visible and near infrared, several single photon sources are available, on the contrary in the telecom bands single photon emitters are scarce. Organic color-centers grafted onto carbon nanotubes are among the short list of potential telecom band single photon emitters and their discovery a few years ago has been a major step forward. To fully exploit their potential, it is key to deterministically couple such single color centers to advanced photonic resonators. This coupling, in the quantum regime makes it possible to modify the emission diagram, the radiative lifetime (thereby boosting the brightness of the source) and to some extent the working wavelength. In this respect, the use of a versatile cavity geometry, where the parameters can be tuned at will is an invaluable but very challenging asset. We were able to take control over the emission properties of a single NT emitting in the telecom O band by coupling it to a fully reconfigurable miniature Fabry Perot cavity (with a high quality factor and low mode volume). We observe a strong brightening of the emission together with a direct coupling to a single mode fiber resulting in high single photon rate (2.10^7) directly usable for quantum communication protocol and quantum random number generation. Furthermore, we perform an in-depth analysis of various effects of cavity quantum electrodynamics by exploiting our unique experimental setup where we are able to plug or unplug at will the coupling to the cavity for a range of cavity lengths making it possible to change the mode volume and the resonance frequency. We measured high Purcell factors up to 30 and a sizable acceleration of the recombination. We also exploited the peculiar coupling of the exciton to the 1D acoustic phonons to tune the working wavelength of the single-photon source and thereby to obtain an independent estimate of the Rabi coupling g that describes the strength of light-matter coupling.



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IS18

EXCITONS IN CARBON NANOTUBES MEET LAYERED MATERIALS: MIXED-DIMENSIONAL HETEROSTRUCTURES FOR NANOSCALE PHOTONICS

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Due to limited screening of the Coulomb interaction in one dimensional systems, unique exitonic properties exist in single-walled carbon nanotubes. Recent research on two-dimensional semiconductors such as transition metal dichalcogenides has also revealed rich optical phenomena where layer numbers and twist angles play important roles. Here we discuss our recent efforts on 1D/2D mixed-dimensional semiconductor heterostructures [1,2]. We demonstrate that hexagonal boron nitride, a widely studied two-dimensional insulator, is an ideal substrate for carbon nanotube photonics [1]. Using boron nitride flakes as ultrathin spacers for nanotubes and photonic crystal nanobeam cavities, deterministic coupling of a nanotube emitter to a cavity is demonstrated by a newly developed transfer process [2,3]. Single-crystalline anthracene is used as a medium which readily sublimes by mild heating, leaving behind clean nanotubes and thus enabling bright photoluminescence. We are able to position nanotubes of a desired chirality with a sub-micron accuracy under in-situ optical monitoring, thereby deterministically coupling a nanotube to a cavity. The anthracene assisted transfer process can also be used to transfer 2D materials with negligible contamination, allowing for investigation of atomically thin materials integrated with nanocavities [3].

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IS19

THEORETICAL CHALLENGES TO SCALING UP PROPERTIES IN CARBON NANOTUBE FIBRES

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The desire to scale up the electrical and mechanical properties of CNT fibres from individual tubes and bundles to macroscopic ropes and tows involves several interesting theoretical and computational challenges, which include simulating their network structure and characterising the orientational order of the structural subunits. Recently, experimental studies have shown that enhancing CNT alignment in fibres by using a double-drawing technique [1] and application of electromagnetic fields in situ during synthesis [2] can result in significant improvements in properties. We describe a procedure for recovering the true three-dimensional orientational distribution function from two-dimensional experimental data [3] and compare this with the network structure of coarse-grained simulations of CNT networks under various assumptions. We then investigate the predicted fracture behaviour and compare to previous experimental results looking high-strain rate failure in fibres [4].

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IS21

FIELD-EFFECT ON TWO-DIMENTIONAL MATERIALS AND THEIR COMPLEXES

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Two-dimensional covalent networks with moderate structural flexibility and chemically inert surfaces make atomic layered materials starting materials to form complexes with other atomic layered materials, atoms, and molecules. These complexes exhibit unique electronic properties those basically exceed the simple sum of those of constituent components because of the interface and border effects in the complexes. In addition to these complexes, the external field leads to further unique electronic properties in these atomic layer materials and their complexes. In this paper, we reported our recent theoretical calculations on heterostructures of atomic layered materials and electric field-effects on them using the density functional theory combined with the effective screening medium method. Our calculations demonstrated that the electronic structures of these complexes can be tuneable by controlling constituent elements and their arrangement in atomic layered materials, mutual arrangements, and external electric field [1,2,3,4,5,6].

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IS22

DISPERSION OF NANOMATERIALS BY TRAPPING: APPLICATION IN 3D PRINTING OF POLYMER COMPOSITES

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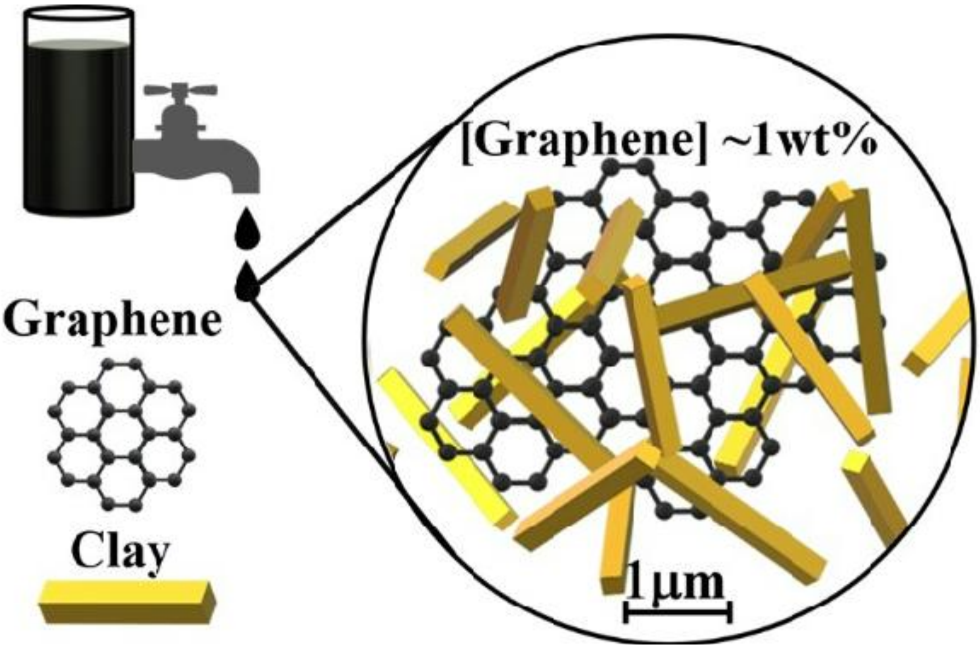
An efficient dispersion of nanocarbons (e.g., nanotubes or graphene sheets) in liquids and solids can enhance their transport properties like thermal and electrical conductivity. Yet, such dispersions are difficult to achieve since these nanocarbons are prone to aggregate and subsequently precipitate due to their strong van der Waals interactions. Conventional dispersion approaches, such as surface treatment of the nanocarbons either by surfactant adsorption or by chemical modification, may prevent aggregation. Unfortunately, surfactant-assisted graphene dispersions are typically of low concentration (< 0.2wt%) with relatively small graphene sheets (<1 µm lateral size) while chemical modification is punished by increased defect density within the sheets. We investigate here a new approach in which the concentration of dispersed nanocarbon in monomer solution is enhanced by the addition of a fibrous clay mineral, sepiolite [1-2], as shown in FIgure 1. The trapped graphene dispersion was applied in additive manufacturing (vat polymerization) where the thermal conductivity of the 3D printed polymer composite was enhanced by 160% compared to the neat polymer.



Graphene trapped in clay network

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IS23
NANOARCHITECTING LOW-DIMENSIONAL MATERIALS AT LIQUID/LIQUID INTERFACES: THIN FILMS FOR BROADER TECHNOLOGICAL APPLICATION

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A novel and versatile way to prepare thin, transparent, flexible and homogeneous films of advanced and multi-component materials has been developed by our research group, based on immiscible liquid/liquid interfaces [1]. The so-called liquid/liquid interfacial route (LLIR) is simple, efficient and unique for several materials, allowing the film deposition over any kind of substrates, plastics included. This talk will demonstrate the preparation of novel and exclusive films of multicomponent nanomaterials based on carbon nanotubes (CNTs), graphene and 2D materials (black phosphorous, MoS2), and their nanocomposites with conducting polymers, Prussian blue analogues or metal/metal oxide nanoparticles, followed by the application of the resulting materials in different fields as electrodes in aqueous and transparent Na- or K-ion batteries, solar cells, transparent electrodes, electrochromic displays, catalysts and sensors [2-8]. It will be shown that the properties of these films can be modulated controlling the morphology and interaction between the components. Based on the selected examples, it will be demonstrated that the LLIR is a new pathway to design materials combining synthesis and processing in one single-pot and single-step, allowing the production of multi-components and multi-functional thin films for application in different fields. Authors acknowledge financial support from CNPq, CAPES/COFECUB, CAPES/PRINT, INCT Nanocarbon and INCT NanoVida.

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IS24

CONTROLLED PREPARATION AND APPLICATIONS OF CARBONENE FIBERS

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The development of lightweight and high-strength fiber is one of the eternal themes in the field of materials. With the rapid change of applications and demands, more structural and functional requirements have emerged in aerospace, national defense, military, energy, biology and other fields. Carbonene materials (mainly including carbon nanotubes and graphene) have the advantages of low density, high mechanical properties, excellent electrical and thermal conductivity, and are ideal base materials for building next-generation lightweight, high-strength, high-toughness, functional and smart fibers.[1] This report mainly introduces our research progress in controlled preparation and application of carbonene fibers, including the controlled preparation methods of carbonene materials, the preparation of high-mechanical-property and multifunctional carbonene fibers, the exploration of structure-regulation method and property-transfer rules of carbonene materials in carbonene fibers, as well as the mass production technology of carbonene fibers and their application prospects in individual protection and artificial muscle.

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IS25

SINGLE CHIRALITY SWCNTS ENRICHMENT GOVERNED BY CONJUGATED POLYMER CHARACTERISTICS

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A number of single chirality single-walled carbon nanotubes (SWCNTs) have been successfully enriched using a variety of conjugated polymers in toluene. The polymer characteristics greatly influence the chiral selectivity and yield in the enrichment. For example [1], fluorene homopolymers such as poly(9,9-di-n-dodecylfluorene) (PFDD) and copolymer with anthracene such as poly[(9,9-dihexylfluorenyl-2,7-diyl)-co-(9,10-anthracene)] result in high (7,6) selectivity from the SG76 CNT source up to 67% and 72%, respectively. The selectivity is calculated by optical absorption using known extinction coefficient. In contrast, poly[(9,9-dioctyl-2,7-divinylenefluorenylene)-alt-co-(9,10-anthracene)], with a double bond spacer, results in (9,5) dominant extractions with the purity of (9,5) up to 80% after ultracentrifugation, which is believed to be the first report on successful enrichment of (9,5) by conjugated polymers. The chiral selectivity is also greatly impacted by the length of alkyl sidechain of fluorene homopolymers. Interestingly, a chiral selection transition from (7,6) to (8,6) occurred using poly(9,9-di-n-tetradecylfluorene) (PFTD) after a few enrichment cycles. The chiral purity of (8,6) was greatly improved from 50% to 86% after slow filtration. Molecular dynamics simulation confirms that different length of sidechain of polyfluorene has different wrapping stability towards specific chirality, where PFTD shows greater stability towards (8,6) than (7,6) (Figure 1). Polymer molecular weight also plays a role to the selectivity and yield. The good quality of the enriched (7,6) was demonstrated by the performance of thin film transistors fabricated with (7,6) ink as the channel materials.

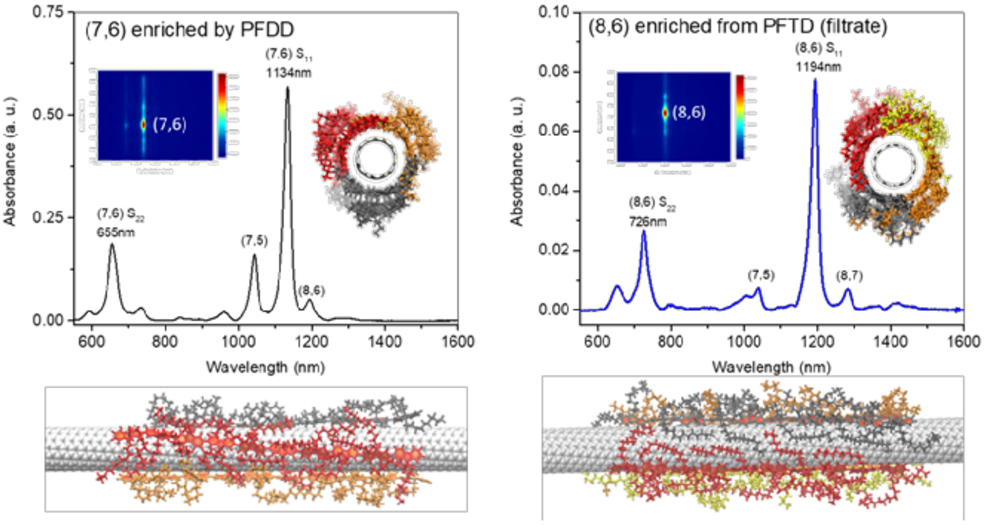

Figure 1. Absorption spectra of enriched (7,6) and (8,6) as well as their PLE maps and optimal polymer binding geometries obtained from molecular dynamics simulations.

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'The impact of conjugated polymer characteristics on the enrichment of single chirality single walled carbon nanotubes'
ACS Appl. Polymer Mater. 4, 6239–6254, 2022.

IS26

MONOELEMENTAL 2D MATERIALS – CHEMISTRY AND APPLICATIONS

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Two dimensional materials are already almost 20 years in the forefront of material science. However the graphene discovery started this new direction of research, beyond graphene are several other monoelemental 2D materials including elements in 14th group (silicene, germanene) as well as elements in 15th group (phosphorene, arsenene and antimonene) and several others. These two-dimensional allotropes are significantly more difficult to prepare due to its lower thermodynamic stability and higher reactivity in comparison with graphene. The contribution will discuss current methods for the top-down synthesis of monoelemental 2D materials from the group of pnictogen and tetrels and their chemistry [1,2]. Various methods of surface functionalization suitable for surface functionalization of silicene/germanene as well as phosphorene and arsenene will be shown. Precise control of surface functionalization allowed various application covering energy storage, catalysis as well as electronic and sensors. The potential applications of surface functionalized monoelemental 2D materials from 14th and 15th group will be demonstrated for the energy storage, electronic and catalysis.

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IS27

HETEROSTRUCTURES BASED ON TWO-DIMENSIONAL MATERIALS

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Low-dimensional materials, including one-dimensional (1D) carbon nanotubes and two-dimensional (2D) graphene, boron nitride (hBN), and transition metal dichalcogenides (TMDs, Fig. 1), provide an exciting platform for exploring novel physics and chemistry at the nanoscale. Low-dimensional materials have attractive physical properties, and importantly, they allow us to explore novel superstructures such as heterojunctions, heterostacks, and superlattices, opening up even more possibilities. We have explored two different methods to create low-dimensional superstructures: (1) crystal growth using metal-organic chemical vapor deposition (MOCVD) and molecular beam epitaxy (MBE) method, and (2) stacking of individual components using the dry transfer approach [1]-[3]. These methods produce various low-dimensional nanostructures as intended.

This talk will focus on our recent research results on low-dimensional lateral/vertical heterostructures, including ultrathin 2D MoS_2/WS_2 heterojunctions and heterostacks of hBN, TMD, and CNT; the 2D MoS_2/WS_2 junction width can be in the sub-nanometer range. In addition to fabrication details, photovoltaic properties investigated by microspectroscopy will be discussed [4],[5].

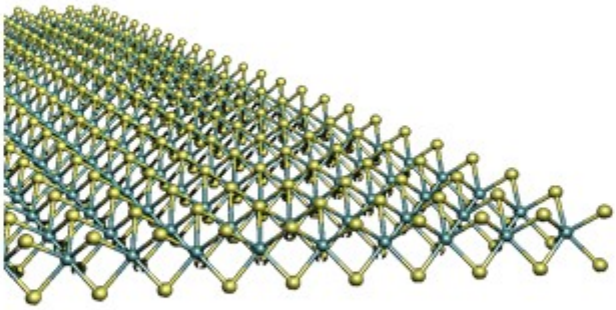

Fig. 1. A ball-and-stick representation of a monolayer transition metal dichalcogenide. Green and yellow balls correspond to transition metal (Mo,W, etc) and chalcogen (S, Se, Te) atoms, respectively.

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IS28

SINGLE-WALLED CARBON NANOTUBE FILM AS AN EFFICIENT CONDUCTIVE NETWORK FOR SI-BASED ANODES

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Silicon-based anodes are considered ideal candidate materials for next-generation lithium-ion batteries due to their high capacity. However, the low conductivity and large volume variations during cycling inevitably result in inferior cyclic stability. Herein, a dry method without binders is designed to fabricate Si-based electrodes with single-walled carbon nanotubes (SWCNTs) network and to explore the different mechanisms between SWCNT and multiwalled carbon nanotubes (MWCNTs) as a conductive network. As expected, higher initial discharge capacity (1785 mAh g^{-1}), higher initial Coulombic efficiency (ICE, 81.52%) and outstanding cyclic stability are obtained from the SiOx@C | SWCNT anodes. Furthermore, its lithium-ion diffusion coefficient (D_{Li+}) is 3–4 orders of magnitude higher than that of SiOx@C | MWCNT. The underlying mechanism is clarified by in situ Raman spectroscopy and theoretical analysis. It is found that the SWCNTs can maintain good contact with SiOx@C even under tensile stresses up to 6.2 GPa, while the MWCNTs lose electrical contact due to alternating compressive stress up to 8.9 GPa and tensile stress up to 2.5 GPa during long-term cycling. Under such very large stresses, the more flexible SWCNTs and their stronger van der Waals forces ensure that SiOx@C still has good contact with SWCNTs.

IS29

A. Siria*

IS30

OPTICAL PROPERTIES OF SINGLE GRAPHENE QUANTUM DOTS

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Recent years have shown an increasing number of studies focused on new light emitters for various applications and in particular for quantum technologies. In this context, nanographenes have great assets since bottom-up chemistry allows a total control on the structure, which opens the way to wide customization of their optical, and spin properties [1–3]. The full benefit from these opportunities needs addressing nanographene intrinsic photophysical properties. To do so, single molecule photoluminescence experiment is a powerful tool [4]. Here, we will focus on small nanographenes where electrons a confined in the three dimensions of space, the so-called graphene quantum dots (GQDs). We will show that our degree of control on the structure allows us to address both the influence of the size and of the symmetry of the GQD on its properties: emission wavelength, polarization selection rules, oscillator strength... We will report on experiments performed at the single molecule level and from room to cryogenic temperatures. We will show that the experimental results are well predicted by extensive DFT/TDDFT calculations combined with molecular dynamics simulations. [5-7].

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IS31

EVALUATION OF DISPERSION STATES OF SINGLE-WALLED CARBON NANOTUBES AND PREPARATION OF THEIR LIQUID CRYSTALLINE DISPERSIONS

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Dispersion of carbon nanotubes (CNTs) in liquids is a crucial process in the fabrication of advanced CNT-based materials. However, quantitative evaluation of the dispersed CNTs remains one of the least investigated aspects of CNTs. Recently, we found that centrifugal sedimentation analysis is an effective and useful tool to characterize the size distribution of CNTs [1]. In addition to the size, the porosity of the agglomerated CNTs can also be measured by changing the rotational velocity of the centrifugation. By using this method, surfactant-stabilized single-walled carbon nanotube (SWCNT) dispersions that show liquid crystal (LC) phases can be effectively prepared [2,3]. As the SWCNT concentration increases, the dispersion undergoes an isotropic to nematic phase transition in which the spindle-shaped LC droplets, or the so-called tactoids, and the Schlieren textures can be observed in the intermediate biphasic state and the nematic phase, respectively [2]. The arrangements of SWCNTs in the tactoids and the Schlieren structures are directly investigated by polarized optical microscopy. We also investigate the effects of SWCNT aspect ratios and surfactants on LC behaviors [3]. For example, the isotropic-to-nematic phase transition occurs at a lower concentration for the SWCNT dispersion with a larger aspect ratio, which is expected by the Onsager theory. The well-aligned film is successfully fabricated from the dispersion with the higher SWCNT aspect ratio by the simple blade coating suggesting that the CNT orientations can be controlled by the normal surfactant-assisted method.

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IS32
DIAMETER-DEPENDENT STACKING OF SQUARAINE DYE MOLECULES INSIDE SINGLE-WALL CARBON NANOTUBES

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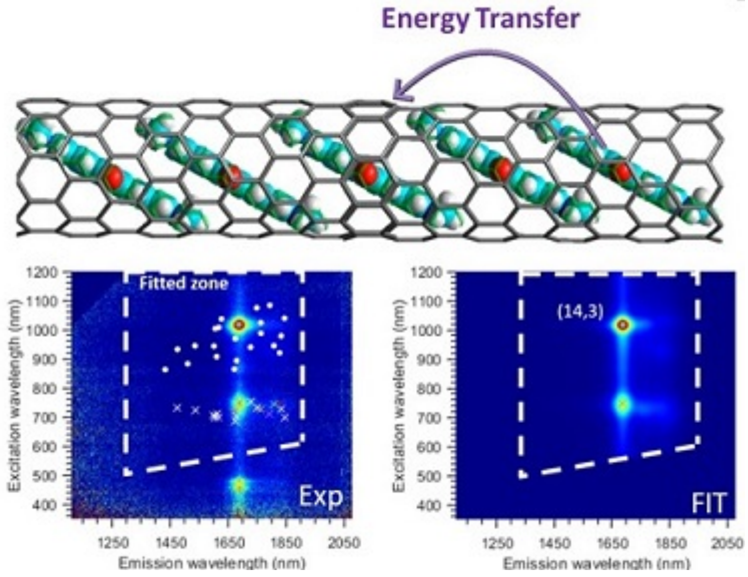
Thanks to the extensive variability of chiral structures of SWCNT, a large variety of electronic and optical properties can be accessed, making them extremely promising for diverse applications such as solar energy harvesting and high-performance (opto-)electronic devices. Besides these very peculiar intrinsic properties, SWCNTs also exhibit a hollow core, which can be filled with dyes giving rise to new one-dimensional hybrids that merge the properties of the nanotube with those of the dyes[1-2]. In this work[3] we report for the first time the combination of extensive chirality-sorting[4] and dye filling, leading to the isolation of nearly single chirality squaraine-filled SWCNTs as shown in the photoluminescence-excitation (PLE) map presented in Figure 1. For each dye@SWCNT chirality combination, we observe a different absorption wavelength of the confined dyes, originating from the different dye stacking driven by the diameter of the surrounding SWCNT. This diameter-dependent dye absorption followed by an energy transfer, is experimentally determined through the measurement and detailed fitting of fluorescence-excitation maps of different chirality-sorted dye-filled SWCNT samples. We, therefore, demonstrate that the diameter of the SWCNT is a lever to tune optical properties of the hybrids, paving the way for future applications in optoelectronics. Moreover, comparison with molecular models provides access to the possible different stacking configurations of the dyes inside the hollow space of SWCNTs with different diameters.



Energy transfer. (top) Schematic view of the new hybrids (bottom) Example of a PLE map and the corresponding fit (left) experimental PLE maps, the white dots represent all the chiralities that have been fitted and the crosses represe nt the energy transfer. (right) Fitted PLE map

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IS33

LAYER-BY-LAYER GROWTH OF MULTI-LAYER GRAPHENE SINGLE-CRYSTALS ENABLED BY PROXIMATE CATALYTIC ACTIVITY

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Direct growth of large-area vertically stacked two-dimensional (2D) van der Waal (vdW) materials is a prerequisite for their high-end applications in integrated electronics, optoelectronics and photovoltaics. Currently, centimeter- to even meter-scale monolayers of single-crystal graphene (MLG) and hexagonal boron nitride (h-BN) have been achieved by epitaxial growth on various single-crystalline substrates. However, in principle, this success in monolayer epitaxy seems challenge to be replicated to bi- or few-layer growth, as the full coverage of the first layer was believed to terminate the reactivity of those adopting catalytic metal surfaces. Here, we report an exceptional layer-by-layer chemical vapor deposition (CVD) growth of large size bi- and few-layer graphene single-crystals, enabled by proximate catalytic activity where the activity of the outermost graphene layer inherits from the platinum (Pt) surface underneath. In-situ growth and real-time surveillance experiments, under well-controlled environments, unambiguously verify that the growth does follow the layer-by-layer mode on open surfaces of MLG/Pt(111). First-principles calculations indicate that the proximate catalytic activity is allowed by an appreciable electronic hybridization between graphene overlayers and Pt surfaces, enabling catalytic dissociation of hydrocarbons and subsequently direct graphitization of their radicals on the outermost sp2 carbon surface. This activity is also proven to be robust for tube-furnace CVD in fabricating single-crystalline graphene bi-, tri- and tetra-layers, as well as h-BN few-layers. Such growth mechanism also promotes the fabrication of graphene spirals where a twisting angle was introduced between adjacent graphene layers. Our findings offer an exceptional strategy for potential controllable, layer-by-layer and wafer-scale growth of vertically stacked few-layered 2D single crystals.

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IS34

MODELLING THE ELECTRONIC STRUCTURE OF BORON-NITRIDE BILAYERS AS A FUNCTION OF STACKING ORDER AND TWIST-ANGLE

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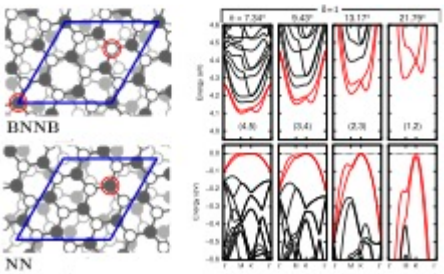
Bilayers of 2D materials have recently emerged as minimal systems where to tune and control the exceptional properties of their constituent layers. By changing the alignment of one layer with respect to the other (twist angle), it is possible to modify the interactions between the two sheets and hence tune their properties in a relatively controlled way. For instance, superconductivity can be switched on in graphene bilayers at some magic twist angle close to 1.1° [1]. In this context, boron nitride twisted bilayers (BNTB) are studied because the twist angle determines the formation and the flatness of several groups of degenerate bands [2]. This leads to a modulation of its optical properties and controls the emergence of correlated phases. Moreover, the presence of two atomic species provides an additional degree of freedom with respect to graphene bilayers, that is the stacking sequence. For example, experimental work shows that, by playing at the same time with the stacking sequence and the twist angle, it is possible to induce ferroelectricity in BNTB and to control the dynamics of the switching on [3]. The last example demonstrates that a correct description of this system must take into account at the same time the twist angle and the stacking sequence. Although some works can be found on the subject, we find that a systematic study is regretfully lacking. Here we present our theoretical results on the evolution of the electronic structure of several BN bilayers upon variations of the twist angle and the stacking sequence [4]. Simulations have been carried out with density functional theory and a tight-binding model we already used successfully in the past [5].



Right panel: different stacking of hBN (BNNB and NN) moiré structures. Left panel: Bottom conduction and top valence of the NN stackings at different twist angles.

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IS35

ATOMIC-LEVEL INSIGHTS INTO CARBON NANOTUBE GROWTH FROM MACHINE LEARNING-DRIVEN SIMULATIONS

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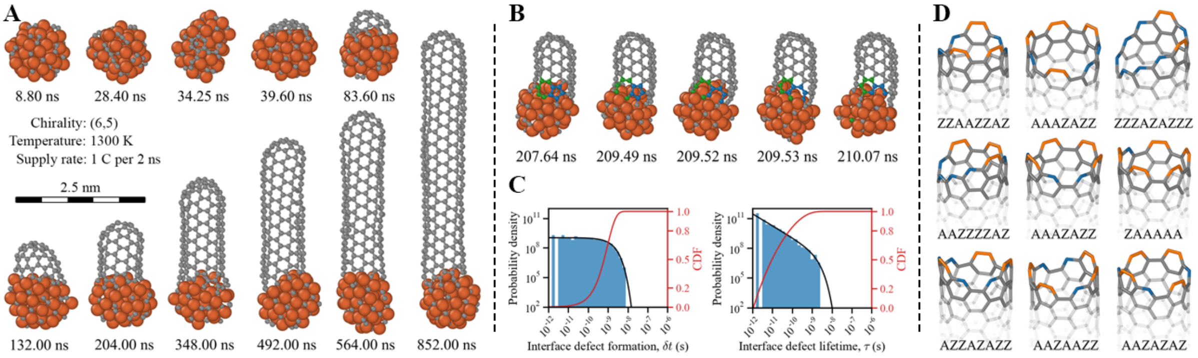
Carbon nanotubes (CNTs) are considered a successor to silicon in future nanoelectronic devices. To realize this technological potential, controlled growth of defect-free CNTs is required. Until now, the understanding of atomic-scale growth mechanisms provided by molecular dynamics (MD) simulations has been hampered by their short timescales. Here we present an efficient and accurate machine learning force field for realistic MD simulations of SWCNT growth on iron catalysts[1]. We simulate growth of SWCNTs on near µs timescales, achieving growth of long, defect-free nanotubes and provide new atomic-level insights into the entire growth process. From the evolution of the tube-catalyst interface and importantly the mechanisms behind the formation and healing of defects. Our results highlight the maximization of configurational entropy at the tube-catalyst interface and how defect-free CNTs can grow ultralong if carbon supply and temperature are carefully controlled.



Growth of a defect-free (6,5) SWCNT on a Fe55 catalyst at a temperature of 1300 K. A shows 11 snapshots of the structure during growth and B illustrates the healing of a 5-7 defect at the interface of the growing tube. Orange and gray spheres represent Fe and C atoms, respectively, in B blue and green spheres depict C atoms initially belonging to the 5-ring and 7-ring defects, respectively. C shows the probability density function and the cumulative distribution function (CDF) for the time between formation of interface defects, δt, and the interface defect lifetime, τ, during growth. D a sample of unique edges present during growth, showing the dynamic nature of the interface. Here zigzag sites are denoted by Z and colored blue in the structure while armchair pairs are denoted by A and colored orange.

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IS36

COULD CARBON NANOTUBE NON-VOLATILE MEMORY REPLACE DRAM?

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The amount of data is growing rapidly, leading to an increase in the data center server market. Data centers currently consume 1% of the world's electricity production, and further growth is expected. Non-volatile memory that doesn't require power is being explored as a replacement for DRAM and is being seen as a potential solution to this problem.

The Japanese government aims to achieve zero greenhouse gas emissions by 2050 and has established the Green Innovation Fund Project (2021~2030) for a total of two trillion yen. As part of the project, Japan Zeon and AIST have been selected to develop Carbon Nanotube Random Access Memory (CRAM) to save energy in data center servers.

CRAM is a type of random access memory that uses carbon nanotubes and has a simple structure that allows for low-cost production. It operates by changing between a low-resistance or high-resistance state when a voltage is applied between the electrodes, making it non-volatile and low power-consuming. Its construction involves sandwiching a carbon nanotube film between electrodes, and it is expected to replace DRAM and contribute to energy savings in data center servers.

In this talk, I will introduce our plans and efforts to develop CRAM. Specifically, we are conducting the development of an "innovative slurry" for forming carbon nanotube films for CRAM, creating a "test device" to evaluate the memory properties of the dispersion solution, and developing "evaluation analysis technology" to better understand the CRAM operating mechanism.

IS37

THERMOELECTRIC PROPERTIES OF ENGINEERED 2D FLAKES

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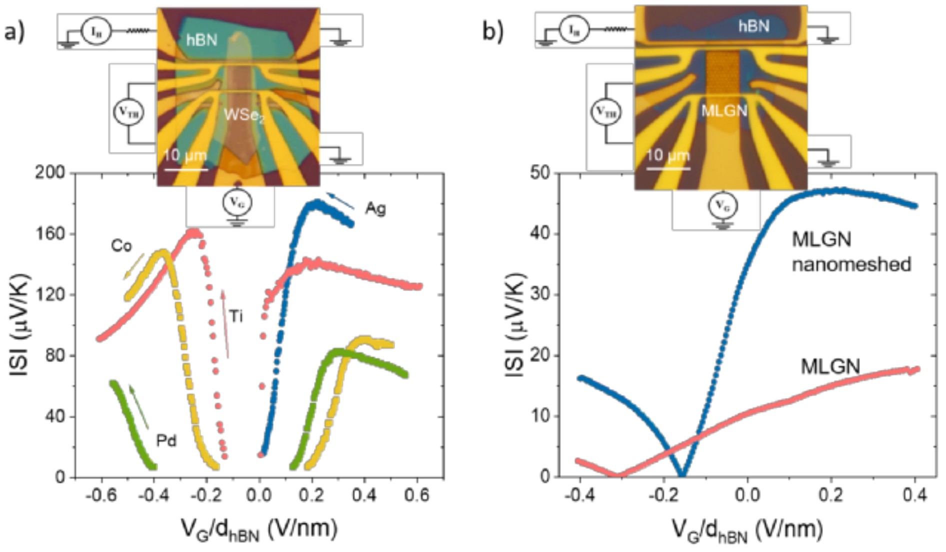
Research on new thermoelectric (TE) devices and materials is highly demanded in nanoelectronics to improve energy conversion at nanoscale. Energy conversion of TE nanogenerators is ruled by TE efficiency ZT, defined as $ZT=S^2\sigma T/k$, with S the Seebeck coefficient, σ the electrical conductivity, k the thermal conductivity and T the temperature. High ZT values (>> 1) are typically sought for a TE material to be exploitable in applications.

In this context, the discovery of 2D materials has opened new routes of investigation. High ZT values have been predicted for example in graphene nanostructures[1] and transition metal dicalcogenides (TMD) have revealed high Seebeck coefficients[2,3]. Due to the complexity of controlling thermal transport at the nanoscale, actual applicability of 2D materials as thermoelectric materials depends on the ability to fully study their pertinent physical properties once implemented in real devices.

I will present our recent contribution in engineering new devices based on 2D materials flakes. In particular we have investigated the electric and thermoelectric properties of hBN/WSe_2 and hBN/MLGN (MLGN=multilayer graphene) heterostructures, where hexagonal boron nitride (hBN) acts as a substrate and as a dielectric spacer efficiently coupling the 2D flake to a local metallic gate. Our investigation reveals the role of the metallic contacts on electronic transport and thermoelectricity in hBN/WSe_2 based devices[4]. Depending on the used metal contact, high values of Seebeck coefficient S up to 180 µV/K can be attained.For hBN/MLGN devices, we find out that a network of holes increases the Seebeck coefficient and reduces the thermal conductivity, by slightly affecting the electronic transport.



(a) hBN/WSe2 and (b) hBN/MLGN based devices for electric and thermoelectric measurements. Absolute value of the Seebeeck coefficient as a function of the gate voltage in hBN/WSe2 and hBN/MLGN (nanomeshed or not) devices.

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IS38

ENERGY-HARVESTABLE PIEZOCOMPOSITE EMBEDDED WITH ONE-DIMENSIONAL P(VDF-TRFE) NANOFIBERS AND SINGLE-WALLED CARBON NANOTUBES

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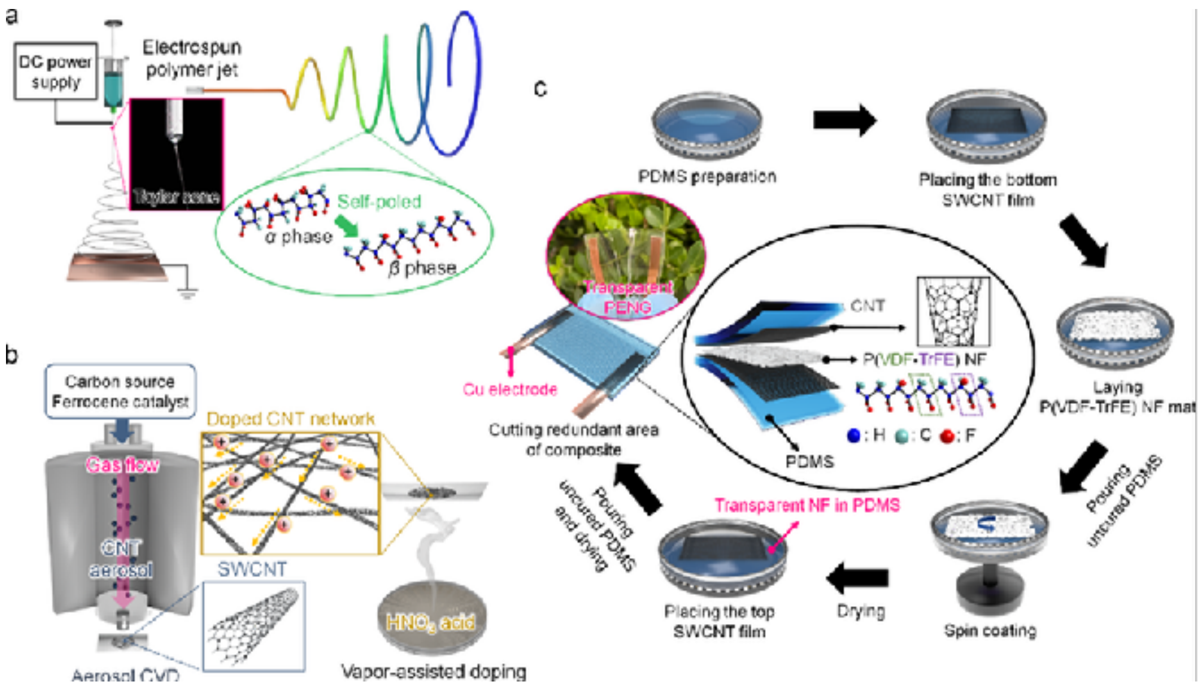
Highly transparent, flexible, and ultrathin piezocomposite, in which electrospun poly(vinylidene fluoride-co-trifluoroethylene) [P(VDF-TrFE)] nanofibers (NFs) and aerosol-synthesized single-walled carbon nanotubes (SWCNTs) are embedded in elastomer matrix, is fabricated. The P(VDF-TrFE) NF mat is exploited as a piezoelectric layer of the piezocomposite while the SWCNT film is applied as a transparent conductive electrode (TCE) thereof. The use of these one-dimensional (1D) nanomaterials allows the piezocomposite not only to have a high transparency along with low diffusivity, but also to exhibit enhanced mechanical properties. In addition, the coupling effect of piezo- and flexoelectricity exhibited from the electrospun NFs and the acid-doping effect conducted on the SWCNTs facilitate a significant improvement in kinetic energy-harvesting performance, leading to a maximum output voltage of 26.8 V. Moreover, electrospinning and aerosol chemical vapor deposition (CVD) methods employed here are facile, scalable, and cost-effective, thus are expected to accelerate the development of industrially feasible next-generation wearable electronics.



IS39

CARBON NANOTUBE-BASED PHYSICAL RESERVOIR COMPUTING

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Reservoir computing (RC) is one of the machine learning methods derived from a recurrent neural network (RNN) and has attracted attention because of the small amount of computation required for learning. In recent years, various forms of physical RC using nonlinear physical systems such as memristors, optical amplifiers, and soft octopus robots have been proposed for low power consumption and high-speed processing. [1] The physical reservoir system needs non-linearity, high dimensionality, and short-term memory. It has also been shown that transient response currents due to electrochemical reactions and ion migration in solution have the ability of reservoirs [2]. In this study, we report physical reservoir systems based on CNT electron devices such as thin-film transistors and memristers.

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IS40

NANOWIRE SYNTHESIS BY FLOATING CATALYST CVD AND LARGE-SCALE ASSEMBLY AS NANOTEXTILES

I. Gómez-Palos [1], M. Vazquez-Pufleau [1], R. Schaeufele [1], Á. Ridruejo [2], A. Mikhalchan [1],
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This talk describes a method to produce macroscopic solids made of 1D nanostructured directly collected as they grow floating in the gas phase, through floating catalyst chemical vapour deposition (FCCVD). Under this synthesis mode, growth is around 1000 faster than in substrate-based processes. The resulting high aspect ratio (> 200) enables the aggregation of nanomaterials in the gas phase and ultimately the formation of network solids similar to nanotextiles. The method, originally used to grow CNTs or BNNTs, has been more recently applied to synthesise nanowires (NW) of Si,1 SiC,2 and MOx, respectively. The first part of the talk discusses progress in our understanding of nanowire growth by FCCVD. It reviews emerging experimental data for the growth rate, diameter distribution and length distribution of NWs and nanotubes.3 This analysis shows that FCCVD is indeed, inherently faster than substrate-based CVD under equivalent temperature and pressure conditions. We ascribe this to faster impingement of precursors into the aerosol of catalyst. Next, the talk presents our efforts to study nanowire aggregation in the gas phase, and the formation of macroscopic network materials. We analyse the conditions for formation of an aerogel through theory of percolation of rigid rods, and apply this analysis to compare the processes for CNT and nanowire assembly. Finally, we show that networks of entangled nanowires can be visualized as nanotextiles both in terms of their structure and their bulk mechanical properties. They are flexible in bending, sustain large strains, have inherent damage-tolerance and are dominated by inter-, rather than intra-particle features, particularly their orientation distribution function.

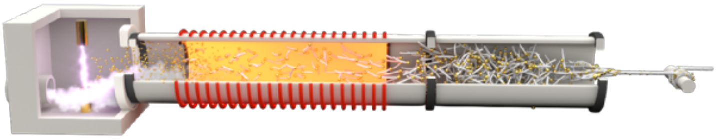

Figure 1. Schematic of nanowire/nanotube synthesis through floating catalyst CVD (FCCVD) and assembly into high-performance network materials.

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IS41
REDUCTIVE NANOCARBON PROCESSING: CHEMISTRY, ASSEMBLY, AND APPLICATION

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Individual perfect nanocarbon structures have exceptional properties; the challenge is often how to exploit their potential in real macroscopic systems. Chemical functionalisation is critical to a wide range of nanocarbon technologies, but needs to be versatile and applicable at scale. Existing approaches tend to rely on liquid phase reactions, often requiring damaging sonication or lengthy work up through filtration or centrifugation. The formation of individualized functionalised single wall nanotubes (SWNTs) and graphenes is a particular challenge.

One particularly promising approach, relies on reductive charging to form pure charged nanocarbon anions which can be redissolved, purified, or optionally functionalised, whist avoiding the damage typically associated with sonication and oxidation based processing [1]. This simple system is effective for a host of nanocarbon materials including MWCNTs, ultralong SWCNTs, carbon blacks, graphenes, and related materials. The resulting nanocarbon ions can be readily chemically grafted for a variety of applications. The chemistry of these discrete nano-ions raises interesting fundamental questions but is also practically useful. Solvated nanocarbon related materials can be assembled by electrophoresis, cryogel formation, or direct cross-linking to form Joule heatable networks, protein nucleants, supercapacitor electrodes, and catalyst supports [2][3]. 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. Combinations with existing commercial carbon fibres can provide opportunities to enhance state of the art performance or introduce new function [3]. The use of nanostructured materials often provides opportunities to simultaneously address otherwise conflicting materials property requirements, such as high ionic conductivity with high stiffness, or self-healing with high absolute strength.

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CS01
SENSING OF PYROPHOSPHATES WITH SP3-FUNCTIONALIZED (6,5)-SWNTS

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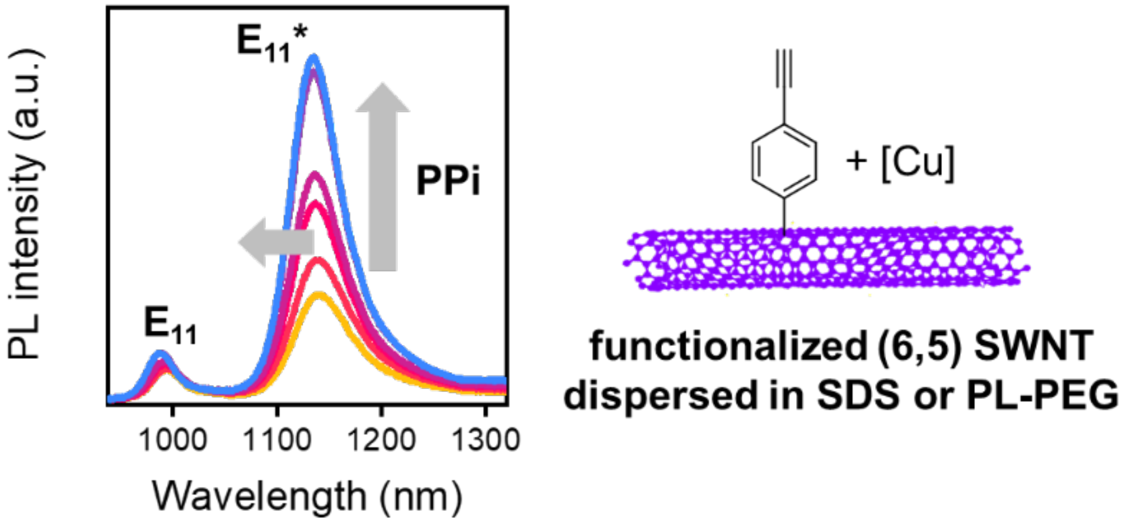
The controlled functionalization of single-walled carbon nanotubes (SWNTs) with luminescent *sp*^{3}-defects has emerged as a powerful tool to enhance their usually low photoluminescence (PL) quantum yields and to employ them for bioimaging and chemical sensing. Here, we demonstrate the spectroscopic detection of inorganic pyrophosphate (PPi) - a cellular ATP hydrolyte that plays a key role in many physiological processes - with the help of *sp*^{3}-functionalized (6,5) SWNTs. We introduce *sp*^{3}-defects bearing an alkyne moiety to ATPE-sorted and sodium dodecyl sulfate (SDS) stabilized (6,5) SWNTs via diazonium salt chemistry. These functionalized (6,5) SWNTs show a high sensitivity towards the presence of Cu(II) ions and strong quenching of the E_{11} and E_{11}* (1130 nm) emission can be observed. Importantly, the defect-induced E_{11}* emission is quenched significantly more compared to the E_{11} emission. The quenching effect can be reversed by addition of Cu(II)-complexing analytes such as PPi. With increasing PPi concentration the E_{11} and E_{11}* intensities are gradually restored. This reversibility enables quantitative detection of PPi. In addition to changes in photoluminescence intensity, the emission peaks shift significantly and can be used as an additional detection metric. Transferring the system from SDS-dispersed SWNTs to phospholipid polyethylene glycol (PL-PEG)-dispersed SWNTs in buffer solution provides the necessary biocompatibility while the sensor remains fully functional with a sensitivity in the range of 10 µM – 2 mM of PPi. With these properties the functionalized (6,5) SWNTs are ready to be used for in vivo sensing and imaging of PPi.



Functionalized (6,5) SWNTs with 4-ethynylphenyl moieties dispersed in SDS or PL-PEG show quenching of near-infrared emission as well as shifts in peak position upon addition of Cu(II) ions. This effect can be reversed by addition of PPi thus enabling the detection of PPi with a sensitivity in the range of 10 µM – 2 mM.

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CS02
TOWARDS TARGETED, FLUORESCENT NANOCARRIER SYSTEMS BASED ON B/N CO-DOPED CARBON NANO-ONIONS

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It is widely known that modern chemotherapy treatments cause severe side effects in patients due to the inability of many cancer drugs to target cancer cells over normal, healthy tissues. One method of circumnavigating this problem is by developing a targeted nanocarrier system. Boron/nitrogen co-doped carbon nano-onions (BN-CNOs) are a novel nanomaterial that could be used as a scaffold for these systems. Their biocompatibility, combined with their nanoscale size [1] gives them promising potential for use in drug delivery and biological imaging applications. Our group has developed a low cost, one-step thermal annealing method to produce BN-CNOs [2]. In the pristine form, BN-CNOs suffer from poor aqueous solubility, like many other carbon nanomaterials. In this work, we have non-covalently functionalised BNCNOs with a hyaluronic acid-1,2-dimyristoyl-sn-glycero-3-phosphoethanolamine (HA-DMPE) conjugate polymer to impart aqueous dispersibility and targetability for cancer cells overexpressing the CD44 receptor. By utilising the hydrophobic interactions between the BN-CNO surface and the phospholipid chains of the HA-DMPE, we have successfully coated the nano-onions with the conjugate polymer, increasing the water solubility of the BN-CNOs [3]. This was confirmed by FTIR, UV-Vis absorption, and dynamic light scattering analyses. We have also attached a fluorescent derivative of the HA-DMPE polymer to the surface of the BNCNOs to allow for cell tracking and bioimaging applications. Our goal is to use this BN-CNO based targeted nanocarrier platform to increase the efficacy and reduce the side effects of existing anticancer drugs.

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CS03
SP³ FUNCTIONALIZED ULTRASHORT CARBON NANOTUBES FOR DEEP BRAIN TISSUE IMAGING

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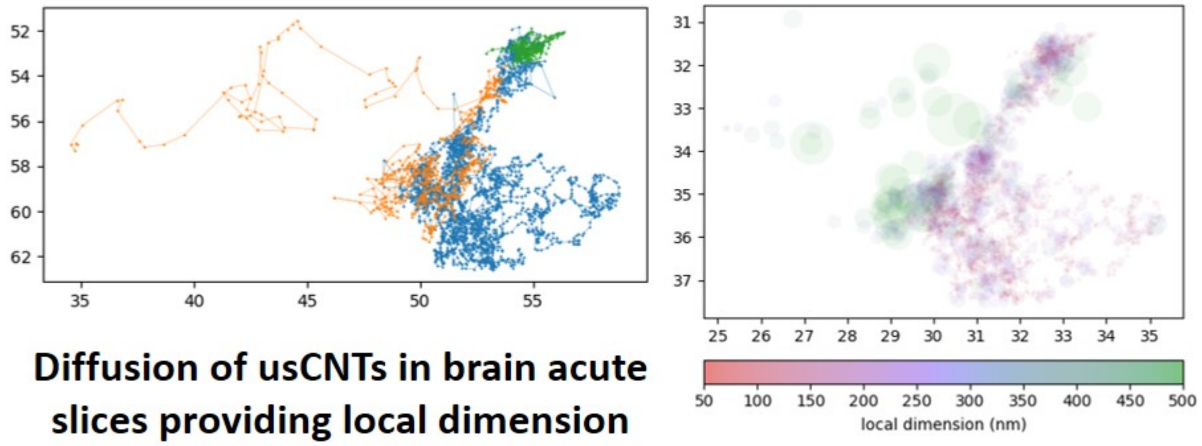
Near-infrared (NIR) microscopy has attracted significant attention for deep tissue imaging due to the combination of low light scattering and absorption by the tissues, especially in the NIR-II window (~1000–1350 nm). In this context, single-walled carbon nanotubes laid the foundation for bio- and sensing applications. More specifically, ultrashort carbon nanotubes (usCNTs) had long been sought for mimicking bio-molecules. Unfortunately, the intrinsic PL is quenched in usCNTs because of their small size compared to the exciton-diffusion-length (<100 nm). Using sp^3 defects, excitons can be prevented from reaching nanotube ends by local trapping, hence resulting in bright fluorescent usCNTs [1]. Herein, we demonstrate the efficient preparation of fluorescent usCNTs specifically designed for biological applications and we show how to create bright and biocompatible usCNTs. More precisely, we adapted a synthesis route where the sp^3 functionalization is followed by chemical cutting [2]. The defect implantation is confirmed by the appearance of a strong red-shifted PL peak at ~1150 nm compared to the pristine CNTs (~980 nm). The length estimated by AFM is in average of ~ 39 ± 12 nm. Subsequently, after surface bio-functionalization by phospholipid-polyethylene glycol, we present our results of usCNTs diffusing in live brain tissue and compare their behavior with that of long sp^3 functionalized CNTs in different compartments of mouse brains [3] (Fig.1).



Sp3 defect introduced bright fluorescent usCNTs for deep tissue imaging in neuroscience.

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CS04

ENGINEERING PH RESILIENCE IN OPTICAL NANOTUBE SENSORS FOR BIOMEDICAL APPLICATIONS

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Optical probes enable real-time monitoring of biomarkers in vitro, in vivo, and in cells. Probes based on the fluorescence of semiconducting single-walled carbon nanotubes (SWCNTs) specifically benefit from photostable near-infrared light emissions that are minimally absorbed by biological tissue. SWCNTs are often solubilized by DNA to enable the optical detection of specific bioanalytes. Despite efforts to engineer the selectivity of the DNA sequences towards only specific analytes of interest, these DNA-wrapped sensors are prone to optical perturbations from fluctuations in pH. In this work, we explore the fluorescence effects of DNA-SWCNT in varying pH. We observe a substantial pH effect that varies with the DNA sequence and exploit this pH sensitivity for applications in cancer detection. Using xeno nucleic acids (XNAs), we further engineer optical sensors that show resilience towards fluctuations in pH, enabling the detection of biomarkers in the absence of contributions from varying pH effects.

CS05

INTEGRATED GRAPHENE FET ARRAY FOR HIGH SENSITIVE DETECTION OF NEW CORONA VIRUS WITH AUTOMATED WASHING SYSTEM

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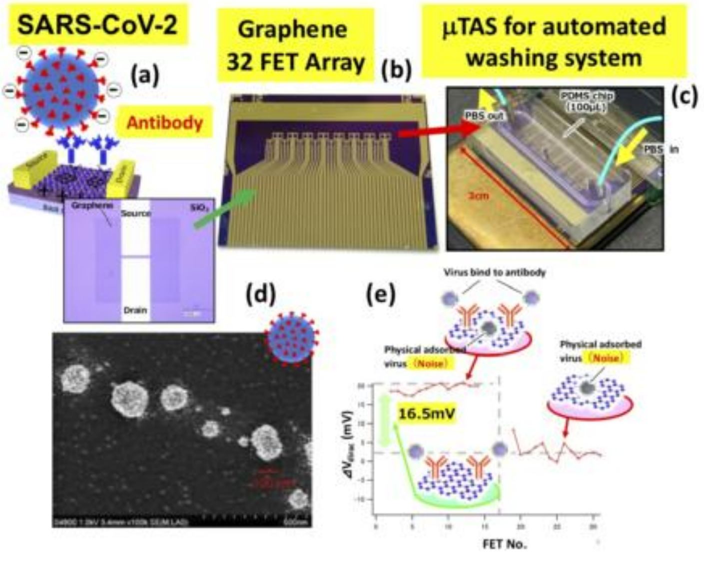
By integrating the 32 graphene FET with antibody modified channel, the new corona virus was detected with 100~1000 times higher sensitivity than the conventional antigen detection kits. The detection time is ~10~20 minutes, which is ~10 times shorter than the PCR system. By using the graphene FET with and without the antibody modification for detecting the signal of virus and for the reference signal, the problems of the signal drift and the physical adsorption of virus were solved. Also by adapting the m-TAS and automated washing system, the restriction of the Debye length was solved and the impurity such as a saliva could be washed away and the pure signal only from the virus which bind to antibody could be detected. Graphene FET was modified by antibody through PBASE which selectively capture the virus. The channel length and width are 10mm and 100mm, respectively. 32 graphene FET's are integrated, and the 13FET's in the left hand side are modified by antibody, and the 13FET's in the right hand side are without antibody modification and used as reference FET. Onto this integrated graphene FET array, the micro total analysis system (m-TAS) made by PDMS was set to introduce the phosphate-buffered saline (PBS) solution from the right hand side inlet and through the graphene FET channel, and to drain from the left hand side outlet. PBS solution was introduced from the reservoir by the computer controlled micropump. In order to control the Debye length, the different concentration of PBS solution should be used for the introduction of virus and for the detection of the charge of virus. Using these process, ~40 new corona virus on the graphene FET channel could be detected clearly which is 100~1000 times higher sensitivity than the conventional antigen detection kits.



Virus Detection by Graphene FET Arrays. (a)Schematic structure of graphene FET with antibody modification and optical image of FET. (b) Optical image of integrated graphene FET array. (c) Optical image of micro-TAS on graphene FET array. (d) New corona virus combined to antibody on graphene FET observed by SEM. (e) Dirac point shift of graphene FET with(left) and without(right) antibody modification by introduction of negatively charged virus.

CS06
GIANT CIRCULAR DICHROISM EFFECT OF TWO-DIMENSIONAL SEMICONDUCTING CARBON NANOTUBE COIL

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Chirality refers to a geometric feature of an entity that allows it to be distinguished from its mirror image, which is responsible for distinct optoelectronic effects. A prevalent approach to construct chiroptical nanomaterials involves the co-assembly of chiral molecules or geometrically helical structures with the host materials. Here, we report another route to directly fabricate chiroptical molecules via templated self-assembly. One-dimensional carbon nanotubes (CNTs) are taken as a representative — a typically chained aggregate of carbon atoms with their chiroptical properties depending on the helicity. Monodispersed semiconducting CNTs were kinetically synthesized and sorted under the assistance of high-voltage electric field. With a single spherical droplet template, individual semiconducting CNTs were nondestructively manipulated into a two-dimensional coiled morphology with well-defined topological structures. Arising from the perfect atomic structure and crystal momentum matching, collective photon-excited carriers were allowed efficient pumping and moving through the whole CNT coil while drastically enhancing the dipole-dipole interactions and chiroptical performances. Chiroptical signals of a single CNT coil collected by Rayleigh scattering circular dichroism (Ray-CD) showed the giant Ray-CD effect with orders of magnitude gain without polarization dependence compared with that of pristine straight nanotubes. This study exhibits new opportunities for CNTs in the chiral optoelectronics and will shed new light on the self-assembly or functionalization of chiral one-dimensional molecules.

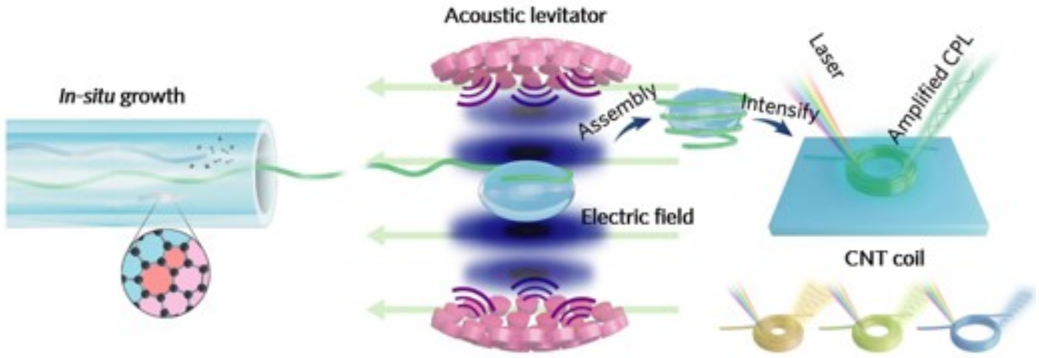

Figure 1. Schematic illustration of the assembly and chiroptical characterization of nanotube coils

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CS07

ROLE OF LOCALIZED IMPURITIES ON NON-RADIATIVE DECAY IN DOPED CARBON NANOTUBES

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Intrinsic and doped semiconducting single-walled carbon nanotubes (s-SWNTs) have far-reaching potential for optoelectronic applications [1-4], which is attributed to near-infrared photoluminescence (PL) of strongly bound excitons and trions as well as favorable charge transport characteristics [5]. So far, optical applications have been hampered by low PL quantum yields (PLQY) on the order of 1% and short excited state lifetimes, both of which are pointing towards efficient non-radiative (NR) decay [6]. However, no consensus has been reached about the NR decay mechanism as either being homogeneous (location independent) or inhomogeneous (location dependent) [6,7]. Here, we present a steady-state PL and transient absorption study regarding the doping dependence of exciton and trion dynamics. Our data reveal that even small doping levels further reduce the PLQY by an order of magnitude. Moreover, we show that exciton kinetics is diffusion-limited for intrinsic and moderately doped s-SWNTs whereas trion decay is monoexponential. In combination with doping-induced spectral changes, these dynamics suggest that doping is best described as inhomogeneous with localized surplus charges acting both as centers for mobile exciton quenching as well as for trion generation and decay. Our study shows that low PLQYs in carbon nanotubes are based on the exciton's large diffusion coefficient and its high susceptibility to frequent local perturbations. Thus, NR decay might be impeded by reducing either the exciton mobility or the inhomogeneities in the nanotube surroundings.

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CS08

EXCITON DECAY AND ANOMALOUS INELASTIC CROSSSECTION IN FREESTANDING GRAPHENE

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Graphene is the ultimately thin dielectric sheet. We combine angle resolved electron energy loss (AR-EELS) spectra in transmission with an energy and momentum resolution as good as 45 meV and 0.04 Å^{-1} (FWHM) and ab inito calculations at different levels of theory. [1] I will present the complete picture of inelastic scattering on a truly 2D electronic system. We can quantitatively distinguish in-plane and out-of plane components of the involved momentum transfer (q) that manifest in a stark contrast to conventional bulk scattering theory. Noteably the crosssections of the π and σ plasmons of graphene do not diverge in the optical limit ($q \rightarrow 0$) according to bulk scattering theory, but their intensity drops in a 2D sheet to zero. The opening of an excitation gap with increasing in-plane q traces out the electronic Driac cone and is very well modeled on the level of DFT+RPA alone. Yet the linear dispersion of the π plasmon is only correctly described on the GW+BSE level. They provide insight on the momentum depdendent excitonic nature of interband transitions in graphene. The exciton picture is only applicable up to to a critical $q_c \sim 0.1$ Å^{-1} beyond which we observe an exciton decay as the independent particle picture becomes applicable for electrons in graphene.

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CS09

UPCYCLING OF PLASTIC WASTES INTO HIGH VALUE-ADDED PRODUCT-CARBON NANOMATERIALS IN ENERGY STORAGE

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Nowadays, many common thermoplastics are widely used in our society, which are enriched carbon carriers compared to biomass. However, these waste plastics are one of the main resources for the formation of “white pollution.” Facing the increasing pressure from white pollution of waste plastics, it is still a great challenge how to treat these wastes. In light of the traditional way does not fully take use of polymer and waste energy, it is really promising to find a proper way to recycle waste plastics into highly valuable products (such as carbon nanomaterials) to reduce the white pollution in the world.[1,2] However, the carbonization yield of plastic is low and the microstructure of carbon materials is hard to control. To address these issues, we have developed a series of methods to produce carbon materials from plastic wastes with controllable morphology and size. More importantly, the obtained carbon nanomaterials were used in energy storage, such as lithium-ion batteries and supercapacitors.[3] The results prove that it is a potential way to recycle these plastic wastes into high-value-added products.

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CS10

STABLE, HIGH ENERGY-DENSITY SIO-NCM FULL CELL BASED ON THREE-DIMENSIONAL CURRENT COLLECTOR OF CARBON NANOTUBES AND PARTIAL PRELITHIATION METHOD

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Silicon monoxide (SiO) is an anode material having high capacity (>1500 mAh/g_{SiO}) with superior stability. SiO is normally coated with polymetric binders, conductive filler on thick and heavy current collector of metal [1], resulting in low capacity per electrode mass. We have previously developed a self-supporting carbon coated SiO (SiO/C)-carbon nanotube (CNT) electrode without using metal foils and polymetric binders that achieved high SiO/C content and high electrode-based capacity [2]. However, there is an issue of irreversible capacity at the 1st cycle due to Li silicate formation [1] and side reaction of electrolyte decomposition on CNTs with large surface area [3], leading to low energy density in full cells. To solve this problem, we here propose a new prelithiation process by two-stack electrodes. The SiO/C-CNT electrode was prepared via dispersion-filtration process [3] of ~1 μm-sized SiO/C particles and submillimeter-long few-wall CNTs synthesized by our fluidized bed [4] (SiO/C 85 mass%, ~0.88 mg_{SiO}/cm^2). The SiO/C-CNT electrode was prelithiated using Li foil and electrolyte (1 M $LiPF_6$ + 3.8 mass% FEC in EC + DEC (1:1 v:v)) for 24 hours. Then another SiO/C-CNT electrode was stacked on the prelithiated electrode to make partially prelithiated SiO/C-CNT electrode. Full cells were fabricated using the partially prelithiated SiO/C-CNT negative electrode, a NCM811-CNT positive electrode (NCM 97 mass%), a polypropylene separator, and the same electrolyte as prelithiation. Under the conditions of 0.45 mA/cm^2 with negative/positive (N/P) capacity ratio of 1.0 and areal capacity of 3.0 mAh/cm^2, the full cell worked stably, achieving high energy density per total electrode mass of negative and positive electrodes (466 Wh/$kg_{electrode}$ at the 100th cycle) (Fig. 1) compared to conventional electrode [5].

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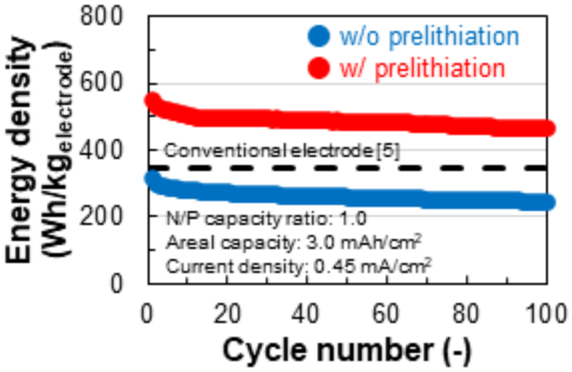

Cycle performance of CNT-based SiO||NCM full cell

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CS11

MAXIMIZING ION ACCESSIBILITY IN MXENE-KNOTTED CARBON NANOTUBE COMPOSITE ELECTRODES FOR HIGH-RATE ELECTROCHEMICAL ENERGY STORAGE

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Improving the accessibility of ions in the electrodes of electrochemical energy storage devices is vital for charge storage and rate performance. In particular, the kinetics of ion transport in organic electrolytes is slow, especially at low operating temperatures. Herein, we report a new type of MXene-carbon nanotube (CNT) composite electrode that maximizes ion accessibility resulting in excellent rate performance at low temperatures. The improved ion transport at low temperatures was made possible by breaking the conventional horizontal alignment of the two-dimensional layers of the MXene Ti3C2 by using specially designed knotted CNTs. The large, knot-like structures in the knotted CNTs prevent the usual restacking of the Ti3C2 flakes and create fast ion transport pathways. The MXene-knotted CNT composite electrodes achieve high capacitance (up to 130 F g-1 (276 F cm-3)) in organic electrolytes with high capacitance retention over a wide scan rate range of 10 mV s-1 to 10 V s-1. This study is also the first report utilizing MXene-based supercapacitors at low temperatures (down to -60 °C) [1-2].

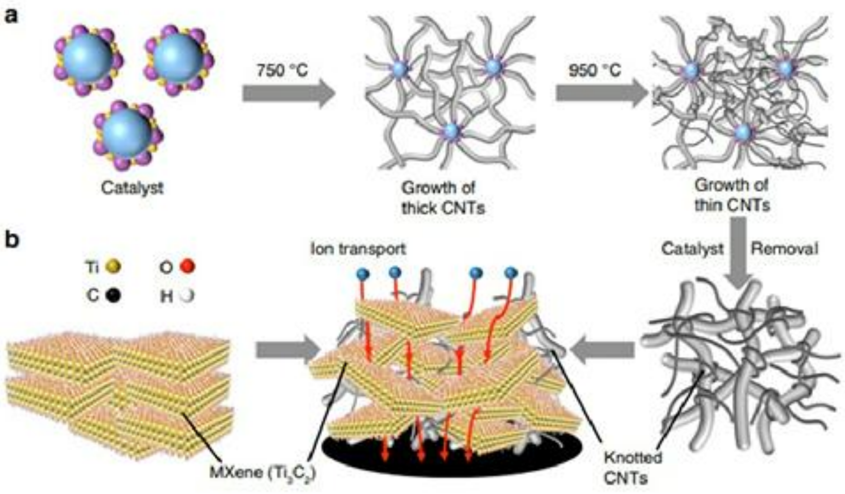

Fig. 1. Design of the MXene-knotted CNT composite electrodes for efficient ion transportation.

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CS12
ROLL-TO-ROLL PRINTING STRETCHABLE OPTOELECTRONIC SYNAPSE TRANSISTOR ARRAY AND THEIR APPLICATIONS

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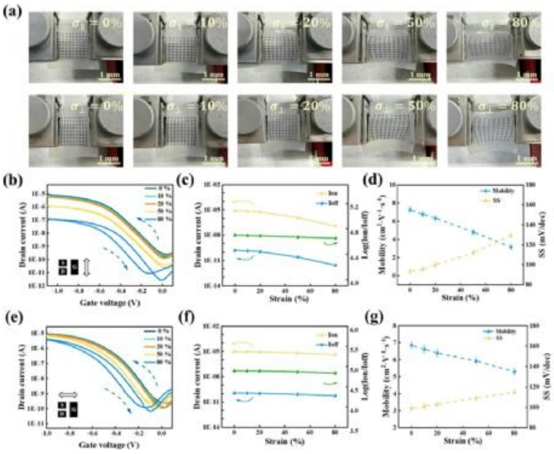
High-performance stretchable optoelectronic synaptic transistor arrays are key units for constructing and mimicking simulating neuromorphic vision systems. In this talk, we report the ultralow-power-consumption and low-operation-voltage stretchable all-carbon optoelectronic synaptic thin film transistors (TFTs) using sorted semiconducting single-walled carbon nanotubes (sc-SWCNTs) modified with quantum dots as active layers on ion-liquid based composite elastomer substrates. The resulting stretchable TFT devices show the enhancement-mode characteristics with excellent electrical properties, mechanical tensile properties and optoelectronic synaptic plasticity with ultralow power consumptions at the low operating voltage. No significant changes of these properties within 20% strain stretching can be observed, and they can remain correct even after 80% strain stretching. More importantly, we designed the nonvolatile of conductance which stimulated by UV light and bending angle to simulate stretchable neuromorphic vision systems (the functions of the crystalline lens and optic cone cells as bionic eyes) for detecting the atmospheric environment for the first time. The maximum accuracy of neural network combined with iterative synaptic weight update can reach up to the record 95.1% as bionic eye.



Optical images and electrical properties of stretchable SWCNT optoelectronic synaptic TFTs under different stretching strains at the vertical and horizontal directions

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CS13

DISTINGUISHING WATER CONFINED INSIDE A NANOTUBE FROM WATER ADSORBED OUTSIDE WITH AN INDIVIDUAL SWCNT-FET

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Single-walled CNTs (swCNTs) have recently gained interest as an intriguing host for the nanoscale confinement of fluids, with a variety of unexpected phenomena such as spontaneous filling, frictionless mass transport, unusual phase diagram, etc. [1]. The majority of these phenomena are still under debate and require experimental confirmation. However, it is challenging in this field to find experimental methods sensitive enough to carry out measurements at the level of individual nanotubes. On the other side, the electronic properties of swCNTs were shown to be sensitive to their diameter, defects, doping, adsorbates, and environment via swCNT field effect transistors (swCNT-FETs) [2], [3].

In this contribution, we show that individual carbon nanotube field effect transistors (CNTFET) are the perfect tool for achieving this goal, enabling for the first time to accurate identification of water confined inside the nanotube. By investigating the electrical performances of several unopened and opened CNTFETs submitted to different atmosphere and temperature treatments, such as dry air, humidity, secondary vacuum, and current annealing, we demonstrate that it is possible to distinguish between water being outside and inside of the nanotube, just outside, or the nanotube free from water. Precisely, we found that secondary vacuum and current annealing both shift the threshold gate voltage of opened swCNTs towards more negative values. However, the secondary vacuum had no effect on closed swCNTs compared to current annealing. We also demonstrate that this behavior is universal across all devices' metallicities, assuming that the nanotube's surface has been pre-cleaned using current annealing. We will also discuss the mechanism behind the coupling of electronic transport and the presence of water.

Our findings open up the possibility of using CNTFET to address long-standing issues in the nanofluidic community regarding the behavior of water confinement at the nanoscale, and also to use them for reliable, sensitive, and selective chemical and biological sensors.

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CS14

DEVICE APPLICATIONS OF ONE−DIMENSIONAL VAN DER WAALS HETEROSTRUCTURE NANOTUBES

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One-dimensional van der Waals heterostructure nanotube [1] is composed of coaxially assembled nanotubes and each layer maintaining its original properties because of the weak van der Waals forces between layers. Therefore, the different combination of van der Waals layers in the hetero-nanotubes would enable novel applications in electronics and optoelectronics, such as a radial semiconductor-insulator-semiconductor heterojunction diode [2] due to the inner p-type semiconducting single walled carbon nanotube (SWCNT), middle insulating boron nitride nanotube (BNNT), and the outmost n-type semiconducting molybdenum disulfide nanotube (MoS2NT). Moreover, when the inner SWCNT is metallic, the three-layer van der Waals hetero-nanotube is behaving like a metal-insulator-semiconductor tunneling diode. In the diode cases, the thickness of the middle BNNT layer is critical to ensure sufficient tunneling current. Besides, the insulating BNNT can also work as a dielectric layer for SWCNT transistors so that the two-layer SWCNT-BNNT van der Waals hetero-nanotube can be made into an efficient transistor with lower hysteresis and improved working stability. Furthermore, additional SWCNT layer outside of BNNT can enable gate-all-around field-effect transistor with the three-layer SWCNT-BNNT-SWCNT hetero-nanotube owing to the metallicity of large diameter SWCNTs.

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ACKNOWLEDGMENTS
Part of this work was supported by JSPS KAKENHI Grant Numbers JP20H00220, and by JST, CREST Grant Number JPMJCR20B5, Japan. Y. F. is financially supported by a JSPS Fellowship (P21364).

CS15

ELECTRICAL MONITORING OF ORGANIC CRYSTAL PHASE TRANSITION USING MOS2 FIELD EFFECT TRANSISTOR

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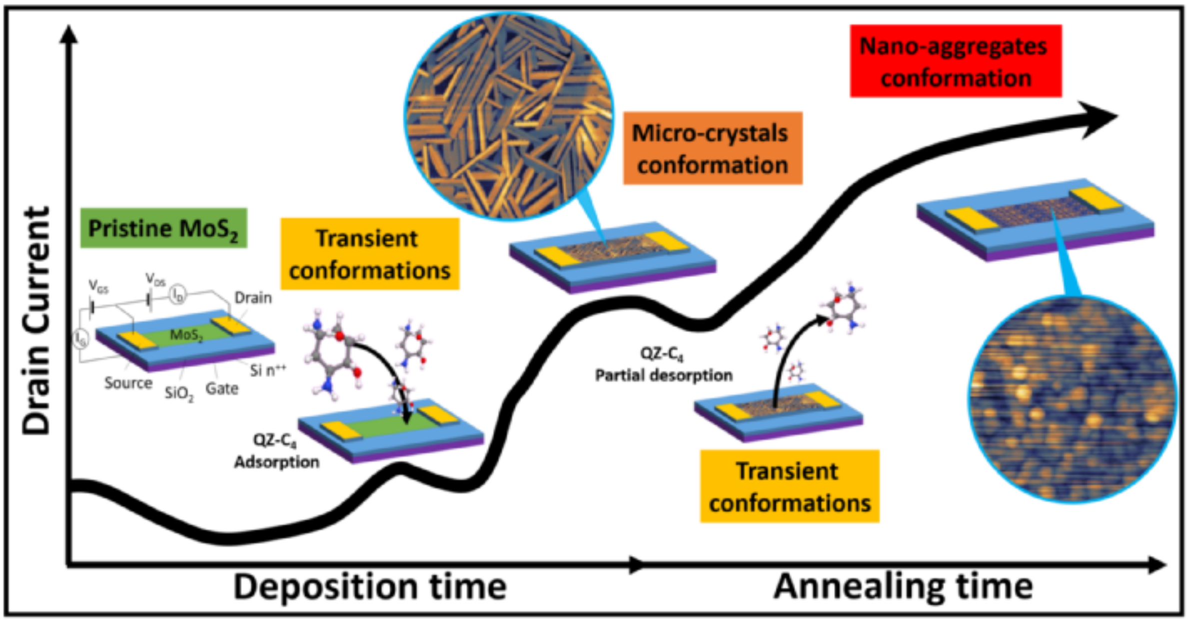
Hybrid van der Waals heterostructures made of 2D materials and organic molecules exploit the high sensitivity of 2D materials to all interfacial modifications and the inherent versatility of the organic compounds [1-3]. In this study, we are interested in the quinoïdal zwitterion/MoS2 hybrid system in which organic crystals are grown by epitaxy on the MoS2 surface and can reorganize in other forms after thermal annealing [4]. By means of field effect transistor measurements and atomic force microscopy, we demonstrate that the charge transfer between organic molecules and 2D materials strongly depends on the conformation of the molecular film. This work shows the great sensibility of MoS2 transistors for sensing molecular events occurring at the nanoscale providing a new experimental tool in addition to the usual microscopies and spectroscopies techniques.



Drain current at different stages. This figure shows the evolution of the drain current of the MoS2 transistor at different steps of the experiment, from deposition of the organic molecules to their annealing. This changes of the drain current allows us to follow the shapes of the crystals grown of the surface.

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CS16

EXPLORING THE BEST CVD CONDITIONS FOR GROWTH OF SMALL-DIAMETER SINGLE-WALL CARBON NANOTUBES USING AN AUTONOMOUS RESEARCH SYSTEM

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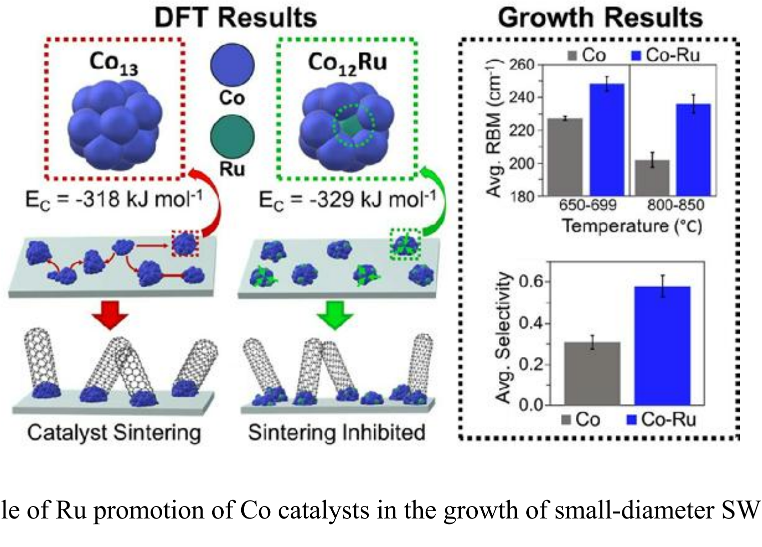
Due to the breadth of parameters that affect growth of single-wall carbon nanotubes (SWCNTs) via chemical vapor deposition, rapid experimentation is a powerful tool for investigating conditions for selective growth of small-diameter SWCNTs. Here we utilize an Autonomous Research System (ARES)—an automated, high throughput, laser-induced CVD system with in situ Raman spectral feedback—to study the roles of Ru promotion of Co catalyst and type of feedstock in the growth of small-diameter SWCNTs at different temperatures. We demonstrate through over 200 growth experiments in ARES and ex-situ multi-excitation Raman spectroscopic characterization that Ru-promoted Co catalyst nearly doubles the selectivity of small-diameter SWCNTs (diameters below 1nm) between growth temperatures of 650°C and700°C in comparison to pure Co. At elevated temperatures between 800 and 850°C, Ru stabilizes Co catalyst nanoparticles and increases the selectivity of small-diameter SWCNTs by almost a factor of three. Results reveal SWCNT diameters are not only dependent on the size of the catalyst but also on the precursor chemistry as selectivity towards small-diameter SWCNTs decreases in the following order: ethylene > acetylene (1% in He) > FTS-GP (Fischer-Tropsch synthesis gaseous product mixture). Density functional theory (DFT) simulations using 13- and 55-atom clusters with similar Ru/Co ratios provide mechanistic insight into the observed phenomenon, revealing increased cohesive energies of Co clusters after the addition of Ru irrespective of the location. Our findings indicate the presence of ~10% Ru in Co increases the sintering resistance and stability of small nanoparticles, as well as selectivity towards small-diameter SWCNTs.



Graphical abstract. Role of Ru promotion of Co catalysts in the growth of small-diameter SWCNTs.

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CS17

SYNTHESIS OF STRAIGHT SINGLE-WALL NANOTUBES DIRECTED BY ELECTRIC FIELDS IN AN ENVIRONMENTAL TRANSMISSION ELECTRON MICROSCOPE

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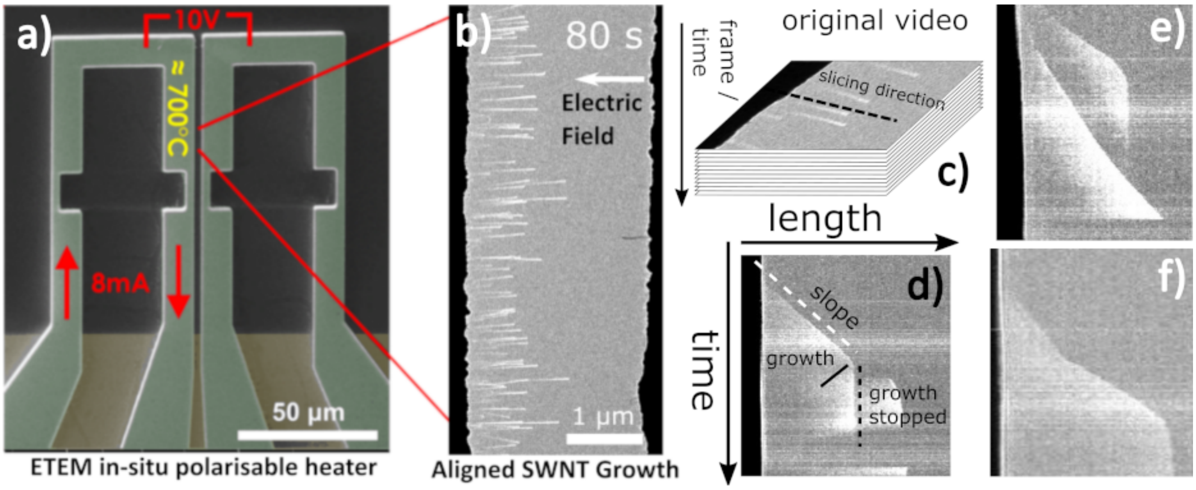
Real-time observations are presented of the aligning effect of electric fields on the synthesis by chemical vapor deposition of carbon nanotubes (CNTs) in an environmental transmission electron microscope (ETEM). The CNTs were grown within the gap of a micro-capacitor incorporated in a specifically designed heating micro-chip. Individual CNTs are easily resolved during this “Electric-Field-Directed-Synthesis” (EFDS) as they appear as extremely straight lines growing parallel to the field. They are predominantly Single Wall CNTs (SWNTs). Unprecedented excellent determination of their growth rates (R) are obtained and followed dynamically. Constant R is mostly observed but other behaviors are observed such as growth rate acceleration. For low applied voltages the growing SWNTs can cross the gap and connect to the opposite electrode upon which some are destroyed by mechanical failure or during the contact. For high applied positive voltages, Field Emission (FE) can occur and the lengths are limited within the gap because the FE leads to new saturation or destruction processes. This can result in the remarkable configuration where a nanotube can simultaneously grow at the base while it is evaporated at the apex. These first in-situ EFDS experiments allow us to envisage many complementary experiments eventually coupled with other characterization techniques such as HRTEM growth observations at the catalyst level or better characterization of the SWNTs produced to determine their metallic or semiconductor character and their chirality.



a) SEM image of the active part of the micro-chip. One cantilever is Joule heated and the second cantilever is polarized to apply the electric field in the gap. b) Observation of an EFDS for a polarization of +50 V. SWNTs appear as straight bright lines. c) Video processing to obtain kymographs for growth rates, R, measurements. d) kymograph obtained on a nanotube showing a constant rate of R = 22 nm/s. e) kymograph showing R accelerating. For the longer SWNT, R increases regularly from 11 to 20 nm/s. f) kymograph showing an abrupt R variation (16 to 33 nm/s).

CS18

ONE-DIMENSIONAL VAN DER WAALS HETEROSTRUCTURE: SINGLE-WALLED NANOTUBES OF TRANSITION METAL DICHALCOGENIDES ISOLATED BY BORON-NITRIDE NANOTUBES

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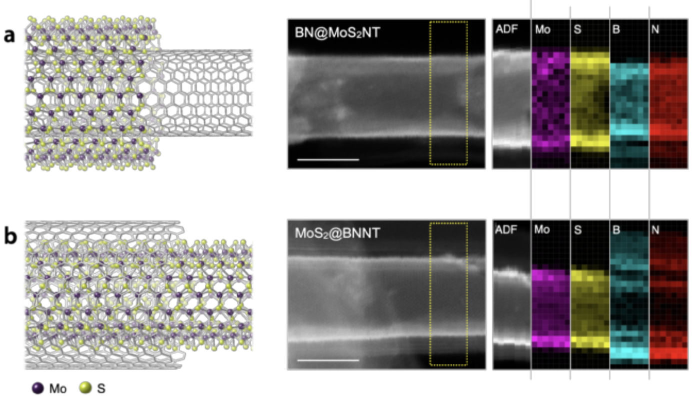
A wealth of chemistry and physics research on carbon nanotubes (CNTs) has spurred experimental and theoretical interest in inorganic nanotubes, particularly for transition metal dichalcogenides (TMDs). Single-walled TMD nanotubes (SW-TMDNTs) are expected to exhibit tunable electronic properties depending on their chirality and chemical composition, making them attractive for a variety of applications. However, conventional bulk syntheses exclusively produce multi-walled structures, and the structural and electronic properties of SW-TMDNTs have been much less explored. In contrast to the traditional syntheses, the recently developed template reactions have yielded crystalline SW-MoS2NTs wrapped around CNTs and boron-nitride nanotubes (BNNTs) [1,2]. In particular, insulating BNNTs (bandgap is ~6 eV) can serve as "nano-test-tubes" that hardly interfere with the intrinsic electronic properties of guest materials, while their practical use as 1D templates has been severely hampered by their poor dispersibility. Here we present a coaxial growth of SW-TMDNTs using BNNTs as templates. We have developed the surfactant-assisted preparation of well-dispersed BNNTs and the BNNT-templated synthesis of 1D van der Waals heterostructures [3]. Our methodology enables the versatile synthesis of TMDNTs with different diameters, chiral angles, and compositions [4]. By utilizing the inner space as well as the outer wall of BNNTs, we have synthesized SW-MoS2NTs with various diameters, including 5 nm or less. The few-nm-wide MoS2NTs are stabilized within protective BNNTs to facilitate their characterization. The chiral indices (n,m) of SW-MoS2NTs have been individually assigned by using transmission electron microscopy, and statistical analyses reveal a broad distribution of their chirality. The BNNT-templated reaction can be applied to extend the variations of their chemical constituents, such as selenides, ternary alloys, and Janus structures. Our study lays further groundwork for the study of structural and electronic properties of TMDNTs towards chirality-controlled synthesis and potential applications in optoelectronics.



Schematics and electron micrographs of single-walled MoS2NTs (a) wrapped around BNNTs and (b) confined within BNNTs.

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CS19

EFFICIENT CONTROLLED GROWTH OF SINGLE-WALL CARBON NANOTUBES AND THEIR DERIVATIVES

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Single-wall carbon nanotubes (SWCNTs) with uniform structures are highly desired for fabricating high-performance electronics. Great efforts have been devoted to controlled synthesizing structure-specific SWCNTs[1, 2]. However, there is a conflict between the growth efficiency and structural uniformity of SWCNTs prepared by chemical vapor deposition, which seriously limits their application exploration. We tried to figure out the reason by systematically investigating the thermodynamic and kinetic factors from a chemical reaction view. It was found that kinetic parameters should be matched with the catalyst with suitable size and composition[3], small-size metal nanoparticles with high thermal stability are critical for achieving efficient growth of structural uniform SWCNTs. To obtain SWCNT-based derivatives with fascinating properties, SWCNT was respectively used as a nanoreactor and template. SWCNTs were cut by defect-induced etchingand used as reactors to prepare WO_3 nanowire@SWCNTs with excellent radiation resistance[4]. Free-standing SWCNT@h-BN films were efficiently prepared by a defect-induced epitaxial growth mode[5]. This provides new insights and a platform for exploring the application of SWCNTs.

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CS20
GRAPHENE QUANTUM DOTS FOR CANCER THERAPY AND DIAGNOSTICS

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Graphene quantum dots (GQDs) are a class of carbon nanomaterials that can possess a number of advantageous properties engineered via controlled synthesis or functionalization. GQDs have recently found their use in many biomedical applications from disease detection to treatment and drug delivery. Cancer is one of the most prominent disease targets of carbon nanomaterials-driven therapeutic approaches due to its staggering mortality rate. However, the translation of GQDs into clinic has been hampered by their lower biocompatibility and accumulation-driven toxic responses. Our recent work is focused on the development of biocompatible and biodegradable GQDs synthesized from biological precursors and enabling near-infrared fluorescence image-based diagnostics. These GQDs are produced via a single-step hydrothermal microwave-assisted method allowing for concomitant doping, while retaining product biocompatibility at above 1 mg/mL concentrations. Metal-doped GQDs possess the capability ultrasonic contrast imaging that can be utilized for deeper tissue cancer diagnostic applications. The 10-fold ultrasound imaging enhancement is observed with metal-doped GQDs in tissue phantom as well as animal tissue. GQD intrinsic fluorescence can itself serve as a non-invasive diagnostic sensing tool, as it can be affected by the binding of different drugs, genes and biomolecules to the GQDs. This optical sensing mechanism is used in our work for identifying trace quantities of cancer-generated genes for early personalized cancer detection. Such sensor prepared from the GQDs complexed with the bait DNA sequence complementary to the target pancreatic cancer miRNA exhibits successful detection of the stem and loop portions of the target gene discriminating against non-complementary sequences. Therapeutic applications of the GQDs developed in our work involve both drug delivery and direct GQD-driven therapy. GQDs targeted to CD44 receptor overexpressed in a variety of tumors are utilized as drug delivery/imaging agents transporting redox therapeutics to breast cancer cells. While targeting increases local therapeutic concentrations, the electron rich GQD platform advantageously enhances the redox action mechanism of the delivered therapeutic. Direct cancer treatment applications developed with these GQDs include in vitro photothermal therapy. GQDs irradiated with 808 nm laser can increase the temperatures of local cellular environments up to 54.5°C sufficient to decrease HeLa cancer cell viability down to 22.9%. Successfully demonstrating cancer therapeutic, delivery and diagnostic capabilities, these biocompatible GQDs can help advance carbon nanomaterials to clinical applications.

CS21
THREE-DIMENSIONAL SINGLE-PARTICLE TRACKING OF SWCNTS AT DEPTH IN COMPLEX (BIO)ENVIRONMENTS

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The nanoscale architecture of living organs is often heterogeneous and tortuous. In the brain extracellular space (ECS), for instance, this complex maze is delimited by cellular walls where ions and signaling molecules diffuse, and its architecture is acknowledged to be important for proper function [1]. However, its precise structure is still mostly unknown. To address this challenge, recent advances in single-particle tracking based on SWIR emitting single-walled carbon nanotubes (SWCNTs) opened the avenue for exploring the ECS at the nanoscale at depth in living tissue [1]. However, in current approaches, the optical microscope point-spread function (PSF) limits the tracking of fluorescent nanoparticles to the two-dimensional imaging plane, restricting access to the axial information of the structure under study. PSF engineering can overcome this limitation by changing the shape of the PSF through phase modulation of the fluorescence signal [2], but it still needs to be adapted to the SWIR domain and in the context of dynamic imaging at depth. We will show how three-dimensional tracking of SWCNTs can be achieved using a customized double-helix phase mask [4] operating in the SWIR. Because nanotubes are not spherical objects, 3D angular diffusion of the nanotubes shall also be considered. Applications to the study of the brain ECS structure will then be presented.

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CS22

THERAPEUTIC TARGETING OF CDK4 KINASE IN PANCREATIC CANCER USING FUNCTIONNALIZED SINGLE-WALLED CARBON NANOTUBES

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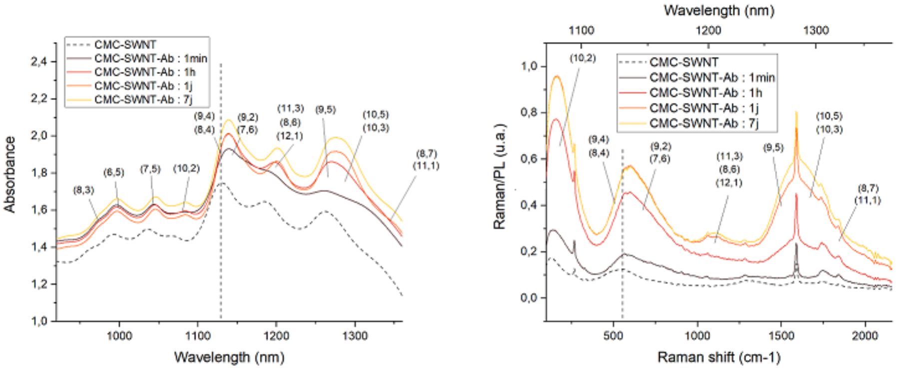
Pancreatic cancer is one of the deadliest cancers with an increasing incidence due to a lack of early-stage diagnostics and effective treatment [1]. The RAS/RAF/MAPK/CDK4 pathway is frequently dysregulated in pancreatic cancer and CDK4 constitutes an attractive target since several drugs (eg Abemaciclib, Ribociclib and Palbociclib) have been approved by the FDA to inhibit its activity [2,3]. However, these inhibitors are not efficient in. To propose an efficient therapeutic strategy to target CDK4 in pancreatic cancer, we propose to deliver Abemaciclib into pancreatic cancer cells using carbon nanotubes. Carbon nanotubes are promising materials for nanomedicine applications and especially for drug delivery [4]. Here, we study the adsorption of Abemaciclib onto single-walled carbon nanotubes (SWNT) dispersed in water using carboxymethylcellulose (CMC), for subsequent delivery of the drug into pancreatic cancer cells. The adsorption is followed by the changes in the optical signatures of SWNTs in the near-infrared (NIR) using coupled NIR absorption, photoluminescence and Raman spectroscopies [5]. We discuss the results in terms of changes of the dielectric environment of the nanotubes, leading to modulation of their excitonic and optical properties. In order to quantify the amount of adsorbed drug on SWNT, HPLC-MS measurements have been performed. In addition, we compared the adsorption kinetics and adsorbed amounts of Abemaciclib with those of Doxorubicin, another anti-cancer drug, which fluoresces in the visible. [6] We have further investigated the inhibitory potential of SWNT-Abemaciclib on proliferation of PANC1 cells and have determined the toxic threshold of SWNT dispersed in CMC.



NIR absorption (left) and Raman/PL (excited at 1064 nm, right) series of spectra probing the kinetics of adsorption of Abemaciclib on aqueous suspensions of SWNT dispersed with CMC

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CS23

NEAR INFRARED FLUORESCENCE LIFETIME IMAGING OF BIOMOLECULES WITH CARBON NANOTUBES

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Single wall carbon nanotubes (SWCNTs) are versatile building blocks for biosensors. Their fluorescence in the near infrared (NIR) enables detection of small molecules as well as proteins or pathogens in the NIR optical transparency window. The selectivity of such sensors is tailored by modification of their organic corona. Interaction of the corona with an analyte changes the fluorescence intensity of the sensor. However, optical signals like fluorescence intensities can be biased by external factors as sample movement or fluctuation in excitation light, which do not affect the other features of fluorescence signals such as the fluorescence lifetime.Here, we show that changes in the fluorescence lifetime can be used as a readout for sensing small molecules. Therefore, we tailored a laser scanning confocal microscope (LSCM) for NIR signals (>800 nm) and employed time correlated single photon counting (TCSPC). $(GT)_{10}$-DNA functionalized SWCNTs are known to increase their fluorescence in response to the neurotransmitter dopamine. Fluorescence lifetime (980 nm) of such sensors increases by up to 25 % with detection limits in the nM range. Applying the lifetime sensor as a paint covering cells, we were able to image extracellular dopamine. Utilizing a laser scanning confocal microscope reveals spatial information in 3D and also allows to trace the sensor response in a small confined volume to increase the temporal resolution. We demonstrate for the first time, that NIR fluorescence lifetime of SWCNTs can be used to monitor small molecules in solution. Furthermore, lifetime imaging with confocal microscopy allows detection of biomolecules in well-defined locations around cells. In perspective, this approach will help to gain deeper understanding of chemical signaling between cells.

CS24

CARBON NANOMATERIALS FOR BIOMEDICAL APPLICATIONS – A CASE STUDY

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Carbon nanotubes (CNTs) have been intensively researched for both fundamental studies and applications since its discovery about three decades ago. The diverse physical and chemical properties of CNTs are useful in various applications, such as electronics, automotive and aerospace vehicles, and biomedical systems. We found that the cytotoxicity of multiwalled carbon nanotubes (MWNTs) depend on their concentration, size, and surface chemical groups (e.g., -COOH). MWNTs and MWNT-COOH could accumulate in human lung macrophage cells (U937), but they did not produce overt cell toxicity within the concentration range of 5-50 µg/ml up to 24 h. However, there were morphological alterations at low doses of MWNT-COOH and significant reactive oxygen species (ROS) generation for MWNTs at higher doses, indicating a distinguished possible cellular stress response and DNA damage from both materials. MWNTs also induced DNA damage in mouse embryonic stem cells. These studies underpin subsequent research, which demonstrated that carbon nanomaterials could act as efficient phototherapy agents for a large variety of phototherapeutic applications, including cancer treatment.

CS25

CHARGE INDUCED EXCITON LOCALIZATION IN SEMICONDUCTING SINGLE-WALLED CARBON NANOTUBES

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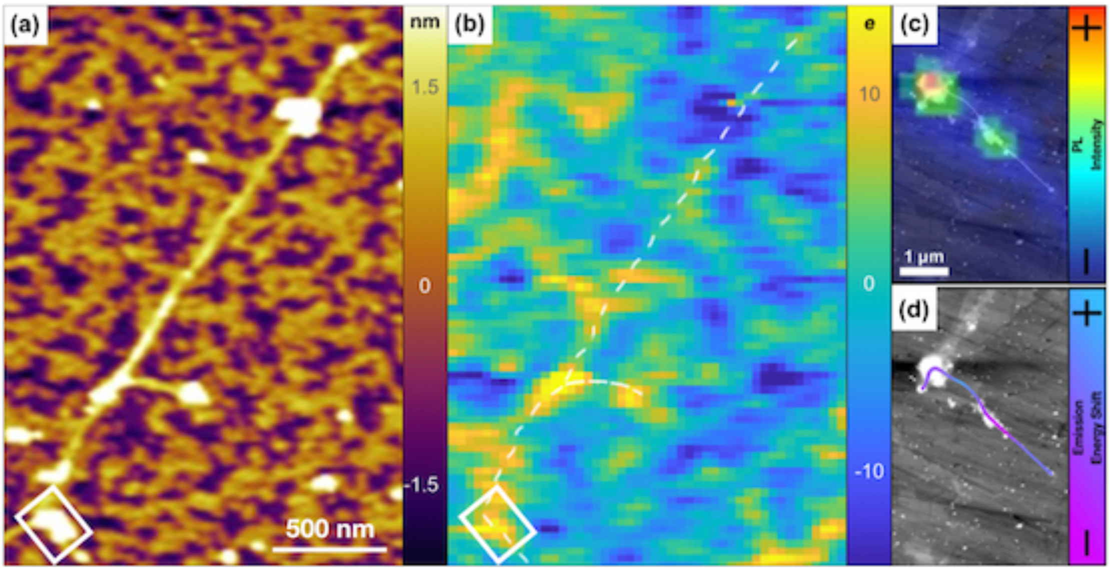
As-synthesized, semiconducting single-walled carbon nanotubes (SWCNTs) are nominally charge neutral. However, ionic surfactants that are commonly used to disperse SWCNTs in solution can lead to significantly charged aggregates adsorbed to the nanotube. In this presentation, we will discuss how electrostatic force microscopy (EFM) was used to characterize the static-charge interactions between an individual SWCNT and its local environment. We report nonuniform spatial charge distributions with highly varying magnitudes ranging between ±15 e associated with surfactant coverage on long SWCNTs (length >1.5 μm). EFM images acquired after resonant photoexcitation demonstrate charge carrier localization due to electrostatic interactions with charged surfactant aggregates. Charge densities as measured by EFM are used to estimate the depth of this electrostatically induced potential well, calculated to be on the order of hundreds of millielectronvolts, suggesting that surfactant charges heterogeneously covering SWCNTs provide traps for excitons potentially leading to their localization. This result is most apparent in our correlative AFM and single molecule optical measurements, showing that charged, surfactant-covered areas on the nanotube result in photoluminescence that is highly localized when compared to the NT length. The localized photoluminescence is significantly brighter, and has redshifted spectra by several nm, relative to neutral charge regions. This work provides the framework for controlling the photophysical properties of SWCNTs and has encouraged efforts to impart control over exciton localization.



AFM and PL images of SWCNT. (a) Topographic and (b) charge profile image of a sodium cholate coated SWCNT. The white box in (a) and (b) surrounds a surfactant aggregate with a calculated charge ~10 e per EFM resolution. (c) Correlated PL image overlaid onto an AFM topographic image. PL is (c) brighter and (d) redshifted at the sites of charged surfactant aggregates.

CS26
TUNABLE MAGNETIC INTERACTION IN HOMOBILAYER MOIRÉ TMDS

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Transition metal dichalcogenide hetero- and homobilayer moiré systems have established themselves as a versatile platform for exploring Hubbard model physics. Their constituent monolayers are notable for a single spin-valley locked pseudospin degree of freedom. However, heterobilayer moiré systems intrinsically break the layer degree of freedom, and most TMDs transition from direct to indirect bandgap semiconductors in the bilayer, complicating homobilayer moiré physics. Here, we employ magneto-optical measurements to probe a near-AA stacked homobilayer MoTe2 moiré system. Doping dependent photoluminescence reveals electric field tunable correlated states, and demonstrates the retention of a direct bandgap at the K and K' points in bilayer. Additional magnetic circular dichroism measurements show signatures of tunable magnetic interactions. The behavior demonstrated via this suite of optical probes establishes moiré MoTe2 as a promising platform for observing correlated and topological physics.

CS27
CHARGED INTERLAYER EXCITON CRYSTALLIZATION PHENOMENA IN BILAYER TMD HETEROSTRUCTURES

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We develop the theory of the crystallization phenomena for charged interlayer excitons (CIE) discovered recently in highly excited transition-metal-dichalcogenide (TMD) heterobilayers [1]. We derive the ratio of the average potential interaction energy to the average kinetic energy and discuss the ’cold’ long-range crystallization phase transition for the many-particle CIE system with and without a perpendicular magnetostatic field applied [2,3]. In zero-magnetic-field case, the strongly correlated phases are predicted — crystal and Wigner crystal for the unlike-charge and like-charge CIEs, respectively, — that can be selectively realized for TMD bilayers of properly chosen electron-hole effective masses by just varying their interlayer separation distance. In non-zero-magnetic-field case, we generalize the effective g-factor concept previously formulated for interlayer excitons [4] to include the formation of CIEs [2]. We show that magnetic-field-induced Wigner crystallization and melting of CIEs can be observed in magnetophotoluminescence experiments with TMD heterobilayes of systematically varied electron-hole doping concentrations (see Fig.1). Our results extend potential capabilities of TMD bilayer heterostructures and can be used for coherent photon emission control, charge transport and spinoptronics applications with this new family of transdimensional quantum materials [5-7].

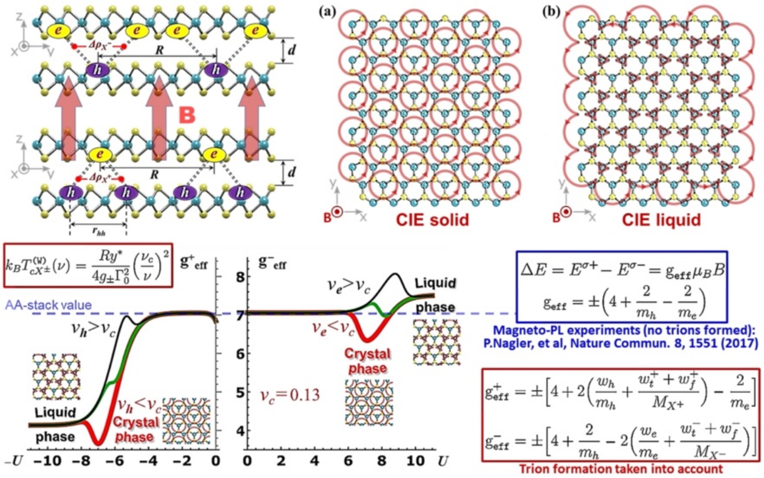

Fig.1. TOP LEFT: Schematic of TMD bilayers under study, with negative (upper bilayer) and positive (lower bilayer) CIE complexes subjected to a perpendicular homogeneous magnetostatic field. TOP RIGHT: Top view of the crystal phase (a) and liquid phase (b) for the negative CIEs in the strong magnetic field directed upward. BOTTOM: Effective g-factor behavior as predicted by the magnetic-field-induced Wigner crystallization model for the positive (left) and negative (right) CIEs in a generic AA-stacked TMD heterobilayer with doped carrier energy U in the strong field regime [line thickness increase indicates stronger field; nu_c=0.13 is the critical filling factor value; the upper (lower) sign in the equations on the right is for the AA(AB)-stacked bilayer].

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CS28

CAN EXCITON-PHOTON POLARITONS INCREASE THE DISTANCE AND EFFICIENCY OF ENERGY TRANSFER IN THIN FILMS OF CARBON NANOTUBES IN PHOTOVOLTAIC DEVICES?

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When strong optical absorbers with large exciton binding energy, like semiconducting carbon nanotubes, are embedded into an optical microcavity, new quasiparticles called polaritons are formed due to coupling between the exciton and microcavity photon modes. The polaritons have both excitonic and photonic properties, including the potential to be spatially delocalized like photons. The behaviors of carbon nanotube exciton polaritons in microcavities are just beginning to be explored,[1-3] including their potential usefulness in light harvesting devices.[4] We recently reported in Ref. 5 on the long-range energy transfer of excitons from (6,5) to (7,5) semiconducting carbon nanotubes across an insulating barrier 150 nm thick in an optical microcavity, mediated by moderate and strong exciton-photon polariton coupling and measured via two-dimensional, white-light spectroscopy. This result lends itself to a scientifically interesting and potentially technologically important question: Can exciton-photon polariton coupling increase the distance and efficiency of energy transfer in thin films of carbon nanotubes in photovoltaic devices? To answer this question, we have embedded nanotube-C_{60} photovoltaic devices in microcavities and quantified the efficiency of energy transfer to the nanotube-C_{60} heterointerface via photocurrent readout, as a function of nanotube film thickness and coupling strength. A moderate improvement both in incident photon to collected electron efficiency (ICPE) and adsorbed photon to collected electron efficiency (APCE) are indeed observed in the presence of both moderate and strong exciton-photon coupling. This result opens the door to new exciton and energy transfer physics in nanotube thin films and the potential for new routes for more efficiently leveraging nanotubes as the light harvesting components of photodetectors and possibly solar cells.

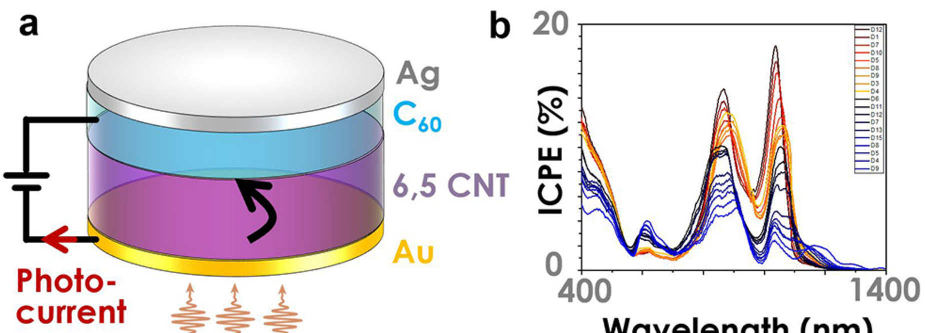

Fig. 1. (a) Nanotube (CNT) / C60 heterojunction in microcavity. (b) Representative ICPE data for different CNT film thicknesses.

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CS30

THEORETICAL STUDIES ON THE CHIRALITY CONTROL TOWARDS SINGLE-WALLED CARBON NANOTUBES

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Based on the unique structures and outstanding chirality-based electronic properties, single-walled carbon nanotubes (SWNTs) are regarded as one of the core candidates in the new-generation of carbon-based materials. Therefore, chirality-controlled growth of SWNTs is the paramount object in the field. We have been dedicating on the growth mechanism towards the chirality control and achieved a series of works. Thermodynamically, we have designed a new growth model, i. e. anisotropic growth when using W-based bimetal with high melting point as the catalysts[1-4]. Combining with the chirality-specific growth of (2m, m) when using metallic carbide as the catalyst, we have proposed the symmetry control mechanism[5] and further designed a new route for chirality control, i. e. symmetry control, dynamic control, and size control. Kinetically, we proposed the chirality mutation theory for conventional catalysts such as Fe, Co and Ni, which explained the experimental observation on the enrichment of near-armchair SWNT[6]. Based on the symmetry control mechanism[7], we further put forward symmetry-breaking theory for Pt group catalyst with larger atomic size and revealed the growth mechanism of armchair SWNTS that grows kinetically unfavorably on the Pt-group surfaces and predicted that the Pd might be the excellent catalyst for the growth of armchair SWNTs. In summary, we have consummated the chirality-specific growth mechanism on SWNTs and discover the key factor for chirality control, which can be used as the guide for the next experimental design.

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CS31
EXCITONIC EFFECTS IN ENERGY LOSS SPECTRA OF FREESTANDING GRAPHENE

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We unravel the importance of many-body effects on the finite momentum EELS (electron energy loss spectrum) of freestanding graphene by comparing very recent experimental measures obtained with high resolution in energy and momentum with ab initio calculations [1]. Calculations are performed at increasing levels of theory, elucidating the importance of the e-e interaction in the quasi-particle properties (included with the GW method) and the e-h interaction (included by solving the Bethe-Salpeter equation). Both interactions needs to be included in the description of the EELS spectrum to obtain a quantitative agreement with experiments, and we observe that while the excitation gap dispersion is dominated by e-e interaction, the dispersion of the π plasmon is governed by an expected constant e-e and an unexpected e-h interaction increasing with momentum transfer. Both the shapes of the onset and the π plasmon are significantly affected by the e-h effects. This project has received funding from the European Research Council (ERC) under the European Union’s Horizon 2020 research and innovation program (MORE-TEM ERC-SYN project, grant agreement No 951215.

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CS32
PREPARATION AND APPLICATION OF GRAPHENE GLASS FIBER

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Graphene glass fiber (GGF) is a new advanced graphene composite material developed through chemical vapor deposition (CVD) method with graphene covering on the surface of glass fiber. Glass fiber is a commercial lightweight structural material with high mechanical strength and flexibility, and has been widely used as a reinforcing material in aircraft, automobiles, etc. Considering the intrinsic excellent infrared properties of graphene and glass fiber, a dual-infrared-emitter design was reasonably constructed in this new composite. Dual-emitter GGF followed the law of gray-body radiation, showing high infrared radiation capability[1]. Meanwhile, the infrared radiation of GGF can be effectively modulated through the band structure engineering of graphene. Graphitic nitrogen doping can regulate the infrared emissivity of GGF from 0.96 to 0.68 under the premise of keeping high solar absorption[2]. This infrared radiation management showed promising potentials targeting the high-performance photothermal conversion for electric-energy-free crude oil collection.

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CS33

EXPLORATION OF GROWTH PARAMETERS FOR HIGH YIELD FCCVD SYNTHESIS OF SWCNT TCFS UTILISING TOLUENE AS CARBON SOURCE

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The outstanding optoelectronic properties of single-walled carbon nanotubes (SWCNTs) have made them perfect candidates for transparent conducting films (TCFs) over the last years. Following our last research work (Er-Xiong Ding et.al[1]) toluene was utilized as a carbon source for SWCNTs synthesis and the growth conditions were furtherly explored to understand better the effect of temperature, feeding rate and hydrogen flow on the sheet resistance of the manufactured SWCNT TCFs. All samples characterized through detailed optical and microscopy techniques and the chiral angles of them were determined via TEM electron diffraction patterns (ED). By optimizing the growth parameters of the reactor, extremely higher yields of SWCNT TCFs were achieved, making a determined step forward for industrial scale production of TCFs.

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CS34

EVALUATING THE EFFICIENCY OF BORON NITRIDE COATING IN SINGLE-WALLED CARBON NANOTUBE-BASED 1D HETEROSTRUCTURE FILMS BY OPTICAL SPECTROSCOPY

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Single-walled carbon nanotube (SWCNT) films represent exceptional optical and electrical properties, showing wide potential for scalable integrated devices [1]. Previously, we have demonstrated CVD synthesis of a one-dimensional heterostructure film, where an SWCNT film serves as a template, while boron nitride nanotubes (BNNT) and molybdenum disulfide nanotubes (MoS_2NT) are coaxially nested over the SWCNT networks [2].

Here, we further developed this synthesis method for successfully controlling the BNNT coating in SWCNT@BNNT heterostructure films. The morphology and crystalline structures of SWCNT@BNNT heterostructures were observed by scanning electron microscope (SEM) and high-resolution transmission electron microscope (HRTEM). Raman spectroscopy is a powerful tool for investigating the strain and doping effect of low-dimensional materials as was previously demonstrated by Lee et al. for graphene [3]. In this work, we use it for studying the strain effect induced by BNNT wrapping on the SWCNTs in the SWCNT@BNNT heterostructure film and demonstrate that the shifts of SWCNT's G and 2D (G') modes can be used as a probe of the efficiency of BNNT coating. In addition, we developed a vacuum annealing method to remove the initial doping effect on the SWCNTs caused by exposure to the ambient atmosphere and investigated the chemical doping effect of MoO3-doped SWCNT films by UV-Vis-NIR spectroscopy and Raman spectroscopy. This work will contribute to a better understanding of the strain and doping effect of SWCNTs, which will be useful for future applications of carbon nanotube-based one-dimensional heterostructures.

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CS35

ELECTRICAL PROPERTIES OF CARBON NANOTUBES BASED COMPOSITE 3D PRINTED BY DIGITAL LIGHT PROCESSING

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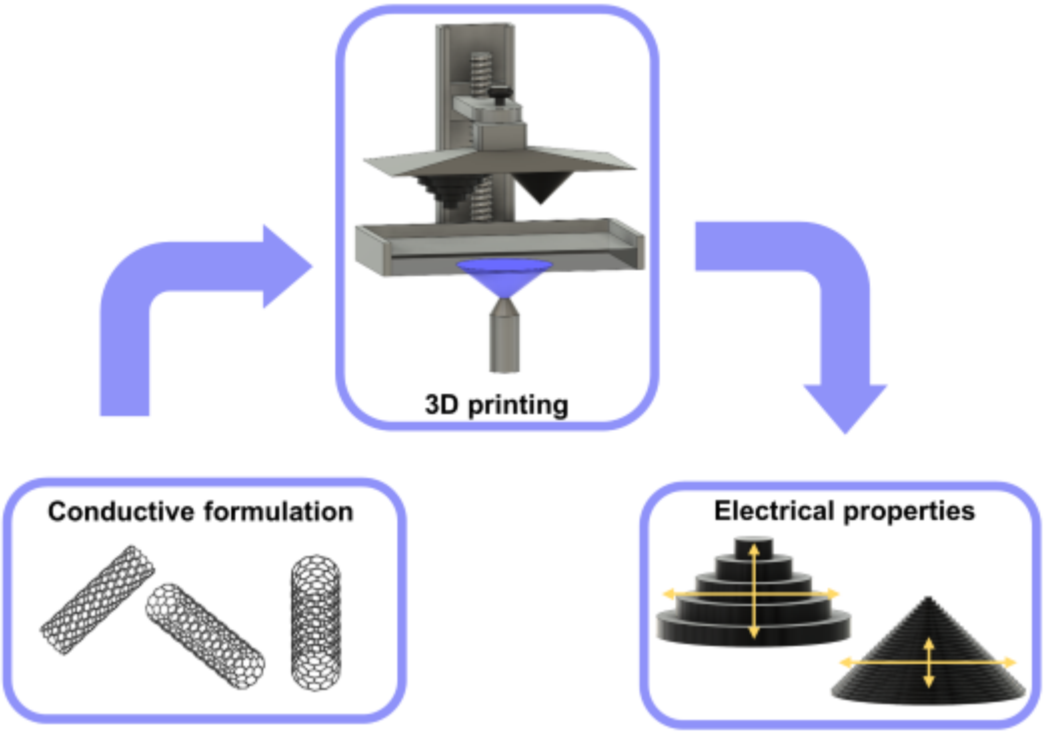
Digital Light Processing (DLP)[1] is an additive manufacturing technology based on a Vat photopolymerisation process. 3D objects are manufactured layer upon layer by projecting 2D light patterns onto a liquid photocurable resin. This fast and accurate process is usually limited to insulating and transparent resins. Loading resins with carbon nanotubes (CNTs) or graphene particles to make conductive and functional objects would significantly broaden the spectrum of applications of the DLP technology. However, several challenges are faced towards this objective. These challenges include the stabilization of nanocarbon particles into the resin, the achievement of acceptable transparency to UV-light in order to photo-polymerize the resin, and the realization of conductive materials formed by a percolation network. We will present work how these objectives can be met with the efficient dispersion of CNTs or graphene particles in acrylic resins [2], and the achievement of highly conductive materials. Special attention will be given to enhancements of electrical properties by thermal annealing and to the conductivity anisotropy of the 3D printed materials.



Schematic approach of conductor carbon nanotube composites made by Digital Light Processing and the impact on the electrical properties.

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CS36
MICRO AND MACROSCOPIC STRUCTURE EVOLUTION OF FEW-WALLED CARBON NANOTUBE BUNDLED NETWORK BY HIGH TEMPERATURE ANNEAL

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High temperature anneal is important to produce nanocarbon-based materials possessing superior functions and performances. However, a full understanding of annealed nanocarbon assembly structures has been challenging. We propose the micro and macroscopic structural analysis of 0.8-3.4 nm diameter few-walled carbon nanotube (CNT) bundled network in a multiple manner. The CNT films were annealed under Ar over 1200-3000°C as the case study. Up to 1800°C nanospace among nanotubes, i.e. interstitial channels important to design multiple functions, was secured by removing carbonaceous impurities. Beyond 1900°C nanometer-scale graphitic particles were formed on the nanotube bundles, then became micrometer size toward 3000°C. Along with the particle growth, small diameter (less than 1.2 nm) nanotubes became undetectable at 2200-2400°C with a reduction in available interstitial channels, finally creating the nontubular, graphitized network structures at 2600-3000°C. The anneal at 1200-1800°C can provide the high purity CNT bundled network structures, and the higher temperature anneal formed the high crystallinity graphitized network structures (Figure). To elucidate the structural evolution, we utilized 14 different analytical approaches, and two-dimensional correlation analysis from the collected data clarified the synchronous and asynchronous structural parameters along the annealing temperature. Thus, the structural alteration was found to occur in 3 phases of 1200-1800°C, 1900-2400°C, and 2600-3000°C. On the other hand, the structure change gradually decreased the electrical conductivity of the CNT film. Our findings would advance carbon material science and pave a way toward nanocarbon applications with the films, fibers, and composites [1].

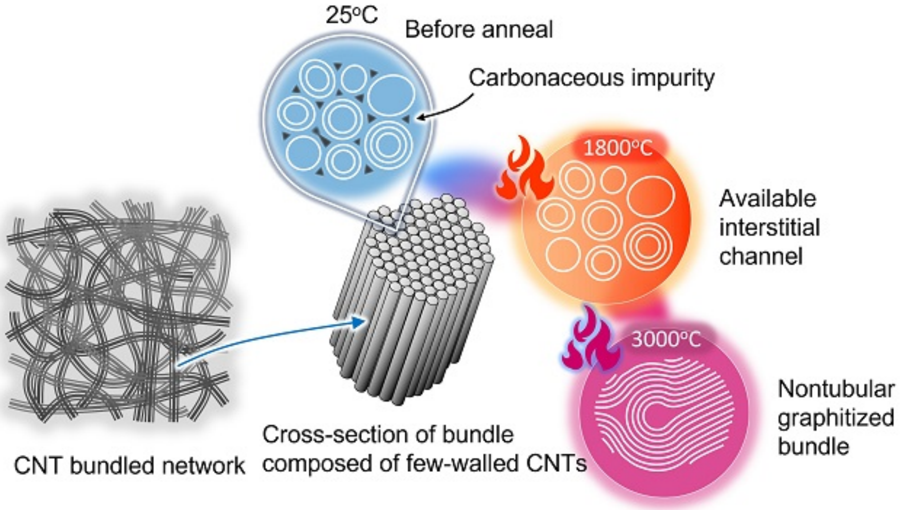

Figure. Scheme on structure evolution of few-walled CNT bundled network by high temperature anneal.

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CS37

ISOLATION OF THE (6,5) SINGLE-WALL CARBON NANOTUBE ENANTIOMERS BY SURFACTANT-ASSISTED AQUEOUS TWO-PHASE EXTRACTION

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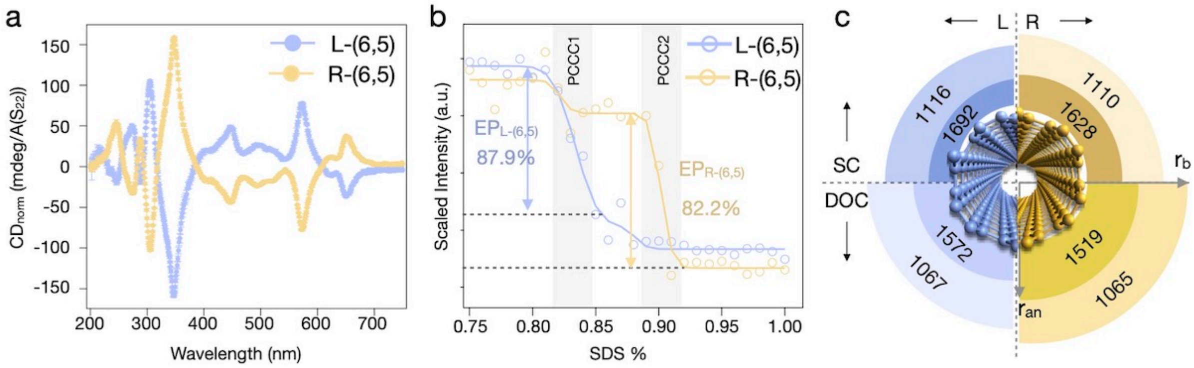
Sorting single-chirality enantiomers is the ultimate goal of single-wall carbon nanotubes (SWCNTs) separation. Although several approaches have been used to produce enantiomeric separation,[1,2] developing a technique with both high accuracy and efficiency is still a challenge and the underlying mechanism requires further in-depth investigation. In this work, aqueous two-phase extraction (ATPE) is used to obtain highly purified (> 80%) left- and right-handed (6,5) SWCNTs with limited experimental steps.[3] The optimized surfactant conditions are studied, and analytical ultracentrifugation (AUC) and near-infrared photoluminescence (PL) measurements are used to examine the surfactant wrapping and partition coefficient change conditions (PCCCs) required for separation (see Fig.1). Our study provides valuable insights into the underlying mechanisms behind surfactant-assisted SWCNT separations and facilitates the use of SWCNT enantiomers in fundamental studies and applications in the future.



(a) CD spectra of the L-(6,5) and R-(6,5) prepared by ATPE. (b) PL intensities of the L- and R-(6,5) as a function of SDS concentration for the DOC/SC/SDS ternary-surfactant system. (c) Schematic illustration of anhydrous radius (inner and dark-color circles) and buoyant radius (outer and light-color circles) for L- and R-(6,5) with DOC and SC respectively. Anhydrous densities and buoyant densities (kg/m3) of L- and R-(6,5) in different surfactants are also marked in the circles.

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CS38
TOWARD HIGH-PURITY SORTING OF SINGLE-CHIRALITY SWCNTS WITH STEPWISE EXTRACTION STRATEGY

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Single-chirality SWCNTs (sc-SWCNTs) are promising materials for upcoming electronics and optoelectronic applications in the post-Moore era. In particular, single-chirality SWCNTs with diameters distributed in a range of 1.2-1.4 nm have been regarded as ideal candidates for nanoscale FETs due to their structure and electrical properties. However, the isolation of sc-SWCNTs becomes rather challenging when the diameter of the nanotube is greater than 1.0 nm. Herein, a stepwise extraction strategy is introduced as an effective approach for the selective and precise separation of single-chirality SWCNTs. Some novel methods have been developed based on stepwise extraction strategy. With these combined methods, several monochiral species were successfully obtained. Three pyridine-containing copolymers with different copolymer units or functional groups, successfully achieved the isolation of (9,8) (10,8) and (12,5) SWCNTs with all the diameters around 1.2 nm at high single-chirality purity (82%, 92.3%, and 95.6%, respectively). In summary, regulating the conjugated structure provides the basis for selectivity determination, and controlling the start materials at each step during separation is critical to the stepwise extraction strategy.

CS39
THE STRUCTURAL COLORATION OF CARBON NANOTUBES

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Carbon nanotubes (CNTs) are promising candidates for numerous cutting-edge fields because of their excellent properties. However, the inherent black color of CNTs cannot satisfy the aesthetic/fashion requirement, and the flammability of CNTs severely restricts their application in high-temperature environments with oxygen. Here, we realized a structural coloration of CNTs by coating them with inorganic oxides layers. By tuning the layer thickness, both CNT fibers and membranes exhibited controllable and brilliant colors. The structural coloration of CNTs substantially improves their performance and broadens their applications.

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CS40

N-TYPE DOPED DRY-SPUN FEW-WALLED CARBON NANOTUBE YARNS FOR THERMOELECTRIC ENERGY HARVESTING

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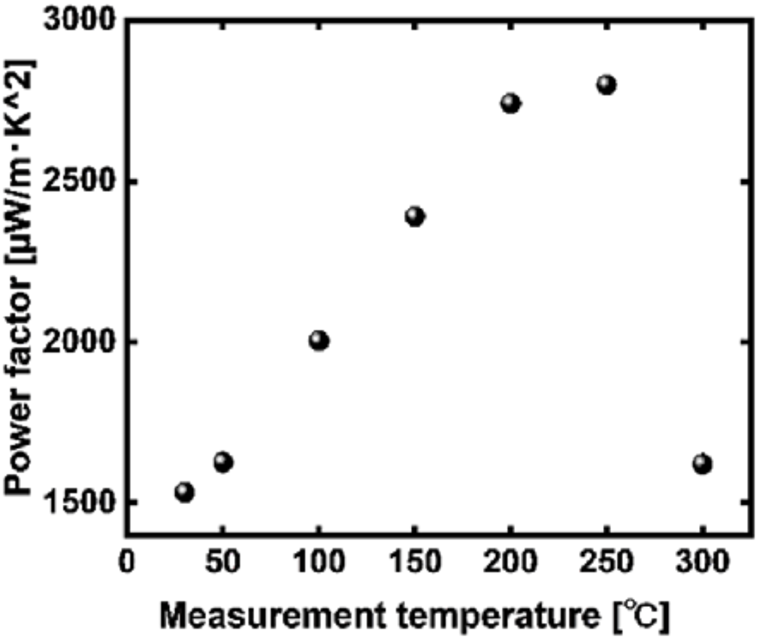
Carbon nanotube (CNT) spun yarn is a potential thermoelectric (TE) material owing to its narrow band-gap energy, high charge carrier mobility, and excellent mechanical property, which is conducive for flexible and wearable TE devices. As-grown CNT yarns exhibit *p*-type properties. Therefore, a high-performance and long-term stable *n*-type doping method is necessary. In this presentation, we report the results of applying 1,3-dimethyl-2-phenyl-2,3-dihydro-1 H-benzimidazole (N-DMBI) [1], which has recently attracted attention as a high-performance n-type doping agent, to CNT yarn. CNT yarn treated with joule heating was doped with N-DMBI in various solvents and conditions, and the *n*-type doping properties were evaluated and investigated. Based on Raman spectra, the crystallinity of CNT yarns was significantly improved by electric joule heating treatment at a high temperature of 3170 K for one second. After doping with various solvents that dissolve N-DMBI, it was found that 1,2-dichlorobenzene could be used as a solvent to achieve a high doping effect without any post-immersion heat treatment. A high power factor (PE) of 1534 $\mu W/m\text{-}K^2$ at around 30 °C was obtained by optimization of the N-DMBI solvent, the crystallinity of the CNTs, and the doping time. A PE of 2390 $\mu W/m\text{-}K^2$ was obtained at 150 °C, where N-MDBI doping is thermally stable. Finally, a *p*-type TEG with 20 windings made of as-grown *p*- and *n*-type CNT yarn was fabricated and operated at a temperature difference of 20 °C, yielding a maximum power of 5.7 nW.



Thermoelectric properties of n-type CNT spun yarn. Thermoelectric properties of n-type CNT spun yarn doped with N-DMBI measured at various temperatures.

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CS42

A HIGH-RATE SUPERCAPACITOR WITH A 90% CAPACITANCE RETENTION AT -100 °C ENABLED BY A HYBRID-ALIGNED STRUCTURAL DESIGN

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In the development of low-temperature storage devices, ultralow-temperature tolerance, rate performance, and the trade-off between performance and working temperature represent critical obstacles, which stem from the problem of inhibited ion mobility.[1-3] Here, we report a unique hybrid aligned CNT structure where adjacent aligned bundles with large space connected with traversing CNTs were synthesized in a single assembly. This architecture affords the formation of highly orientated ion-transport channels due to its large and low tortuous ion-transport channels. Neutron scattering in conjunction with other techniques revealed that the presence of orientated macropore channels created by the specially designed hybrid aligned CNT architecture was the key for the enhanced electrolyte permeability, even allowing electrolyte to be infiltrated into the deepest inner volume of the electrode, thereby mitigating the degradation of ion kinetics at low temperatures. At -100 °C, a capacitance retention of 90% was achieved at a scan rate of 20 mV s^{-1}, breaking the commonly observed trade-off between the electrochemical performance and working temperature. Finally, a highest-reported power density of 40 kW kg^{-1} and an energy density of 75.3 Wh kg^{-1} were presented at -100 °C, far surpassing the previously reported low-temperature supercapacitors.

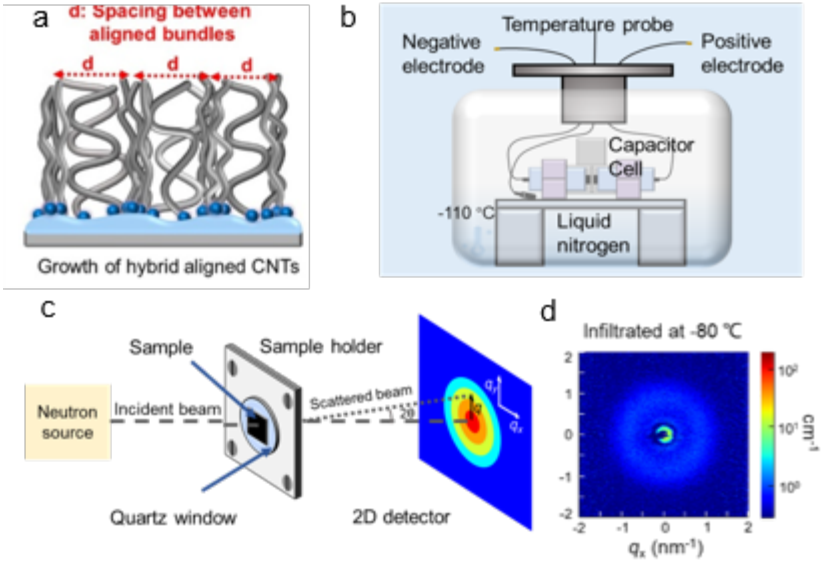

Figure 1. Structure design of a) hybrid aligned CNTs, b) Device assembly, c) Schematic of experimental setup for SANS measurements of electrolyte-infiltrated CNT electrodes, d) 2D SANS images for the hybrid aligned CNTs after electrolyte infiltration at -80 °C.

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CS43
QUANTIFICATION OF SP³ DEFECTS IN DIFFERENT (N,M) SPECIES OF SINGLE-WALL CARBON NANOTUBES BY RAMAN SPECTROSCOPY

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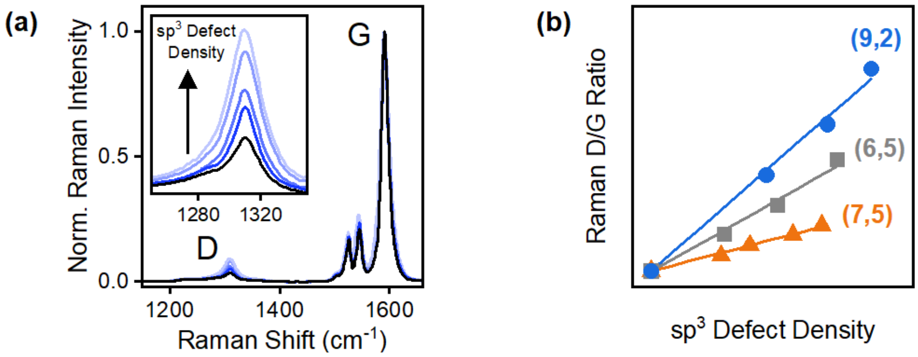
The controlled functionalization of semiconducting single-wall carbon nanotubes (SWCNTs) with luminescent sp^3 defects leads to increased photoluminescence (PL) quantum yields and single-photon emission in the near-infrared due to efficient trapping of fast-diffusing mobile excitons. While the choice of reaction parameters allows for a precise control of binding configurations and PL emission wavelengths of these sp^3 defects [1,2], the direct quantification of their number density in SWCNTs is very challenging. We have recently introduced an absolute quantification method for sp^3 defects in (6,5) SWCNTs by combining the change of the integrated D/G ratio in Raman spectra with the calculated sp^3 defect densities obtained from PL quantum yield measurements [3]. Here, we expand this approach to other SWCNT species and show that the linear relation between Raman D/G ratios and calculated sp^3 defect densities remains valid for a variety of chiralities. We also demonstrate that in addition to the characteristic D-mode, other defect-activated modes in the Raman intermediate frequency region also scale linearly with the sp^3 defect density. Furthermore, the dependence of the Raman D-mode intensity on excitation energy is examined to enable an excitation energy independent quantification of sp^3 defects in SWCNTs via Raman spectroscopy.



Raman data of functionalized SWCNTs. (a) Raman spectra of (6,5) SWCNTs with different degrees of sp3 functionalization. (b) Linear correlation of the integrated Raman D/G ratios with the calculated sp3 defect densities for different SWCNT chiralities.

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CS44
PROPERTY ANALYSIS OF 1D AND 2D NANOSTRUCTURES USING IN SITU TRANSMISSION ELECTRON MICROSCOPY

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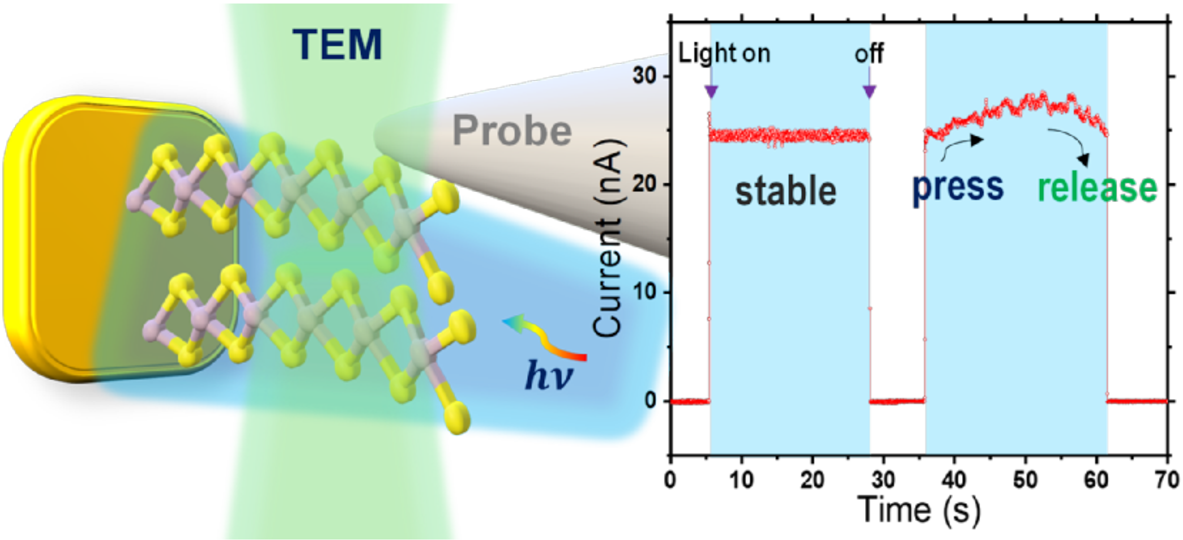
Carbon and boron nitride nanotubes, transition metal dischalogenide and MXene nanosheets are engineered and studied in a high-resolution transmission electron microscope using various *in situ* TEM holders and manipulators. Electromechanical properties of nanotubes and nanosheets are analysed using a mechanical resonance technique while applying alternating currents to the electrode assembled within the *in situ* electrical TEM holder frame[1], and/or direct tensile tests on nanostructures within the TEM column (Young's modulus, tensile strength, fracture toughness)[2], and three terminal transistor-like electrical setups (metal-to-semiconductor transitions)[3]. In addition, optomechanical and optoelectronic responses of molybdenum selenide nanosheets bent in different crystallographic directions inside the TEM column are measured while using light illumination through the optical fiber inserted into the pole piece of the electron microscope[4]. The author is grateful to many former and current group members, in particular, to Drs Xin Zhou, Ovidiu Cretu, Daiming Tang, Mingsheng Wang, Xianlong Wei, Naoyuki Kawamoto, Masanori Mitome and Yoshio Bando (NIMS, Japan), and Drs Chao Zhang, Joseph Fernando and Konstantin Firestein (QUT, Australia) for their key experimental contributions to the *in situ* TEM projects over the years.



Experimental setup inside the transmission electron microscope for analysis of optoelectronic and optomechanical properties of MoSe2 nanosheets under in situ TEM deformation.

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CS45

BNNTS FILLED WITH DYES EMITTERS: IN AXIS MODULATION OF THE LUMINESCENCE THROUGH MECHANICAL STIMULI

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Single walled carbon nanotubes (SWCNTs) have been used as a 1D template for assembling various organic and inorganic compounds thanks to their hollow, crystalline and cylindrical architectures. However, It has been demonstrated that the overlap of the emission bands of the adsorbed dyes with the absorption bands of semiconducting nanotubes in the visible range (2-3 eV) leads to effective energy transfers that both readily quench the dyes fluorescence and sensitize the nanotube host.[1,2] As other material candidate, boron nitride nanotubes (BNNTs) have been used as template for fluorescent molecular assembly, capitalizing on their wide-gap semi-conductors of 5.5 eV.[3] In this presentation, we will first discuss on the polarization properties of the luminescence of confined sexithiophene 6T molecules inside BNNTs : Combining aberration corrected high resolution transmission electron microscope (ac-HRTEM) analysis and polarized micro luminescence imaging, we will explain why extinction ratio values of the polarization as high as 700 at room temperature can be reached in 6T@BNNTs. We will also show that this polarization property at the nanoscale can be expanded in macroscopic transparent polymeric thin films loaded with aligned 6T@BNNTs.[4] In a second part, we will present that mechanical stretching could induce a strong modulation of the luminescence signal along the axis of a 6T@BNNT. We will show that this mechanism leads to the formation of periodic luminescent chains of aligned molecules with chain lengths ranging from 400 nm to 2 microns.[5] (Fig1) Finally, we will demonstrate that a deterministic positioning of this in-axis modulation of the luminescence can be obtained through photo-induced mechanism, leading to single to aggregated emitters aligned along the BNNT axis.[6]These results open the doors to customizable and deterministic positioning of emitters for encoding light in advanced photonics building blocs.

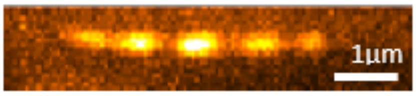

Figure 1. Example of periodically encoded dipolar chain inside an individual BNNT. Confocal luminescence image recorded at 600 nm.

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CS46

CHARACTERIZATION AND MODULATION OF THE INTERLAYER INTERACTIONS IN 2D MATERIALS AND THEIR HETEROSTRUCTURES

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The interlayer van der Waals (vdW) interactions are critical in determining the novel properties of two-dimensional (2D) materials and their vertical heterostructures. Therefore, a precise and quantitative characterization and modulation of the interalyer vdW interactions is essential for both scientific research and applications. In this presentation, a novel scanning probe microscopy technique, namely Angstrom Indentation (Å-I) will be introduced. Å-I enables non-destructive indentation at the Angstrom scale, facilitating the extraction of interlayer elasticity from the force-indentation curves. The interlayer elasticities of various 2D materials were obtained using this method [1]. Additionally, an ultrahard monolayer diamond structure driven from bilayer graphene by Å-I was observed. Local high pressure applied through an atomic force microscope tip on epitaxial bilayer graphene on SiC(0001) induced interlayer sp^3 covalent bonds forming, eventually creating a novel monolayer diamond structure. The elastic modulus of this monolayer diamond was found to be around 1TPa, close to the value of cubic diamond. First principle calculations along with nano-hardness measurements demonstrate that the graphene-diamond phase transition is reversible and cannot be activated when the epitaxial graphene is thicker than 3 layers [2]. The second part of the presentation is focused on the graphene/h-BN vdW heterostructure. We used diamond anvil cell (DAC) to apply up to 10GPa hydrostatic pressure to modulate the band structure of the graphene/h-BN moiré superlattices. Our findings showed that high pressure compresses the interlayer space and enhances the interlayer interactions and the inversion asymmetry, thus effectively tuning the graphene band structure. We were able to enlarge the primary Dirac gap of graphene in the large-twist-angle superlattices from 30meV to 80meV at 8.3GPa and re-open the pre-closed secondary Dirac gap in valence band at 7GPa [3].

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CS47

GAS PHASE CATALYST FREE SYNTHESIS OF LOW-DIMENSIONAL MOS2: A MOLECULAR DYNAMICS STUDY

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Low dimensional (1D and 2D) materials, especially transition metal dichalcogenides such as MoS2, are materials that have seen significant interest in the past two decades due to their unique properties. These properties differ significantly from bulk properties due to their unique structure and quantum confinement effects. Bulk MoS2 is a indirect-gap semiconductor, while monolayer MoS2 is a direct band gap semiconductor and MoS2 nanotubes exhibit tunable band gaps depending on the number of walls, diameter, and chirality [1]. The chemical vapor deposition (CVD) synthesis of TMD materials has proven effective at making high quality, yield and purity TMD nanomaterials. There is a need however to circumvent issues associated with post-synthesis transfer, which can introduce structural defects into the material. In this work we investigate the mechanism of catalyst-free floating CVD MoS2 synthesis [2]. MoO3, S2 and varying amounts of H2 gas were modeled using the tight-binding method GFN-2xTB molecular dynamics. Results show the MoO3 clustering with sulfur binding to the oxygens outside the MoO3 cluster. The amount of Mo-O bonds steadily decrease while Mo-S bonds increase, which shows MoS2 beginning to form by sulfur removing oxygen from the Mo. Hydrogen acts as an inhibitor, binding to the Mo and preventing Mo-S bonds from forming. The results are consistent of preliminary formation of catalyst free floating CVD MoS2

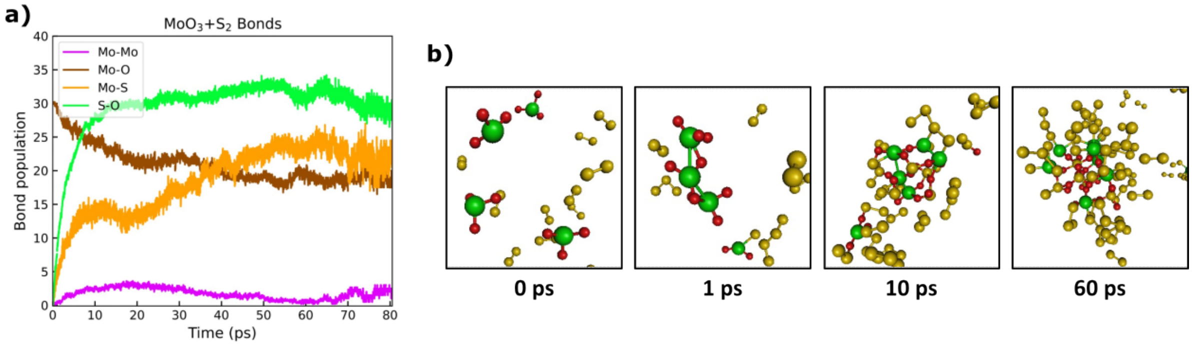

Figure 1. a) Average bond population from the MoO3 + S2 molecular dynamics simulation and b) snapshots showing (from left to right) the initial conditions, agglomeration of MoO3, clumping of S2 around the MoO3 and lastly the S moving O away from Mo.

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CS48

EXPLORING THE BISTABLE GROWTH OF CARBON NANOTUBES: INSIGHTS FROM A SIMPLE MODEL AND KINETIC MONTE CARLO SIMULATIONS

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Recent experiments have revealed a fascinating aspect of carbon nanotube growth on catalytic transition metal nanoparticles by chemical vapor deposition, where the growth proceeds in a bistable manner with alternating segments of fast and slow growth [1]. The growth rate factor between the two regimes is found to be around 1.7, which is observed to be remarkably universal, i.e., independent of the catalyst nanoparticles [1-3]. Additionally, the switches between the two growth regimes occur at random instances, which suggests that they are not related to fluctuations in temperature, pressure, or chemical potential of the carbon feedstock in the growth chamber [3]. To shed light on this intriguing phenomenon, we have developed a simple yet powerful growth model for carbon nanotubes, based on the assumption that the number of carbon atoms at the edge of the nanotube in contact with the catalyst remains constant. On this basis, different configurations of tube edges are explored, with two distinct families of possible types of edges emerging: those with a high amount of so-called armchair motives, where the tube edge is mostly perpendicular to the tube axis, and those with a high amount of zigzag edges, where the tube axis and the normal of the edge form the largest angles. Importantly, insertion sites are much more abundant in the former case, leading to higher growth rates. By comparing the growth rates of these two families of edge configurations, we have recovered the factor of around 1.7 [3]. These considerations are thus based much on considerations pertaining to configurational entropy [4].

In a second step, we have developed more detailed kinetic Monte Carlo simulations based on insertion and removal barriers for pairs of carbon atoms on zigzag or armchair motives within the tube edges [4]. An additional bistability term that separates the two growth regimes is added to the energetic model. It accounts for the fact that flat tube edges better conform to the shape of the catalyst than edges with a hyperbolic paraboloid shape (similar to Pringles chips) [3]. These shapes occur in case of edges at the interface between the two growth regimes, but are repressed due to the energetic penalty due to shape mismatch and keep the growth limited to one of the two growth regimes for a certain amount of time. With these KMC simulations, we explore the growth kinetics of carbon nanotubes in the relevant diameter range of 0.75 - 2 nm.

Overall, our work explores the intriguing bistable growth of carbon nanotubes and provides a framework for further investigations.

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CS49

IN-SILICO TENSILE TESTING OF CNT NANOFILMS: THE EFFECT OF ALIGNMENT

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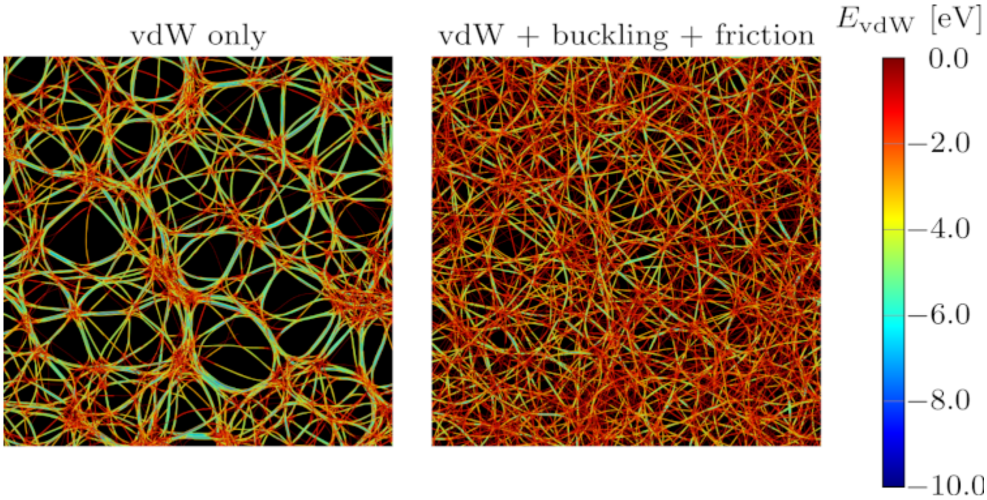
It is known that aligned carbon nanotube (CNT) materials far outperform their unaligned counterparts in terms of mechanical stiffness and strength, see e.g. [1]. While this general trend is observed qualitatively in experiments, it remains difficult to isolate the effects of alignment from those of densification, and to accurately control the degree of alignment in a CNT material. Here, we present a computational study of the effect of alignment on the mechanical properties of CNT nanofilms where we address some of the limitations found in experiments. The CNT nanofilms are simulated using the newly updated version of the MESONT package [2] in LAMMPS, in which CNTs are modelled as elastic chains of interacting cylindrical segments. The mesoscopic forcefield employed in the package accounts for bending-buckling and van der Waals (vdW) interactions. We also present a new mesoscopic model for inter-tube friction which we parametrise using atomistic simulations of CNTs. By investigating the effect of bending-buckling and inter-tube friction, we show that both effects greatly inhibit bundle formation and produce finer network structures compared to simulations in which bending-buckling and friction are neglected (see Fig.). To study the effect of alignment, network structures at specific degrees of alignment are generated and subjected to simulated tensile testing. We demonstrate that in CNT nanofilms, tensile strength and stiffness of the material scale exponentially with the Chebyshev orientation order parameter [3]. Finally, we map our results onto a simple bond percolation model, showing that alignment mainly enhances the load-bearing fraction of CNTs in a nanofilm. Hence, we show that alignment alone (rather than densification) is key in bringing the exceptional properties of individual CNTs to the macroscale.



CNT nanofilms generated using the MESONT package, with and without bending-buckling and friction. The colours indicate the vdW energy, a proxy for bundle thickness.

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CS50

HIGH-PERFORMANCE COMPLEMENTARY TRANSISTORS BASED ON ALIGNED SEMICONDUCTING CARBON NANOTUBE ARRAYS

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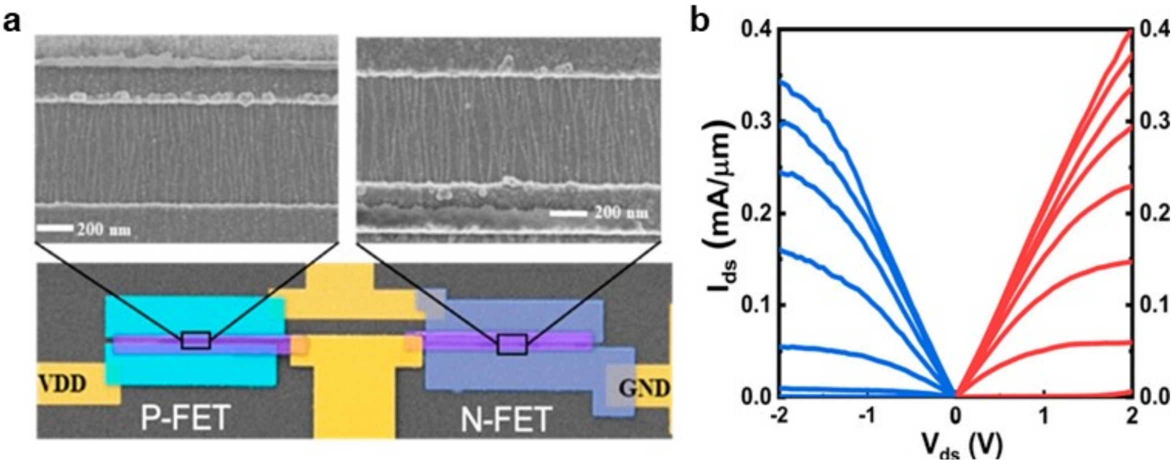
High-density semiconducting aligned carbon nanotube (A-CNT) arrays are promising materials for digital integrated circuits (ICs), and high-performance A-CNT p-type field-effect transistors (P-FETs) have been demonstrated with extraordinary electronic performance [1]. However, high-performance A-CNT n-type FETs (N-FETs) have not yet been implemented. In this work, we reveal the mechanism hindering the realization of A-CNT N-FETs contacted by low-work-function metals and develop corresponding solutions to promote the performance of A-CNT N-FETs to that of P-FETs. The fabricated Scandium (Sc) -contacted A-CNT N-FET with a 100 nm gate length exhibits an on-state current (I_{on}) of 800 μA/μm and a peak transconductance (g_m) of 250 μS/μm, representing the highest performance of CNT-based N-FETs to date. Moreover, CMOS technology has been developed to realize N- and P-FETs with symmetric high performance based on A-CNTs. The fabricated A-CNT CMOS FETs show electron and hole mobilities of 325 and 241 $cm^2V^{-1}s^{-1}$, respectively, which are slightly higher than the corresponding values of Si CMOS transistors. Our scalable fabrication of A-CNT CMOS FETs with comparable electronic performance to Si CMOS will promote the application of CNT-based electronics in digital ICs [2].



Doping-free CMOS FETs based on A-CNTs. (a) False-color SEM images of a typical CMOS inverter with a gate length of 500 nm for both P-FET and N-FET; the enlarged SEM images present the details of channel regions. The scale bar is 200 nm. (b) Output characteristics of the same N-FET (red) and P-FET (blue) in (a).

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CS51

DOPING TO OVERCOME THE N-TYPE CONTACT CHALLENGE IN HIGHLY-SCALED HIGH-PERFORMANCE CARBON NANOTUBE TRANSISTORS

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High mobility and tunable bandgaps in carbon nanotube transistors have attracted interest for logic applications where low contact resistance (R_C) is necessary to preserve the excellent transport of the channel material [1-3]. Palladium metal has been shown to deliver excellent performance as a p-type contact for highly-scaled CNT transistors, with R_c = 6.5 kΩ for contact length (L_C) of 10 nm [4]. However, the leading method for low resistance n-type contact to CNT uses low-workfunction metals (e.g. Scandium, Hafnium, Erbium) which have a small Schottky barrier for electron conduction but struggles with poor yield and high resistance at short L_C due to the tendency to scavenge oxygen from air and surrounding dielectrics [5,6]. This talk will report a novel strategy to utilize stable metals with an excellent interface to the CNT and apply strong n-type doping near the contact to achieve transparent electron tunneling through the Schottky barrier. We first demonstrate tunable n-type doping using Plasma-Enhanced Atomic Layer Deposition (PE-ALD) of an Aluminum Nitride doping film with a HfO_2 dielectric barrier of varying thickness. The mechanism for AlN doping is investigated by systematic experimentation across PE-ALD temperature and HfO_2 barrier thickness. We then measure contact resistance for 50 nm channel length single-CNT transistors with n-type channel doping. N-type contacts are demonstrated which yield down to 12 nm L_C, remain stable for >8 months, and display record-low R_C of 5.1 kΩ per CNT (20.4 Ω-μm for 250 CNT/μm) at L_C = 20 nm. This work resolves one of the few remaining fundamental obstacles towards complementary CNT logic technology.

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CS52

DNA-WRAPPED CNTS: FROM PRECISE ASSEMBLY TO ENERGY-EFFICIENT ELECTRONIC SWITCHES

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Since the invention of the first transistor, the interdisciplinary researches involving chemistry, materials science, and solid-state physics have contributed to the development of semiconductor electronics. At the crossroads towards future electronics, biological systems inspire future evolving of computing architectures and manufacturing framework. For instance, the high-resolution DNA self-assembly from synthetic biology field, have recently been used to construct ultra-scaled CNT transistors at a resolution superior to conventional lithography. DNA templated CNT electronics display fast on/off switching characteristics, as well as high on-state conductance, approaching the intrinsic limits of CNTs. Meanwhile, by wiring multiple individual CNT transistors, we demonstrated Boolean logic gates within the bio-templated electronics. More broadly, we demonstrate the in silico fabrication of diverse semiconductor materials via precise assembly approaches.

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CS53

MAGNETIC FIELD CONTROL OF THE FRANCK-CONDON COUPLING OF FEW-ELECTRON QUANTUM STATES

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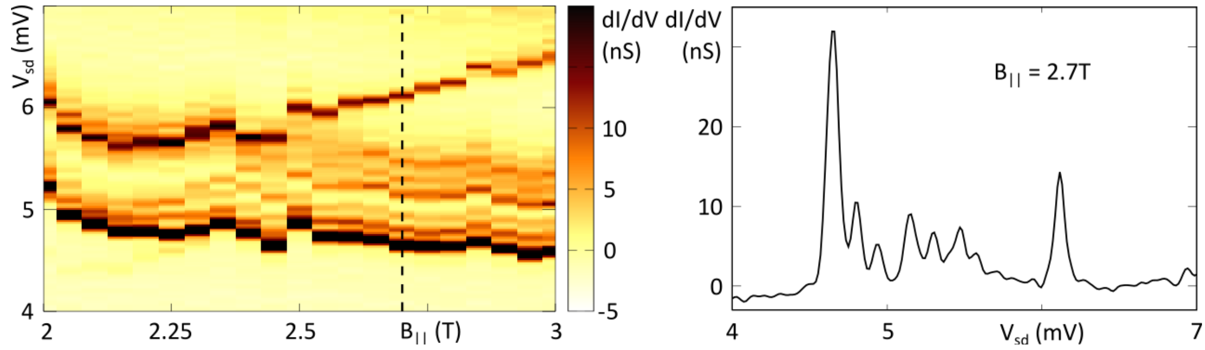
The longitudinal vibration of a suspended carbon nanotube has been observed many times in low temperature transport spectra via distinct harmonic Franck-Condon sidebands [1-5]. Typically, strong Franck-Condon coupling has been attributed to disorder-induced or deliberately targetted charge localization. Here, we present the observation of a strong, tunable coupling in an ultra-clean carbon nanotube with N=1 or N=2 electrons in the conduction band. The clean transport spectrum allows a tentative identification of the electronic base quantum states according to their valley quantum number. Interestingly, the Franck-Condon coupling strength g, as extracted from our data, both depends on the magnetic field and on the precise electronic quantum states participating in transport. While spin-dependent Franck-Condon phenomena have already been observed [6], our results clearly point towards a valley-dependent origin. As possible cause of this phenomenon, re-shaping of the electronic wavefunction envelope by the magnetic field [7-9] is discussed. A simple calculation demonstrates that variations of g as observed in the experiment can be reproduced by the theory, paving the way towards more realistic and detailed quantum-mechanical modelling.



Franck-Condon sidebands in the two-electron excitation spectrum. From [1].

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CS54
LOW-DIMENSIONAL SEMIMETAL-SEMICONDUCTOR CONTACTS

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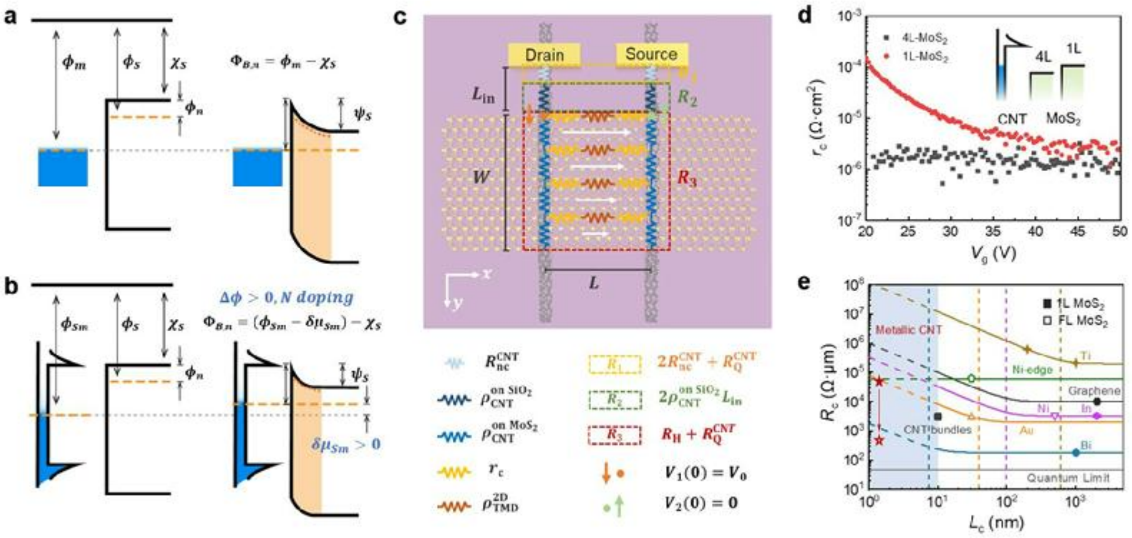
Two-dimensional (2D) semiconductors are promising in channel length scaling of field-effect transistors (FETs) due to their excellent gate electrostatics. However, the deteriorated contact resistance for 2D channels limits the device performance as well as the scaling of contact length. Low-dimensional semimetal-semiconductor (Sm-S) junctions have shown their potentials in electrical contact optimization recently. It is of great scientific significance to study the interfacial behavior of Sm-S systems and develop new high-performance semimetal contacts. Here, we investigate the gate-tunable contact-induced Fermi level shift (CIFS) behaviors in semimetal single-walled carbon nanotube (SWCNT) and graphene[1]. A resistivity comparison methodology and a Fermi level catch-up model are developed to measure and analyze the CIFS. The work function change of semimetal, as a result of CIFS, will naturally introduce a modified form of the Schottky-Mott rule, so that a modified Schottky barrier height can be obtained for the Sm-S junction. On this basis, we further construct a 1D semimetal-2D semiconductor contact by employing single-walled carbon nanotube electrodes, that can push the contact length into the sub-2 nm region[2]. Such 1D-2D heterostructures exhibit smaller van der Waals gaps than the 2D-2D ones, while the Schottky barrier height can be effectively tuned via gate potential to achieve Ohmic contact. A longitudinal transmission line model is proposed for analyzing the potential and current distribution of devices in short contact limit, and used to extract the 1D-2D contact resistivity which is as low as 10^{-6} $\Omega\cdot cm^2$ for the ultra-short contacts. We further demonstrate that the semimetal nanotubes with gate-tunable work function could form good contacts to various 2D semiconductors including MoS_2, WS_2 and WSe_2. The study on Sm-S junctions should be useful for the construction of reconfigurable devices and further miniaturization of electronics in the future.



Low-dimensional semimetal-semiconductor contacts

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CS55

A NEW CONDUCTIVE NETWORK IN CONCRETE DESIGNED BY INTERFACIAL NANOENGINEERING

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Traditionally, conductive fillers are mixed directly with cement matrix before binding with aggregates to develop piezoresistive cement-based sensors. This results in the most vulnerable region, interfacial transition zone (ITZ), from which microcracks are initiated, merely located at the periphery of the conductive network and thus limits the sensitivity of the smart sensor. Recently, we propose a strategy to construct a three-dimensional (3D) conductive network in the mortar with ITZ directly embedded in it, thus greatly increasing both the conductivity and piezoresistivity without significantly sacrificing mechanical property. Highly conductive graphene-coated fine aggregates (termed conductive G@FAg particles) are prepared by adsorption of graphene oxide (GO) onto the fine aggregates (FAg) surface, followed by simple annealing and microwave treatment. The combined usage of conductive G@FAg particles and results in an outstanding electrical conductivity and an excellent fractional change in resistivity under cyclic compressive loading, with a negligible compressive strength loss. The much-improved conductivity and FCR value with such a low weight percentage of conductive carbon materials are attributed to the unique 3D network of conductive channels. Such general strategy of nano-interface engineering with graphene derivatives can also be readily extended to the promotion of other physical properties (strength, EMI, damping, mass transportation, et al), thus opens a new window to optimize properties of cementitious materials.

CS56

HIGHLY EFFICIENT SELECTIVE SYNTHESIS OF PURE SEMI-CONDUCTING SINGLE WALLED CNT HAVING SUPERIOR ELECTRICAL CONDUCTIVITY BY IN-SITU RADIAL MIXING IN FLOATING CATALYST CHEMICAL VAPOUR DEPOSITION

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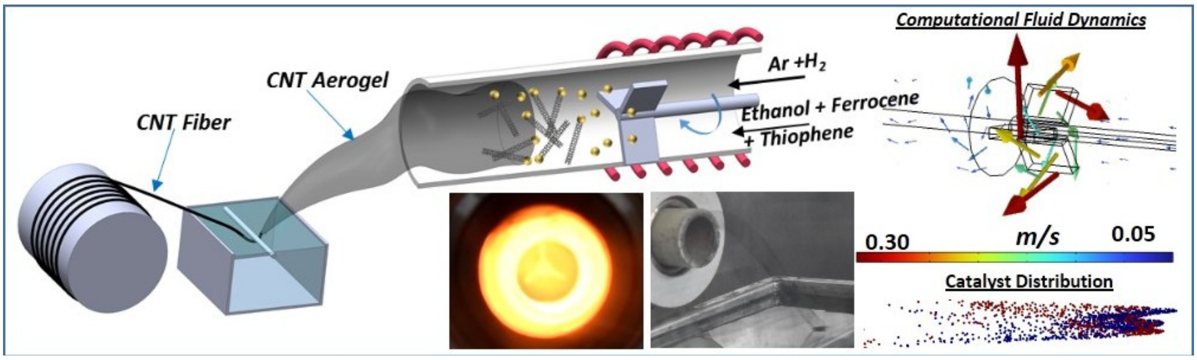
The ability of CNT fiber to translate exotic properties of individual CNTs from nanoscale to macroscale has given it the potential to replace conventional materials. In this work, for the first time, we have significantly enhanced the conversion of CNT fiber synthesis in FC-CVD by in-situ radial mixing inside the reactor using a rotating fan. The mechanism for the enhancement of the conversion has been determined with the aid of computational fluid dynamics. The radial mixing is able to increase the conversion from 4.12 ± 0.21 % to 15.1 ± 0.95 % which is the highest carbon conversion reported in FC-CVD for direct spinning of SWCNT fiber. The radial mixing inside the reactor was able to selective produce SWCNT with 95 % semiconducting in nature. The produced SWCNT has extremely low impurities in the as synthesized condition with no amorphous carbon and only 2.8 % iron as determined by thermogravimetry. The radial mixing was also able to enhance the aspect ratio by 129 %. The improvement in the aspect ratio and purity led to the production of fiber with highest electrical conductivity (8.46 ± 0.45 MS/m) for a semiconducting SWCNT fiber despite not using any post processing.



Graphical Abstract. Schematic of the radial mixing FC-CVD along with the computational fluid dynamics simulation

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CS57

PREPARATION OF MACROMATERIALS FROM NANOCARBONS BY INTERFACE CHARGE INJECTION

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Nanocarbon such as fullerenes, carbon nanotubes and graphene are mostly used in the form of macromaterials, whose properties and functions are sensitive to the interface between nanocarbons and the structural features of the micromaterials formed. Thus, the structural control of macromaterials from nanocarbons is a critical issue, for which the interface tuning technique needs to be further developed. Charge injection has been used to modify the physical properties (e.g., energy level of electrons) but yet to tune the structure of macromaterials. We have found that, by charge injection from α-Li_3N, the stacking of graphite is changed from ABC to AB stackings, at ambient pressure and temperatures below 400 ºC. By charging C_{60} molecules periodically arranged in a face center cubic lattice with α-Li_3N, a novel long-range ordered porous carbon (LOPC) crystal was formed. LOPC possesses the characteristics of both long-range order in the three-dimensional crystal and partially broken C_{60} molecules connected as the building blocks. Interface charge injection offers a new approach for constructing new materials much like using Lego blocks, thus allowing the precise control of interfaces in crystal macromaterials.

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CS58

ULTRAHIGH-PERFORMANCE CARBON NANOTUBE-BASED GRAPHITIC FIBERS

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One-dimensional carbon nanotubes (CNT) with a high aspect ratio have been considered as the ultimate building block for high-performance CNT fibers due to their outstanding properties. Many attempts to develop high-performance CNT fibers have been conducted since 2000. However, the bulk properties of CNT fibers make it difficult to realize the ultimate properties of individual CNT owing to the imperfect alignment, presence of pores, and limited connectivity of elements in the assemblies. Here, we will present the systematic studies of the wet-spinning process for manufacturing the ultrahigh performance CNT fibers by controlling fiber shape, alignment, aspect ratio of CNT, and thermal treatment process [1-2]. Furthermore, thermoelectric properties of thermally annealed CNT fibers will be presented.

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CS59

WEAK LOCALIZATION VERSUS FLUCTUATION INDUCED TUNNELING IN HIGH PERFORMANCE CARBON NANOTUBE FIBERS

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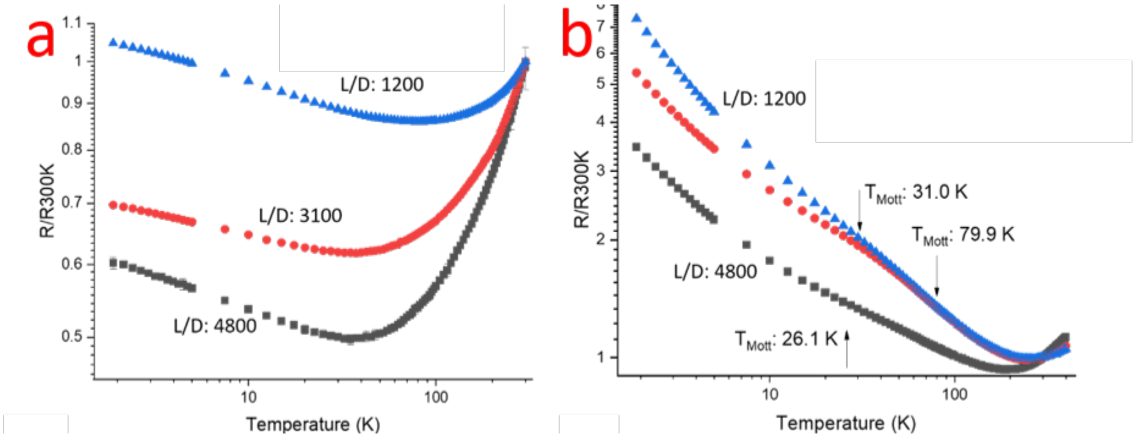
Carbon nanotube (CNT) fiber conductivity nearly exceeds copper's specific conductivity and further improvement is expected with greater aspect ratios[1] and incorporating dopants with long range order[2]. Analogous to the graphitic intercalation compounds, which approached and exceeded copper's absolute conductivity, CNTs have the advantage of bendability and superior mechanically strength[3]. Despite strategic opportunities of CNT fibers as a multifunctional conductor, we find that literature is unknowingly divided on their electrical transport mechanisms. In one prevalent literature narrative (homogeneous conduction), the overall CNT material "order" starts low where localized charge carriers hop to distant sites. As the order is increased experimentally (say by enhancing doping degree[4], microstructure alignment[4], or metallicity[5]) the CNT material undergoes an insulator to metal transition and, with further order enhancement, becomes a metal with either 2D or 3D weak localization. In the other prevalent literature narrative (heterogeneous conduction), long metallic structures are separated by small insulating gaps that delocalized charge carriers must tunnel through[6] [7]. Here, using cryogenic magneto-resistance (MR) measurements on multiple high conductivity CNT fibers made from CNTs with different aspect ratios, we conclusively demonstrate that 1) weak localization is responsible for the negative magneto-resistance; 2) weak localization, however, only accounts for a small portion (< 10%) of the resistance upturn approaching absolute zero; 3) a magnetic-field independent heterogeneous conduction model must account for the bulk of the fiber's extrinsic resistance. These findings are important in that the homogeneous and heterogeneous narratives in literature rarely, if at all, consider the other alternate narrative, while being responsible for most of a CNT fiber's resistance at room temperature.



Resistance versus temperature for CNT fibers with different aspect ratios when a, doped and b, de-doped.

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P000

IN SITU XAFS ANALYSIS FOR CHEMICAL STATES OF METAL CATALYSTS DURING SWCNT GROWTH BY ACCVD

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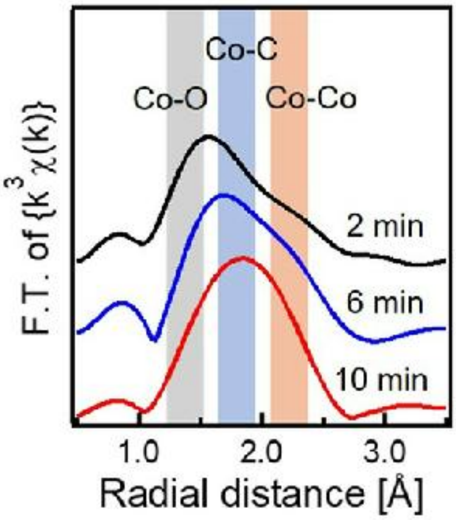
Selective growth of single-walled carbon nanotubes (SWCNTs) with a specific chirality has been a significant issue because their electronic structures are dependent on their chirality. To realize structural control of SWCNTs, it is important to understand the growth mechanism of SWCNTs. However, the details of growth process of SWCNTs from catalyst particles are still unclear, because the catalyst particles are nanosized, showing different properties from their bulk states. To clarify the physical and chemical states of catalyst particles during SWCNT growth, in situ analysis is essential. So far, many groups reported environmental transmission electron microscopy (ETEM) studies for SWCNT growth from iron-group metal catalysts [1-2]. However, compared with the typical growth condition of SWCNTs, they were performed at a relatively low temperature under low feedstock gas pressure.

In this study, we performed in situ X-ray absorption fine structure (XAFS) spectroscopy to investigate chemical states of transition metal catalysts such as Fe, Co, Ni, Ir, and Pt during SWCNT growth by alcohol catalytic chemical vapor deposition (ACCVD). XAFS analysis can be performed even at high temperature and high pressure. Therefore, XAFS is applicable for analysis under the conventional growth condition of SWCNTs. Our results showed that, during SWCNT growth, iron-group metal catalysts were partially carbonized, but that platinum-group ones were maintained metallic [3-4]. We demonstrated marked difference in the degree of carbonization of catalyst particles, depending on the electronic structures of catalyst metals.

This work was partly supported by JSPS KAKENHI Grant Number JP19H02563 and conducted at the Institute for Molecular Science (IMS), supported by “Advanced Research Infrastructure for Materials and Nanotechnology" in Japan (ARIM), Grant Number JPMXP1222MS1001.



RSF of Co catalysts. RSFs of Co catalysts, which were obtained from XAFS spectra during SWCNT growth.

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P001

3D-PRINTED CARBON TILE-MODULATED WELL-INTERCONNECTED POROUS PSEUDOCAPACITIVE ELECTRODE

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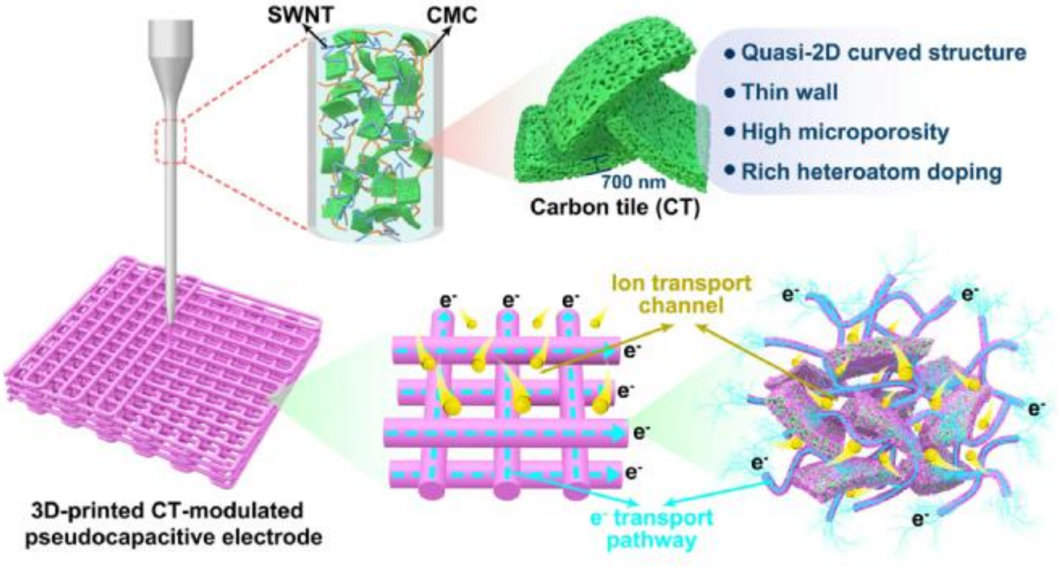
Pseudocapacitive electrode architecture with well-interconnected open pores is essential and critical to the high-performance energy storage. However, challenges remain pertaining to consistent and scalable manufacturing, as well as fast ion/electron transport, especially at a high mass loading of active materials. Herein, with kapok-derived proper-curved quasi-2D carbon tile (CT) featuring thin wall and high microporosity as unique skeleton support, a novel pseudocapacitive CT-single-wall carbon nanotube (SWNT)-NiCo2O4 electrode was constructed via a scalable and controllable extrusion-based 3D printing strategy. The resulting 3D-printed electrode demonstrated abundant well-interconnected hierarchical pores and continuous conductive network built by coupling CTs and SWNTs, thereby enabling uniform and high mass loading of active NiCo2O4 (31 mg cm-2), and meanwhile guaranteeing unimpeded channels and adequate pathways acting as “superhighways” for ultrafast ion diffusion and electron transport throughout the entire device. Benefiting from these prominent features, an asymmetric supercapacitor assembled with 3D-printed CT-modulated electrode delivered high specific capacitance (588 mF cm-2) and energy density (138 µWh cm-2), exceptional long-term cycling stability (82% after 50000 cycles), and superior capacity even at large electrode thickness. This work has shed light on new strategies for fabricating rational pseudocapacitive electrode architectures toward high-capacity and rapidly cycling devices.



Schematic illustration. Schematic illustration of the fabrication process and proposed ion/electron transport model of a 3D-printed CT-SWNT-NiCo2O4 cryogel electrode

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P002

A DFT STUDY OF THE NANOTUBE CATALYST CHARGE TRANSFER DURING CVD GROWTH

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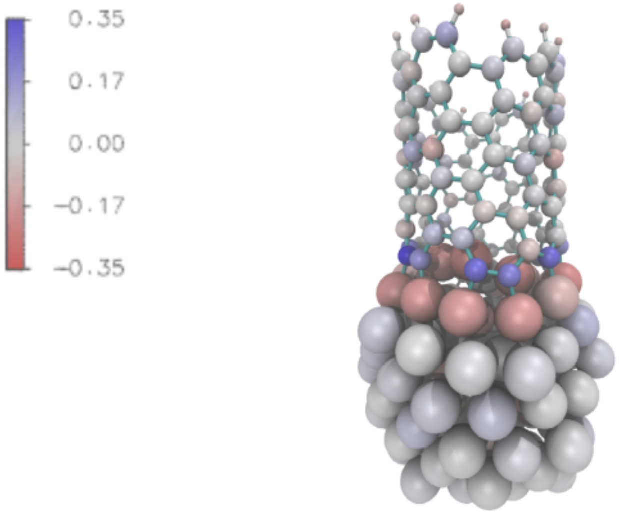
In the context of a soaring demand for high-performance electronic devices, single-walled carbon nanotubes (SWCNTs) have emerged as a promising material with tunable electronic structure. However, a significant challenge lies in the controlled growth of SWCNTs with a specific chiral index (n, m), which determines their electronic properties. Different pathways towards a chirality selective synthesis have been explored, e. g. by catalyst engineering, optimization of CVD conditions or other methods (1,2, 3). An emerging method uses an external electric field to produce highly selective semiconducting samples (4). The interface between the growing SWCNT end edge and the catalyst clusters has been shown to play a crucial role in the CCVD process (5). This contact between the tube and its feeding catalyst is dynamically evolving to enable carbon incorporation in the growing tube and a large number of edge configurations (6) are encountered, where charge transfer (7) might play a role.

In this study, using DFT calculations and a Bader charge analysis, we investigate the charge transfer between nickel nanoparticles and a small number of SWCNTs, considering different edge structures characterized by their numbers of armchair and zigzag edge atoms in each of them.



Nickel catalyst cluster with (8,4) nanotube colored according to their charge transfer

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P003

A SIMPLE MICROPREPARATIVE GEL ELECTROPHORESIS TECHNIQUE FOR PURIFICATION OF NANOSCALE BIOCONJUGATES

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Fluorescent probes are the foundation of optical imaging and sensing technologies. These probes are engineered for different applications by varying the probe size, composition, bioconjugation, and other various properties. The performance of these probes, however, depends strongly on the ability to purify these constructs from their synthesis mixtures. Although a variety of chromatographic and electrophoretic purification techniques can be used to purify probes, such techniques are usually laborious and time-consuming, and they often require complex and costly instalments that are inaccessible to most laboratories. In this work, we introduce a versatile micro-preparative (MP) method based on polyacrylamide gel electrophoresis (PAGE) to purify fluorescent proteins (enhanced yellow fluorescence protein, EYFP), synthetic nanoparticles (graphene quantum dots, GQDs), as well as nano-bioconjugates (EYFP-DNA and GQD-DNA). We demonstrate the successful isolation of EYFP from crude cell extract with 90% purity, comparable to purities achieved using a two-step size exclusion and immobilized metal-ion affinity chromatography purification procedure. The technique was further applied for the size-dependent separation of a commercial mixture of GQDs into three different fractions with distinct optical properties. Finally, we apply MP-PAGE to extract EYFP-DNA and GQD-DNA bioconjugates from a reaction mixture that otherwise could not be readily processed using traditional chromatography techniques. MP-PAGE thus offers a rapid and versatile means of purifying biological and synthetic nanoprobes without the need for specialized equipment.

P004

ACCURATE HEIGHT MEASUREMENT OF CARBON NANOTUBES USING SCANNING PROBE MICROSCOPY

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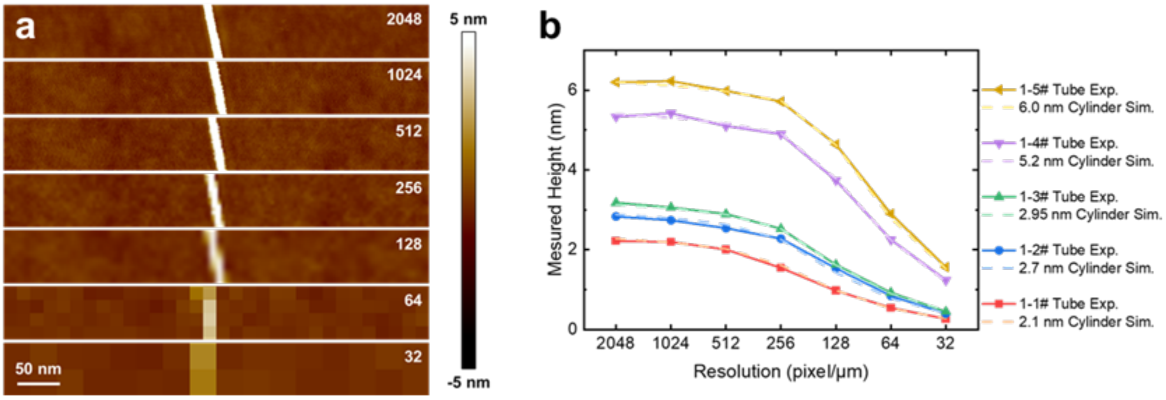
Scanning probe microscopy is one of the most commonly used methods to characterize carbon nanotubes' morphology and properties, with advantages of high resolution, broad applicability, simplicity, and non-destructiveness. However, there are still problems that hinder accurate characterization. Due to the discrete measurement process, atomic force microscopy (AFM) obtains a heightmap with limited pixels, where representative sampling is difficult for zero- and one-dimensional structures with small sizes.

Herein, we simulated the sampling process of height measurement at different pixel densities in the Peakforce Tapping mode of AFM by the Monte Carlo method. These results agreed with experiments, facilitating the correction of distorted apparent height. Our work not only clearly presents the resolution-related inaccuracy in the diameter measurements but also offers way to correct the problems.



AFM images (a) and the experimental and simulated apparent heights (b) of individual carbon nanotubes at different pixel densities.

P005

ADHESION OF VACNT ON ALUMINUM COLLECTOR FOR OPTIMIZED ENERGY STORAGE SYSTEMS

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Vertically aligned carbon nanotube (VACNT) arrays are considered promising candidates as alternatives to active materials, such as activated carbon, for energy storage system electrodes. However, there is little documentation in the literature on studies of the interfaces between VACNT-based active materials and the current collectors of supercapacitors or batteries.

NAWATechnologies developed several types of specific electrodes for applications such as supercapacitors or batteries. The Aerosol Assisted Catalytic Chemical Vapor Deposition method is used for the one-step growth of dense VACNT carpets on aluminium foils at low temperature (615°C) leading to a single-step and continuous process that meets industrial requirements for the development of low cost, highly conducting and light supercapacitors electrodes [1]. In order to optimize their performances, we suggest studying the VACNT/Aluminum interface to improve the adhesion of the VACNTs on the collector while limiting the interface resistance and ensuring optimal power performance of the device. One of the specificities of this work is to combine innovative methods of studying adhesion (in-situ analysis under the SEM) with interface analysis on cross sections or in 3D (FIB). This parametric study is also associated with electrochemical characterizations (electrochemical impedance spectroscopy, cyclic voltammetry, chronopotentiometry, floating) with three-electrode cell and in complete device to analyse the interfacial resistances and the performances in energy, power, cycling. The presentation will provide preliminary results on adhesion and electrochemical performance, with a focus on two aspects of the synthesis. Firstly, the aluminum surface, which is the major factor affecting the reactivity of catalytic particles during the growth of VACNTs on the substrate. This was characterized using various methods, including XPS, confocal microscopy, SEM, roughness testing, and AFM. Secondly, the VACNT synthesis parameters, such as growth rate and cooling temperature, were analyzed to enhance the adhesion properties of VACNTs on aluminum.

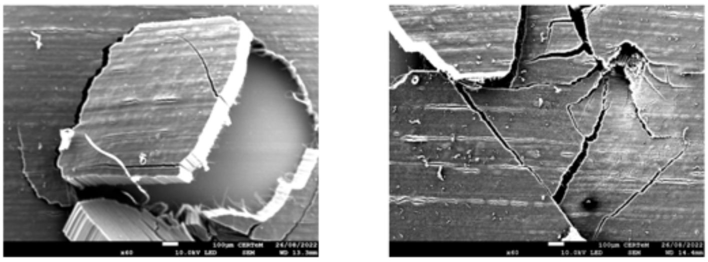

Figure 1: SEM image illustrating the delamination of VACNT

SEM image illustrating the delamination of VACNT

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P006

ALL-SCREEN-PRINTABLE CNT FILM-TYPE PHOTO-THERMOELECTRIC IMAGE SENSOR ARRAY SHEETS

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As the structures of industrial products become increasingly complex, nondestructive testing is indispensable to obtain detailed information on their internal structures and defects. In this context, carbon nanotube (CNT) films are suitable for omni-directional nondestructive imaging testing devices for 3D multilayered objects due to their flexibility and ultrabroadband photo-absorption[1-2]. On the other hand, the integration of devices such as one-dimensional arrays and two-dimensional matrix cameras required alternating combinations of fabrication environments of high vacuum and cooling, and room-temperature atmosphere[3]. Therefore, this situation hinders broad use. To this end, this work reports on the successful fabrication of CNT-based integrated image sensors by screen-printing in room-temperature air. Fig. 1a shows the concept of the presenting device fabrication by screen printing. The channel employs an aqueous solution of the semiconducting-metallic-mixed SWCNTs and performs the chemical carrier doping with an aqueous solution of 15 Crown 5 Ether and KOH, and the electrode formation with a mixture paste of conductive micro filler and binding agent. Fig 1b compares the accuracy of screen printing with the concentration of CNT dispersion. The high concentration of CNT solution enables stable direct drawing due to the high viscosity of the dispersion. As shown in Fig 1c, the conventional device fabrication process(Transfer) causes disconnections at the channel-electrode interface while drying the electrode, however, this work demonstrates improvement. In addition to the above, this work is going to comprehensively report optimal conditions in the printing device fabrication process and the applications of nondestructive inspection at the conference.

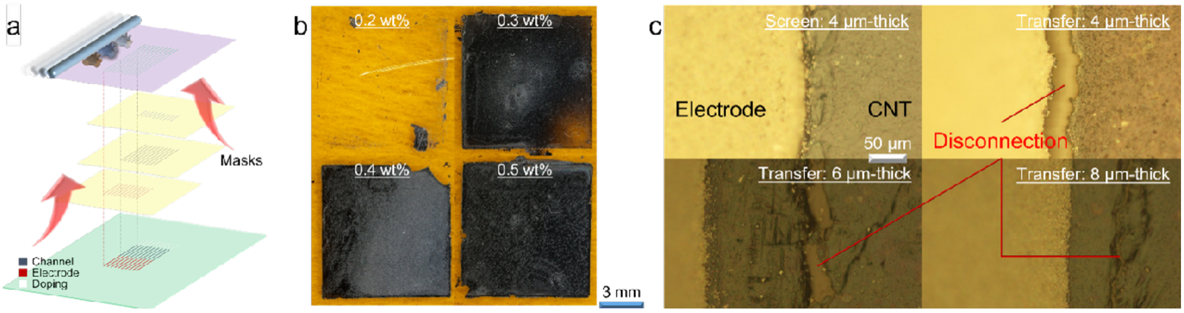

Figure 1. a, Concept of the presenting device fabrication. b, Comparison of printed CNTs channels in response to solution concentration. c, Photograph of the disconnection at channel-electrode interface.

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P007

APPLICATION OF TON-DEGREE CARBON NANOTUBE-BASED MESOPOROUS ADSORBENTS FOR TRAPPING VOCS IN OIL REFINERY FACTORY

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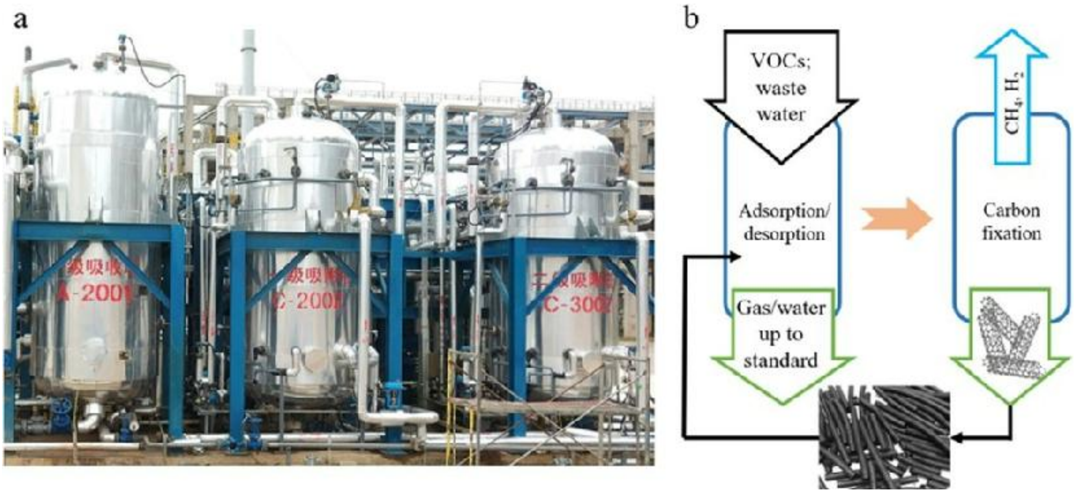
Owing to the special structure configuration, high thermal conductance and non-polar surface property, carbon nanotubes are applicable as adsorbents of trapping aromatics and gasoline-type compounds. For a practical industrial application, the molding of carbon nanotubes to be a strip or particles with macroscopic scale is necessary to avoid the loss carried away by gas or liquid flow. It remained a state of art yet for the fabrication of an adsorbents simultaneously meeting the requirment of the pore design, mechanical strength free of attrition, as well as not sacrifying its effective surface area. It spent 7 years for our team to develop such a multifunctional adsorbent, to realize its mass production in several ten tons degree, and to use them in an oil refinery factory[1-5]. An integrated apparatus was built for the pressurized adsorption of aromatic-type VOCs, for the desorption with steam and the recycle use of condensed aromatic products. A far quick heat start up and close down of apparatus was realized for CNT-based adsorbents, compared to activated carbon adsorbents. Interestingly, we used a CVD process to further convert light hydrocarbon component into carbon nanotubes, where the key includes the high efficeint conversion to meet the emission regulation of non-methane hydrocarbons. Sufficient data allowed us to discuss the carbon nanotube cycle in this operation, as using green electricity as the energy supply. Thus, a near carbon zero emssion cycle can be achieved.

It, we think, is a contribution of carbon nanotube-related technology to the era of carbon neutrality.



VOCs capture by CNT-based adsorbents. Photo of the skid-mounted equipment of adsorption-desorption-carbon fxation process based on CNT-based adsorbent (a). Schematic diagram of industrial closed-loop (b)

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P008

ATOMIC SCALE CHEMICAL ORDERING IN FRANCKEITE—A NATURAL VAN DER WAALS SUPERLATTICE

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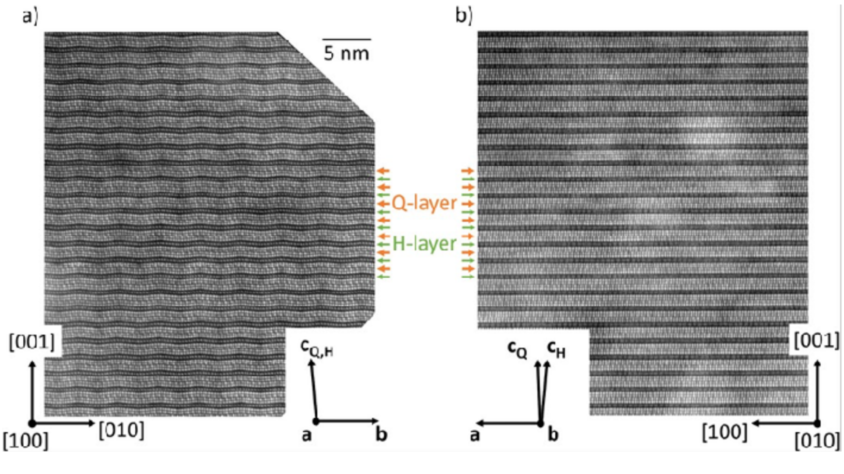
Franckeite is a naturally occurring sulfosalt mineral with a van der Waals superlattice structure, found in Bolivia and first described by Stelzner[1]. This van der Waals heterostructure is composed of alternating incommensurate 2D layers, namely the H-layer (PbS) and Q-layer (SnS_2). Franckeite has attracted attention recently due to its semiconducting and electrochemical properties and the possibility for exfoliation of flakes and their incorporation into devices[2,3]. An extensive review on preceding characterization results is given in the work of Makovicky et al.[4], including a detailed description of the atomic site modulation caused by the incommensurate structure was proposed. Such modulations in franckeite, and the related mineral cylindrite, have been imaged before using transmission electron microscopy (TEM)[5,6] or with high-angle annular dark field (HAADF) scanning transmission electron microscopy (STEM)[7].
Here we present several new experimental observations of franckeite, including atomic structure measurement using state-of-the-art high-angle annular dark-field (HAADF) scanning transmission electron microscopy (STEM) and atom probe tomography (APT). With atomic-number image contrast in HAADF STEM(Fig1). direct information about both the geometric structure and its chemistry is provided, including several new chemical ordering effects. We present mid-infrared reflectance and transmittance spectroscopy measurements of exfoliated franckeite crystallites, where absorption associated with indirect excitons in the superlattice is expected to be observed.



HAADF-STEM images of franckeite: atomically resolved Q-layer and H-layer are distinguishable. (a) In [100] viewing direction, the displacive modulation is visible. (b) In [010], the modulation is averaged along the projection leading to a blurring of the atomic columns when the sample thickness is in the order or larger than the modulation wavelength.

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P009

BIOSENSING MEMBRANE PROTEINS WITH SOLUTION GATED GRAPHENE FIELD EFFECT TRANSISTORS

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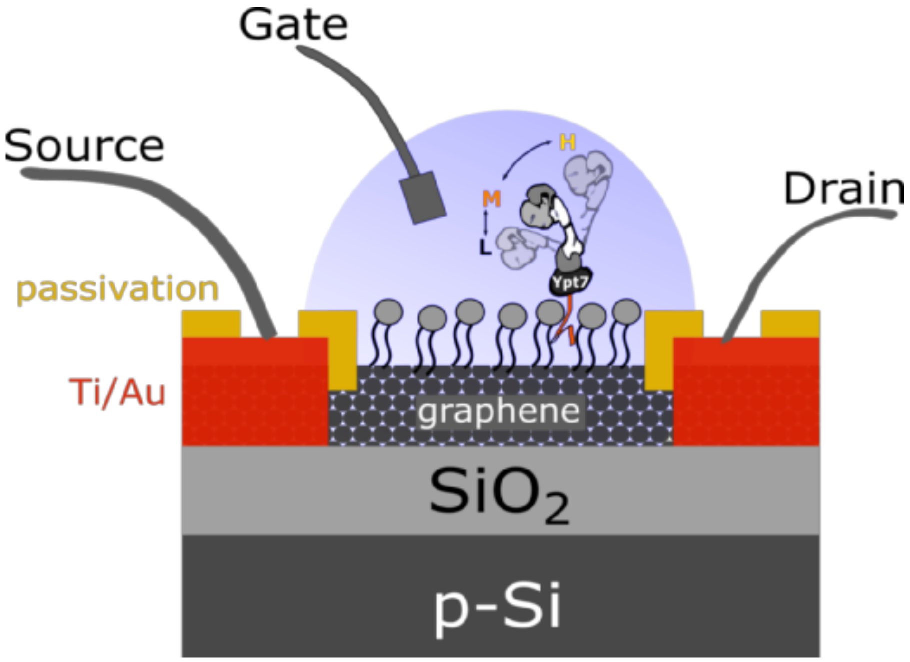
Membrane proteins are crucial for many biological processes, yet their dynamics and function remain poorly understood due to the lack of techniques that provide adequate spatial and temporal resolution. In this study, we present a novel approach using solution-gated graphene field effect transistors (SGFETs) in combination with biomimetic membranes to investigate protein dynamics. Specifically, the histidine-tagged proteins were captured by the tris-NTA complexes conjugated to the lipid membrane on the SGFETs interface [1]. Once the protein was attached, we ensured its reversibility using the imidazole wash as a competitor molecule for the histidine tag. In addition, we utilized SGFETs to track the electrochemical potential while immobilizing HOPS membrane tethering complexes on a lipid monolayer. The dynamics governing the behavior of HOPS were previously reported using graphene-induced energy transfer measurements on dye-labeled complexes [2]. Through noise measurements, we assessed the impact of different functionalization steps on the device's transport properties. We explore the potential of our method to study the dynamics of label-free proteins.



Immobilization of the HOPS complex on the SGFET channel-lipid membrane interface, with schematic representations of potential conformational changes in the HOPS complex in the L (low), M (medium), and H (high) states.

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P010

BOOSTING CO-BASED AEROSOL CVD SYNTHESIS OF SWCNT TRANSPARENT CONDUCTIVE FILMS

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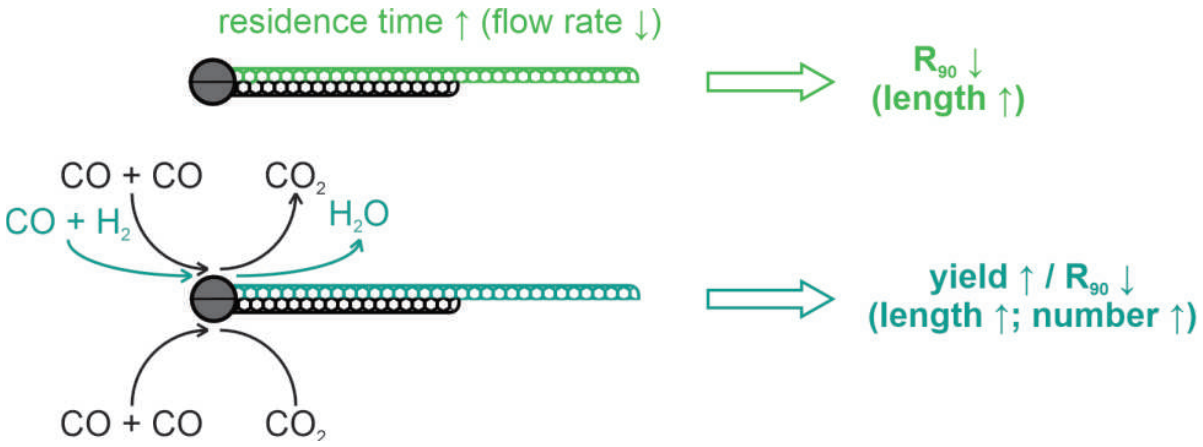
Aerosol (floating catalyst) chemical vapor deposition (CVD) process is one of the most promising methods for SWCNT synthesis since it allows one-stage and scalable production of SWCNTs in various forms – aerosols, fibers, and thin films, which may be considered as a main alternative material to brittle ITO with its depleting resources. Meanwhile, CO-based aerosol CVD nanotube synthesis attracts much attention, since it results in the highest optoelectronic properties achieved. Nevertheless, a significant drawback of the CO-based process is its quite low productivity, as well as optoelectronic performance, is still not reaching an industrial level of ITO (~ 10 Ω/□ equivalent sheet resistance at 90% transparency (R_{90}). Besides, the general aerosol CVD reactor feature is a poor opportunity to study catalyst evolution and nanotube growth processes. In our investigation, we have proposed an approach to tuning SWCNT length while maintaining the catalyst activation stage by an increase in residence time in a flow reactor [1]. Nanotube lengthening was shown to enhance SWCNT film conductivity (we have managed to achieve R_{90} of 54 Ω/□ for doped films). Using this method, in our next work, we have thoroughly studied a CO_2 effect in CO-based SWCNT synthesis on catalyst evolution and have demonstrated that CO_2 considerably decreases catalyst lifetime. In another study, we have switched on a poorly studied reducing growth promoter, H_2, and have shown it significantly increases synthesis yield by another carbon-feeding reaction between CO and H_2. At the same time, at different conditions, H_2 introduction may also result in a decreased R_{90} [2]. Thus, we have proposed different techniques for improving the figure of merits of both the CO-based aerosol CVD process (productivity) and the product – SWCNT thin film (its optoelectronic properties). The authors thank Russian Science Foundation grant No. 20-73-10256.



Schematic representation of residence time and hydrogen effect in the CO-based aerosol CVD synthesis of SWCNT films

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P011

BOOSTING SOLAR-POWERED INTERFACIAL WATER EVAPORATION BY ARCHITECTING 3D POLYMERIC TOPOLOGICAL NETWORK IN CNT CELLULAR STRUCTURE

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Photothermal hydrogel, with an inherently modifiable hydrated network, has been widely demonstrated as a promising candidate for efficient water treatment. However, there are still great challenges in architecting abundant interfacial mass transfer channels and avoiding excessive polarity interaction in polymeric hydrogels.

Here, a 3D interconnected topological porous hydrogel was proposed to enable cellular carbon nanotube (CNT) structures filled with hydrophilic and thermosensitive nanonetworks via infiltration and crosslinking of polyvinyl alcohol (PVA), polyethyleneimine (PEI) and carbon black particles (CBs). In this regard, the obtained hybrid hydrogel, featuring confined capillary channel and weak hydration interaction, achieved a superior water evaporation rate of 3.55 kg m-2 h-1 with an efficiency of 92.0% under 1 sun irradiation, and particularly a high self-evaporation rate of 0.49 kg m-2 h-1 in the dark. More importantly, such hybrid hydrogel demonstrated excellent evaporation performance in weak sunlight and highly humid environments. This work has shed light on new insights to manufacture porous and low-enthalpy photothermal hydrogels for advanced solar-driven water treatment technology.

Keywords: Carbon nanotube, topological hydrogel, hydration, solar steam generation

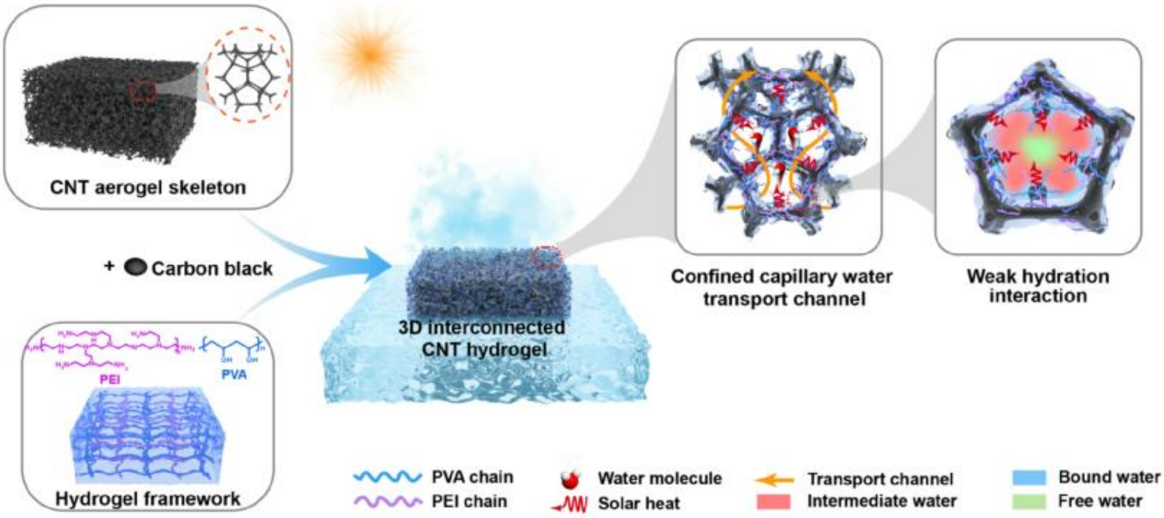

Figure 1. Schematic design of 3D interconnected topological CNT hydrogel

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P012

BOTTOM-UP SYNTHESIS AND PROPERTIES OF GRAPHENE QUANTUM DOTS

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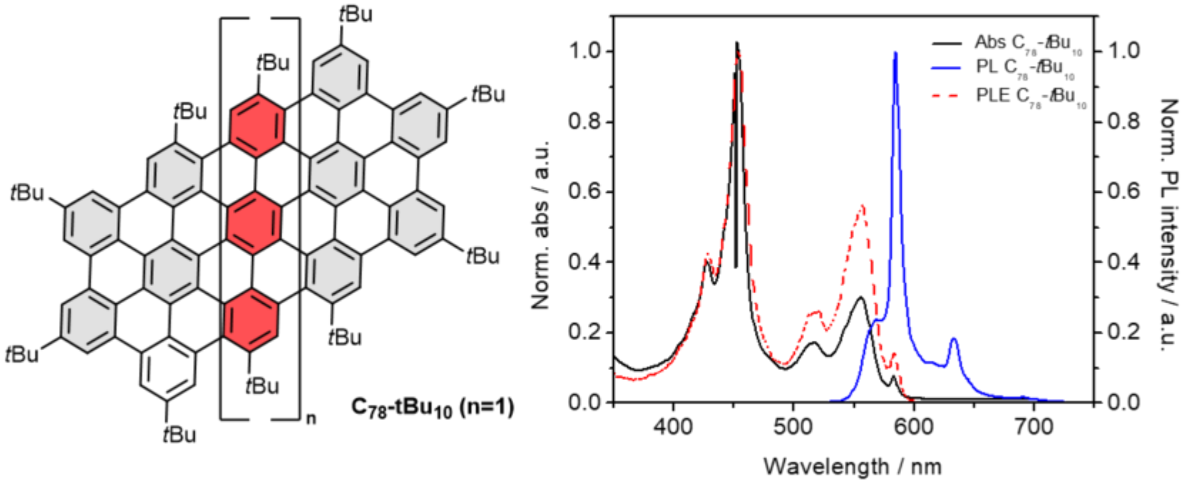
For the last fifteen years, researchers have been interested in the synthesis and properties of graphene materials produced using a method called top-down. In 2008, H. Dai has been demonstrated the formation of graphene quantum dots (GQDs) starting from graphite material.[1] Nevertheless, this method does not allow controlling the structure of the final material at the atomic level. This degree of control is done by a simple method called bottom-up which exploits the chemical synthesis. A benzene ring is the ideal precursor for this approach and the multiplication of these rings forms polycyclic aromatic hydrocarbons (PAHs). The group of K. Müllen has developed a method for the synthesis of polyphenylene dendrimers based on the Diels-Alder reaction. These dendrimers are then oxidized by the Scholl reaction and give PAHs.[2] GQDs have a very low solubility in organic solvents. Optical analyses are tricky because of the molecules that aggregate strongly due to π-π stacking interactions and are therefore not individualized.[3] To remedy this problem, functionalization of the edges of GQDs is possible to increase the steric hindrance of each GQDs, thus limiting π-stacking.[4-5] The new family of GQDs synthesized is "saturated" with tert-Butyl group that makes them highly soluble and individualized in classical solvents.



Structure and photophysics of a C78-tBu10 particle

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P013
CARBON NANOMATERIALS FOR ROOM TEMPERATURE GAS SENSING

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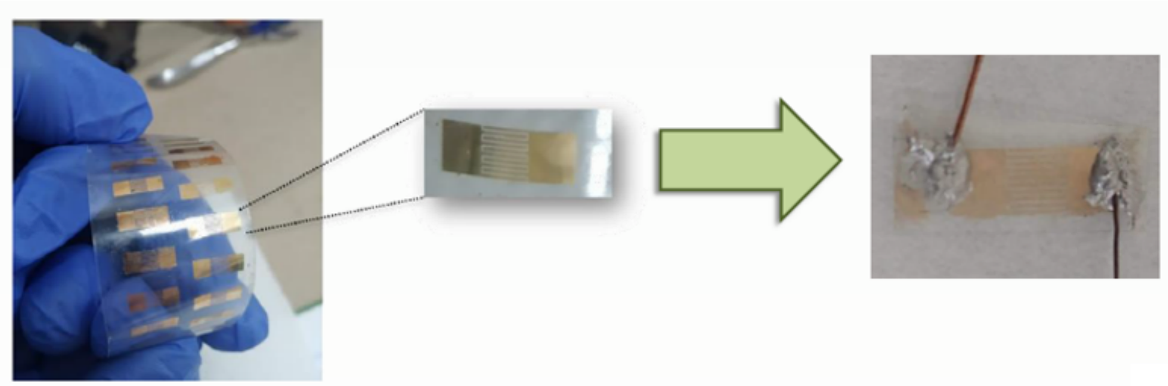
The development of gas sensors with high detection properties operating at room temperature is of great interest due to their low power consumption and long-term stability. Among the various types of semiconductor gas sensors, metal oxide-based sensors are the focus of research due to their high gas response, excellent selectivity, good portability, and low manufacturing cost, but the high operating temperature compromises the application in gas sensors, as maintaining a high and stable temperature system increases its operating cost [1]. Inserting a material that operates at room temperature is a solution to mitigate such facts. Graphene can overcome this deficiency. Graphene is a two-dimensional nanomaterial characterized by high ductility, electrical conductivity, transparency, and flexibility [2]. In this context, a way to reduce the metal oxide-based sensors operating temperature through graphene doping will be presented, maintaining its stability and detection sensitivity [3]. In addition, as a way of implementing the production of nanostructured devices on a flexible substrate, the study and application of plasma treatment at atmospheric pressure on PET substrates were carried out, for the production of sensors [4].



Interdigitated electrode. Interdigitated electrode made on PET substrate for gas sensing.

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P014

CARBON NANOTUBE ELECTRON BLACKBODY AND ITS RADIATION SPECTRA

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An optical blackbody is an ideal absorber for all incident optical radiation, and the theoretical study of its radiation spectra paved the way for quantum mechanics (Planck's law). Herein, we propose the concept of an electron blackbody, which is a perfect electron absorber as well as an electron emitter with standard energy spectra at different temperatures. Vertically aligned carbon nanotube arrays are electron blackbodies with an electron absorption coefficient of 0.95 for incident energy ranging from 1 keV to 20 keV and standard electron emission spectra that fit well with the free electron gas model. Such a concept might also be generalized to blackbodies for extreme ultraviolet, X-ray, and γ-ray photons as well as neutrons, protons, and other elementary particles.

P015

CARBON NANOTUBE MECHANICAL RESONATOR WITH MASS SENSITIVITY OF 70 YOCTOGRAM AT ROOM TEMPERATURE

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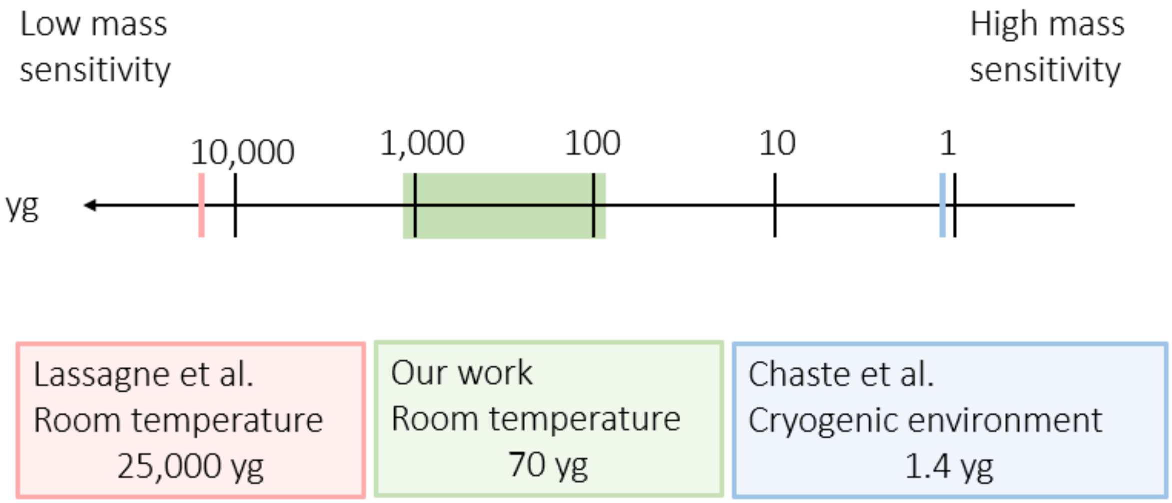
Carbon nanotubes (CNTs) are exceptional mechanical resonators. They are extremely light with masses in the attogram range. As bottom-up materials, they do not suffer from surface defects like their top-down counterparts NEMS usually etched from silicon or nitride substrates [1]. From these two features stems their exquisite mass sensitivity of 1.4 yg, the mass of a single proton, in a cryogenic environment, (1 yg = 10^{-24} g) as demonstrated by Chaste et al [2]. This sensitivity was reported to be much worse at room temperature, about 25 zg [3] (1 zg = 10^{-21}g). This has hindered the use of CNTs as sensors in real-life applications. In this work, we show that CNTs mechanical resonators can also reach exquisite sensitivity at room temperature down to 70 yg: the mass of an individual molecule as small as pentane. We carefully investigated the noise mechanisms that could be limiting the sensitivity: electrical fluctuations, temperature drifts, residual molecules in the gas phase and Brownian motion. It was found our resonator works close to the Brownian noise limit and that it is not bounded to external sources of noise. Increasing the pressure does not seem to degrade the sensitivity, which might be preserved up to ambient pressure. Finally, the exquisite sensitivity observed here is similar for several CNTs, making it a reliable and reproducible asset. This opens up the possibility to perform single-molecule sensing, in various contexts [2,4].



Mass sensitivities using CNTs mechanical resonator

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P016

CARBON NANOTUBE-BASED FLEXIBLE HIGH-SPEED CIRCUITS WITH SUB-NANOSECOND STAGE DELAYS

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High-speed flexible circuits are required in wireless flexible systems that perform real-time information analysis for emerging applications, such as next-generation wearables for personal health care. Scaling the channel length of the transistors into the sub-μm region is one of the keys. Here, we present scaled carbon nanotube-based thin film transistors (CNT-TFTs) with channel lengths down to 450 nm on 2-μm-thick parylene substrates, achieving state-of-the-art performances of high on-state current (187.6 $\mu A\ \mu m^{-1}$) and large transconductance (123.3 $\mu S\ \mu m^{-1}$). Scaling behavior analyses reveal that the performance hike in scaling is attributed to the channel resistance reduction while the contact resistance remains unchanged. Notably, the contact resistance on a single nanotube basis of 180 ± 50 kΩ per tube is comparable to that achieved in rigid ones, indicating huge potential in ultimate scaled flexible CNT-TFTs with high performance comparable to their rigid counterparts where contact resistance dominates the whole device performance. Five-stage flexible ring oscillators are built to benchmark the speed of scaled devices, in which an oscillation frequency of 356 MHz and a stage delay of 281 ps were achieved at a low supply voltage of 2.6 V.

P017

STRUCTURAL DESIGN OF MULTIFUNCTIONAL NANOCARBON MATERIALS FOR EXTREME-ENVIRONMENTAL APPLICATIONS

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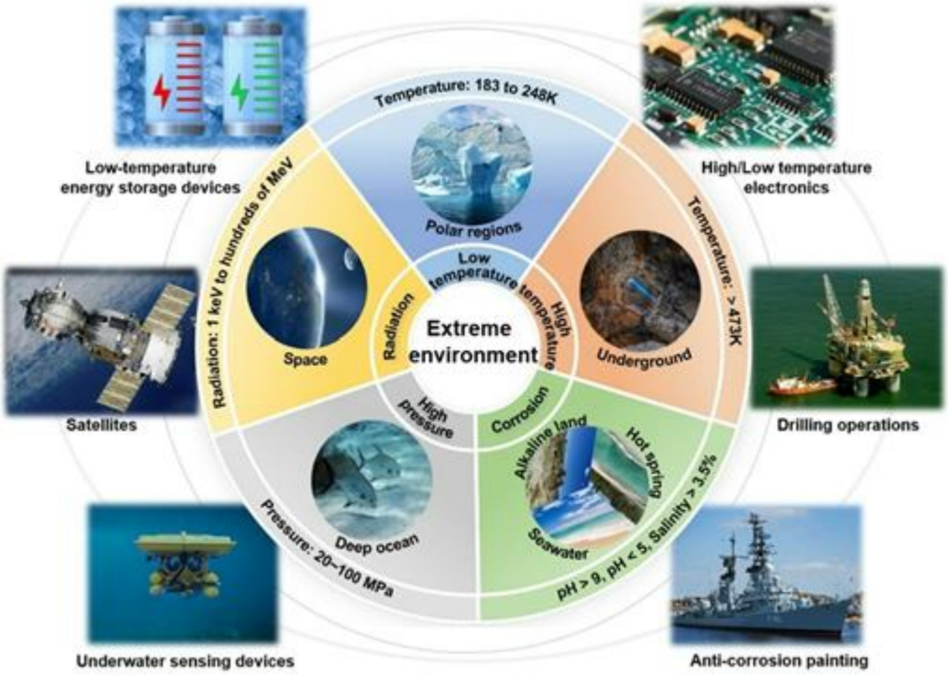
Extreme environments represent numerous harsh environmental conditions, such as temperature, pressure, corrosion, and radiation. The tolerance of applications in extreme environments exemplifies significant challenges to both materials and their structures. Given the superior mechanical strength, electrical conductivity, thermal stability, and chemical stability of nanocarbon materials, such as carbon nanotubes (CNTs) and graphene, they are widely investigated as base materials for extreme environmental applications and have shown numerous breakthroughs in the fields of wide-temperature structural-material construction, low-temperature energy storage, underwater sensing, and electronics operated at high temperatures. Here, the critical aspects of structural design and fabrication of nanocarbon materials for extreme environments are reviewed, including a description of the underlying mechanism supporting the performance of nanocarbon materials against extreme environments, the principles of structural design of nanocarbon materials for the optimization of extreme environmental performances, and the fabrication processes developed for the realization of specific extreme environmental applications. Finally, perspectives on how CNTs and graphene can further contribute to the development of extreme environmental applications are presented. [1-6].



Extreme-environmental applications

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P018

CARRIER DOPING EFFECT OF FUNCTIONALIZED SUMANENES ON CARBON NANOTUBE

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Sumanene $C_{21}H_{12}$[1] has an electric dipole due to the bowl-shaped structure, and the dipole moment can be modified by the termination (H, O, F). Sumanene also exhibits an inversion of the bowl structure by mechanical stress or an electric field,[2] and hence an inversion of an electric dipole.[3] A combination of sumanene and semiconducting carbon nanotubes (CNTs) has great potential to realize a nanoscale molecular memory. In this study, various types of functionalized sumanenes were coated on CNT thin-film transistors (TFTs) to investigate the interactions between sumanenes and CNTs. Functionalized sumanenes were spin-coated on CNT TFTs. Three types of devices were fabricated with monofluoro (F1)-, difluoro (F2)-, and hexafluoro (F6)-sumanene, respectively. The electrical characteristics of CNT TFTs were measured in a glove box after the removal of adsorbed water molecules. The threshold voltage of F1-, F2-sumanene, and F6-sumanene exhibited a negative (Δp=-1.4×10^{11}, -1.3×10^{11} $\mathrm{cm^{-2}}$) and positive (Δp=$+6.7\times10^{10}$ $\mathrm{cm^{-2}}$) shift, respectively, compared to the that of pristine CNT TFT. This result can be explained by the balance between the electron transfer due to the high electron affinity of the F termination and the electric field doping by the dipole of sumanene.

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P019

CHARACTERIZATION OF TWO-TERMINAL SUSPENDED CHEMICAL VAPOR-DEPOSITED GRAPHENE FIELD-EFFECT DEVICES FOR SENSING APPLICATIONS

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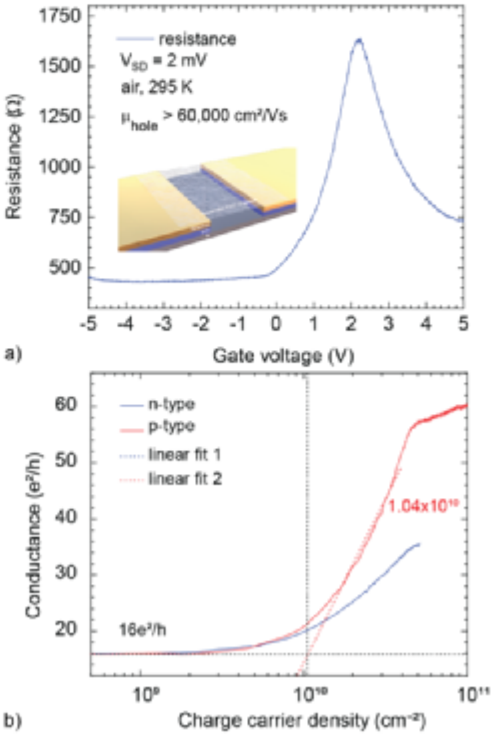
Chemical vapor deposition is a useful method to grow large-area, single-layer graphene films on copper films. Using the polymer-assisted transfer technique, the transfer of large-area graphene films over a wafer scale is achievable. However, challenges related to improving CVD graphene device performance metrics (field-effect mobility) using polymer-assisted methods have remained. Such enhancements of field-effect mobility in graphene devices have been extensively studied under different device architectures. Primary architecture considers the direct fabrication of graphene devices on oxide substrates.[1] Secondary architecture has explored the encapsulating graphene films with insulating 2D material layers using dry transfer methods. Tertiary approaches have explored the suspension of the graphene film using polymer-assisted methods. We demonstrate the realization of such tertiary device architectures with suspended chemical vapor-deposited graphene films using standard microfabrication approaches. Our simplified approach demonstrates >10x improvement in field-effect mobility compared to CVD graphene devices on SiO2/Si substrates.[1, 2] In addition, we demonstrate the use of current annealing techniques under ambient conditions to reduce polymeric surface contamination of CVD graphene devices. Our approach shows the realization of CVD graphene devices with high-performance metrics and offers a viable, scalable alternative to encapsulation and solvent-assisted methods.[3]

Keywords: charge scattering, chemical vapor deposition (CVD), graphene



Characterization of suspended CVD graphene devices. Fig. 1a) Field-effect characteristics of a suspended CVD graphene device, 1b) Conductance vs the charge carrier density profile extracted from the FET characteristics. Note the low residual charge carrier density of ~1x10^10 cm-2 observed in this device.

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P020

CIRCULARLY POLARIZED NEAR-INFRARED PHOTO- AND ELECTROLUMINESCENCE FROM ENANTIOPURE SINGLE-CHIRALITY SINGLE-WALL CARBON NANOTUBES

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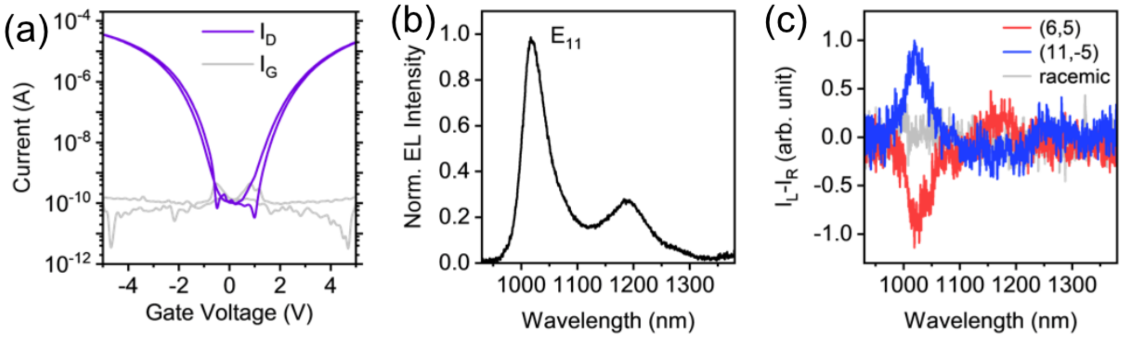
Near-infrared (NIR) light-emitting devices exhibiting circularly polarized luminescence (CPL) have potential applications in spintronics, quantum computing, and optical communication. Especially, the NIR II region above 1000 nm is important for optical diagnostics and bioimaging. However, inherently circularly polarized light-emitting devices in the NIR II region have not yet been realized due to the lack of suitable chiral emitters. Semiconducting single-wall carbon nanotubes (SWCNTs) are chiral materials that exhibit NIR emission in the NIR II region and already have been applied in light-emitting devices [1,2]. Recently, advanced separation techniques [3-5] have made it possible to obtain sufficient amounts of enantiopure single-chirality SWCNTs exhibiting clear circular dichroism (CD). CPL is an analogue of CD and often the associated dissymmetry factors are correlated. Hence, CPL from enantiopure SWCNTs can be expected. Here, we demonstrated NIR circularly polarized photo- and electroluminescence from enantiomer-sorted SWCNTs. Enantiopure (6,5) and (11,-5) SWCNTs were separated by gel chromatography and films were deposited on glass substrates with source-drain electrodes followed by a gate dielectric and gate electrode to create light-emitting transistors. The transistors exhibited ambipolar charge transport and electroluminescence with a peak corresponding to E_{11} of (6,5) and (11,-5) SWCNTs. Circularly polarized electroluminescence and photoluminescence spectra represented by the difference between the intensity of right-handed (I_R) and left-handed emission (I_L) could be recorded with opposite signs between (6,5) and (11,-5). This first observation of CPL from SWCNTs opens up new applications in the NIR II region.



Transistor and optical properties of SWCNT films. (a) Transfer characteristics of a (6,5) SWCNT transistor. (b) Representative EL spectrum of the transistors. (c) CP EL spectrum of transistors with enantiopure and racemic SWCNTs.

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P021
TOWARD 1D/2D HETEROSTRUCTURES FOR NANO-OPTICS

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Since the discovery of graphene, the assembling of 2D semiconductors in van der Waals (VdW) heterostructures results in the emergence of fascinating properties1 with potential impact in nano-optics. However, the presence of intrinsic structural defects and inhomogeneities in 2D semiconductors, associated to indirect band baps and low quantum yields, still limit their study and use in nanophotonics as effective emitters. In contrast, 0D materials such as luminescent organic molecules display strong light/matter interaction and intense light emission properties. On another hand, molecules are fragile, highly sensitive to their environment and difficult to arrange and position.

In this presentation we show that nanotubes can be used as template for the integration of 1D chain of luminescent molecules2–4 in 2D materials. We present preliminary results on the 0D/1D/2D fabrication process, their structural characterization and luminescence properties.

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P022

COMPREHENSIVE MODEL FOR THE THERMOELECTRIC PROPERTIES OF TWO-DIMENSIONAL CARBON NANOTUBE NETWORKS

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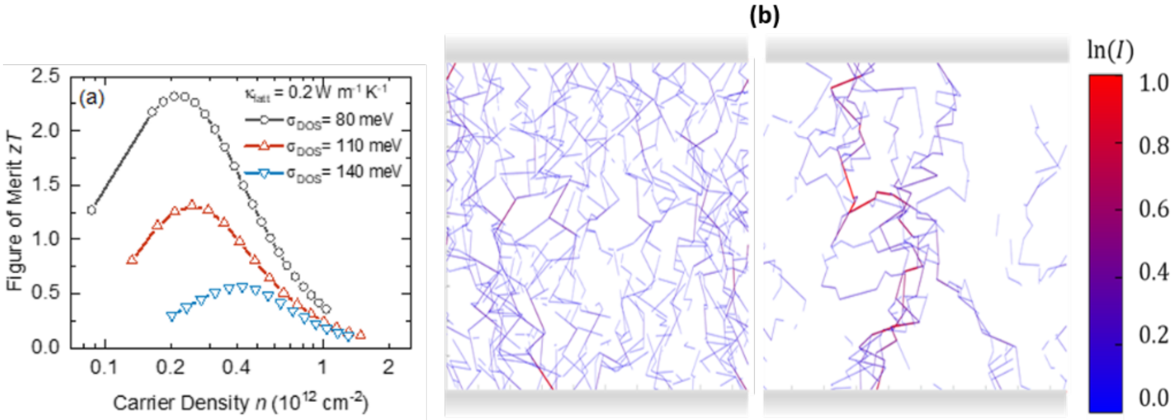
Networks of semiconducting single-walled carbon nanotubes (SWCNTs) are interesting thermoelectric materials due to the interplay between CNT and network properties. We developed a unified model for charge and heat transport determining the thermoelectric properties of 2D CNT mesh-like networks. These meshes can be treated as a random resistor network where disorder-shifted 1D DOS are integrated into the steady state master equation and the Landauer formalism is used for modelling the junction and tube resistances. The model provides a consistent description of a wide range of previously published experimental data for temperature and charge-carrier-density-dependent conductivities and Seebeck coefficients, with energetic disorder being the main factor to explain the experimentally observed mobility upswing with carrier concentration. In more details, electrical and thermoelectric properties of the network are obtained by solving Kirchhoff's laws through a modified nodal analysis, where we use the Boltzmann-transport formalism to obtain the conductivity, Seebeck coefficient, and electronic contribution to the thermal conductivity. Moreover, we show for lower disorder energies, the Lorentz factor obtained from the simulation is in accordance with the Wiedemann-Franz law for degenerate-band semiconductors. Suppressed disorder energy and lattice thermal conductivity can be the key to higher thermoelectric figures of merit, zT, in SWCNT networks, possibly approaching or even exceeding zT = 1.



(a) Calculated thermoelectric figure of merit dependence on carrier density, parametric in energetic disorder. (b) Current distribution in the SWCNT network with varying disorder at constant Fermi energy. Lower to higher disorder from left to right.

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P023

CONTACT ANGLE DEPENDENCE OF CONDUCTANCE BETWEEN CARBON NANOTUBES FROM TIGHT-BINDING SIMULATIONS

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Aligning carbon nanotube (CNT) materials to a high degree can lead to remarkable improvements in their bulk electrical properties [1]. While some previous studies have shown that orbital overlap, alignment and registry effects can improve conductance, those studies are either limited in scope [2] or use simplified tight-binding (TB) models which do not fully consider the local orbital geometry for inter-tube contacts [3]. To account for these shortcomings, we present a large-scale TB study on the effects of registry and contact angle on CNT conductance. The TB model employed in our study accounts for overlap integrals of Slater p and s orbitals, depending on their relative orientation [4]. The study considers 231 distinct pairs of metallic CNTs of different helicities in point contact, in a total of 1,319,472 unique contact geometries. Conductances between all leads connected to the scattering region are calculated using the Landauer-Buttiker formalism in the Kwant package [5]. We show that measured conductances depend strongly on the specific contact geometry, resulting in a highly variable conductance spectrum as the contact geometry changes. Statistical averaging reveals that small contact angles dramatically improve inter-tube conductance due to increased orbital overlap and stronger inter-tube coupling. Likewise, registry effects are also observed where the orientation of the hexagonal lattices of the two CNTs in contact coincide. We further show that registry effects are only significant compared to overall alignment effects when the registry mismatch angle is less than 10°. Additionally, we observe that, regardless of relative helicity of contacting tubes, CNT-CNT contacts are sufficient to cause significant backscattering of Bloch waves in both CNTs, substantially limiting the overall conductance. These findings are used to derive practical design goals for CNT materials which aim to optimise inter-tube conductance whilst minimising backscattering. Our findings confirm that making structures containing fully-aligned near-armchair CNTs is likely the best way to bring the remarkable properties of individual CNTs to the macroscale.

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P024

CONTINUOUS GAS-PHASE SYNTHESIS OF SIZE-PRECISE CATALYST NANOPARTICLES FOR SINGLE-WALLED CARBON NANOTUBE GROWTH

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Prized for their extraordinary properties at the microscale, single-walled carbon nanotubes (SWCNTs) continue to attract interests from multiple research disciplines. Yet it remains a challenge to produce high-quality SWCNTs economically and efficiently. Currently, the two mainstream approaches are post-synthesis sorting and direct growth. As the former often involves solution-based processes that can contaminate or even damage the CNTs, the direct growth is favoured for it better preserves the intrinsic properties of SWCNTs for downstream applications. Nanoparticles (NPs) play a determining role in this latter method for they can directly influence the diameter and chirality of the SWCNTs [1]. However, the lack of capabilities that offer precise control over the particle size still hinders the fundamental research in this realm and subsequent SWCNT manufacturing. Among the myriad of catalysts choices, metals that become liquid during CNT growth (normally Fe, Co, or Ni based) are believed to give better growth kinetics. For the same reason, it is challenging to precisely control their size. By coupling an aerosol furnace reactor with inline size selection and deposition, we report a new technique towards precise and scalable synthesis of small (<2 nm) and monodisperse (geometric standard deviation <1.25) iron catalyst NPs for high-quality SWCNT production [2]. Moreover, the modular approach offers independent control over the catalyst size (1-8 nm), the choice of supporting substrate, and the SWCNT synthesis conditions. This enables us to investigate the correlation between the size of the catalyst NPs and their performance in subsequent reactions. We compared the diameter distribution of SWCNTs grown from size-selected 3.6 nm and 1.8 nm iron-oxide NPs via Raman spectroscopy and observed a constraining effect by NP size on SWCNT diameter that becomes more prominent with smaller NPs: 1.8 nm iron-oxide NPs have a strong preference to produce more 1.2 – 1.4 nm SWCNTs. We also find that as the particle size is further suppressed to less than 1.4 nm, its ability to catalyse SWCNT growth weakens. This gas-phase synthesis route for catalyst nanoparticles, with its capability in mobility-based size-control, shows great potential in achieving scalable production of high-quality SWCNTs. It also creates new opportunities to probe the influence of nanoparticles in often complex processes involved in nanomaterial manufacturing.

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P025

CONTROL OF GRAPHENE ISLAND NUCLEATION ON GRAPHENE/SIC TEMPLATE BY SEQUENTIAL THERMAL PROCESSES IN VACUO WITHOUT AIR EXPOSURE

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Layer-by-layer growth of graphene by chemical vapor deposition (CVD) with ethanol is a potential method for van der Waals (vdW) homo-epitaxial growth of twisted multilayer graphene (tMLG) [1]. In previous publication, we demonstrated the twisted structure of grown graphene layers on monolayer graphene templates by scanning transmission electron microscopy (STEM) and 2D peak analysis of Raman spectroscopy [2]. Unfortunately, the scattering effect of the charged impurity induced by defects in grown graphene layers limited the carrier mobility of the field effect transistors using grown tMLG. Hence, the mechanism of layer-by-layer growth by CVD with ethanol is a key point for vdW homo-epitaxial growth of tMLG. In recent study, the synthesis of tMLG is prepared on graphene/SiC template with atomically flat surface for structure analysis [3]. We verified that moiré pattern appears in the lattice structure of the grown graphene island and the grown graphene islands have the randomly twisted angles. By investigating the temperature dependence of graphene island morphology, the emergence of graphene islands with different twist angles indicates that excessively localized nucleation sites lead to coalescence processes during the lateral growth stage. In this study, to suppress the nucleation sites, we further optimized the surface cleanliness of templated monolayer graphene by sequential thermal (ST) processes, which serially performed annealing treatment and CVD treatment. The high-quality monolayer graphene used as template was synthesized on SiC by the annealing treatment in argon atmosphere at 1725 °C, ~1 bar and then tMLG was grown by the CVD treatment with ethanol after cooling down in the same vacuum chamber. A wide growth temperature ranging from 1000 ºC to 1500 ºC was investigated during the ST processes for comparison with the air-exposure processes [3]. Graphene islands were laterally grown in the temperature range from 1100 °C to 1300 °C, and the temperature dependence of nucleation density is opposite to air-exposure processes. By comparing the surface condition of template graphene after annealing treatment, the growth mechanism of tMLG layer-by-layer growth in two processes can be concluded. The contrasting growth behaviors suggest that the contaminant from air on the graphene template participated in the ethanol decomposition and surface etching process, then increased the nucleation density. From these results, the nucleation density was effectively suppressed in the ST processes with contaminants removed. It is further expected to make progress in the large-area lateral layer-by-layer growth of tMLG.

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P026

CONTROL OF HIGH-HARMONIC GENERATION IN TRANSITION METAL DICHALCOGENIDE BY CARRIER INJECTION

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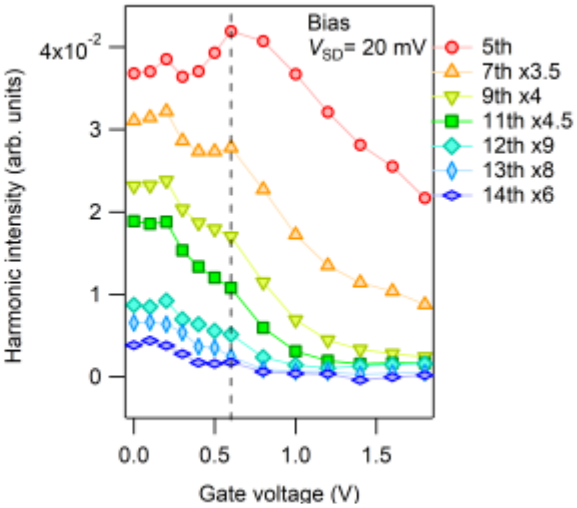
The recent development of a high-power mid-infrared laser enables us to observe high-harmonic generation (HHG), the generation of multiple optical harmonics through the non-perturbative process[1]. There are two distinct mechanisms of HHG: generation from the nonlinear transition of the carriers between bands (interband dynamics) and nonlinear oscillation within a band (intraband dynamics). Previously, we found that the carrier injection strongly influences HHG in semiconducting carbon nanotubes with bandgap energy $E_g = 1.26$ eV [2]. For example, the increase in the carrier density suppresses the 5th and higher harmonics above the E_g, however, we found that it enhances 3rd harmonics, which is below E_g. These results suggest that in the wider-gap sample higher-order harmonics would be enhanced by carrier injection. In this study, we investigate the dependence of HHG on the carrier injection in the molybdenum disulfide (MoS_2), which has $E_g = 1.8$ eV (> 5th harmonics). We expect that the harmonics below 5th would be enhanced by the carrier injection. In addition, we also investigate the behavior of even order harmonics, which can be generated by the lack of inversion symmetry, in the monolayer MoS_2.We used monolayer MoS_2 grown by the chemical vapor deposition method on a sapphire substrate and employed a side-gating device using an ionic liquid, which tunes the Fermi level by a shift of gate voltage V_G. In the measurements, intense 4.8-μm-wavelength lasers irradiate the sample to generate HH. As a results, we found that the 5th harmonics increases as injecting electrons, but the other harmonics decrease almost monotonically. These results agree with what we have expected. In addition, we observed that the even harmonics such as the 12th and 14th orders also decrease as the increase of the injected carriers like 13th harmonics.



Change of HHG by carrier injection. HH intensity in MoS2 as a function of gate voltage.

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P027

CONTROLLED GROWTH OF HORIZONTALLY ALIGNED SINGLE-WALLED CARBON NANOTUBE ARRAYS

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Single-walled carbon nanotubes (SWNTs), especially horizontally aligned SWNT arrays, have become one of the most promising materials for next-generation electronic systems due to their special nanostructure and excellent electrical properties. However, the synthesis of SWNT arrays still faces two major problems, purity and yield. Synthesis determines the future. For further promoting the practical application of carbon nanotubes, growth of SWNT horizontal arrays with controlled structures and high density is imperative. In the chemical vapor deposition (CVD) growth of carbon nanotubes, catalyst is of vital importance. We found that, carbide catalysts with high melting point can maintain their crystal structures at the growth temperature, so the nucleation of carbon nanotubes can be thermodynamically controlled to have the same symmetry with the catalyst crystal plane. Further optimization of growth kinetics can result in the enrichment of carbon nanotubes with specific chirality.[1] In order to increase the yield of SWNTs with controlled structures, we developed an approach of in-situ preparation and continuous loading of solid catalysts: floating solid catalyst CVD (FSCCVD).[2] The carbide catalyst nanoparticles were directly obtained in the carrier gas by decomposition and carbonization of catalyst precursor at high temperature. SWNT horizontal arrays can be obtained on ST-cut quartz substrates after the deposition of TiC catalyst nanoparticles, and the chirality of the grown SWNTs had the same symmetry as the carbide catalyst crystal plane. The enrichment of (16, 8) tubes with a purity of 74% was finally realized. This method can be further used to realize the direct growth of high-density arrays via a spacially confined strategy, which greatly increase the deposition efficiency of the catalyst nanoparticles and the growth efficiency of the SWNTs through a trapping effect. As a result, high-density of ~65 tubes/μm and high semiconducting purity of ~97% were obtained at the same time, benefiting from the titanium-based catalyst structures[3]. We are now trying to untilize the charge-transfer between catalysts and SWNTs with the assistance of illumintion to selectively synthesize semiconducting tubes. From fine structure control to continuous growth, we provides new ideas for preparation of SWNTs with high-density and specific structures, and aims to realize wafer-scale, high-density SWNT arrays with controlled structures.

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P028
THEORY OF SIGMA BOND RESONANCE IN FLAT BORON MATERIALS

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In chemistry, theory of aromaticity and π bond resonance plays a central role in intuitively understanding the stability and properties of organic molecules. Here we present an analogue theory for three center two electron (3c-2e) σ bond resonance in flat boron materials, which allows us to determine the distribution of two-center two-electron and three-center two-electron bonds without quantum calculations. Based on this theory, three rules are proposed to draw the Kekulé-like bonding configurations for flat boron materials and to explore their properties intuitively. As an application of the theory, a simple explanation of why neutral borophene with ~1/9 hole has the highest stability and the effect of charge doping on borophene's optimal hole concentration is provided with the assumption of σ and π orbital occupation balance. Like the aromaticity theory for carbon materials, this theory greatly deepens our understanding on boron materials and paves the way for the rational design of various boron-based materials.

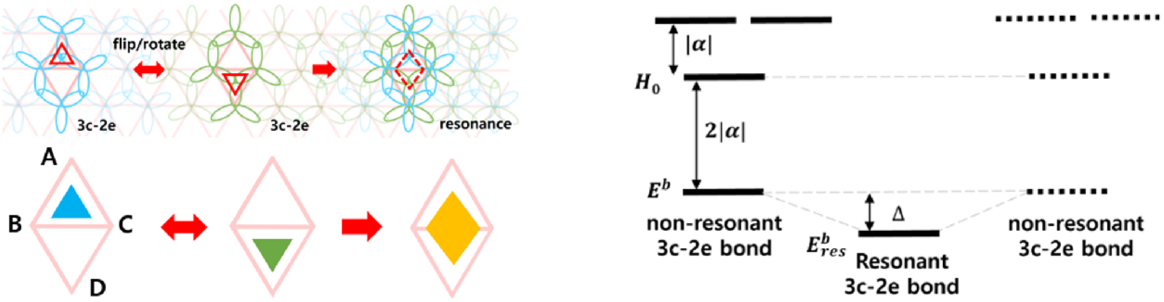

Figure. 1. A resonance model for alternating 3c-2e bonds in a triangular boron lattice(left) and the energy level of the 3c-2e resonance state by the linear combination of atomic orbitals (LCAO).

P029

SINGLE-WALL CARBON NANOTUBE FUNCTIONALISATION AND NETWORK ASSEMBLY

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Single-wall carbon nanotubes (SWCNTs) have attracted attention because of their unique optical, electronic, and physical properties, which lead to potential applications in optoelectronic and bio-sensing devices. However, it is a challenge to organise large networks of SWCNTs for these devices. The main issues regarding this are the economical processability and micro-scale controllability. This project aims to organize large SWCNTs into networks, alongside functionalising the SWCNTs with the aim to control junction formation. We will discuss two methods we developed for the assembly of the large SWCNTs networks. First, a facile-modified filtration method was used to prepare a thickness-controllable SWCNT thin film. The thickness is controlled by the SWCNTs concentration and sample volume. In the second, an external point source vapour system[1] is used. This is to control the SWCNTs depositing behaviour on the substrate, with the fabrication of an arranged pattern expected. Following these assembly methods, various functionalized SWCNTs are introduced. Site controllable functionalisation, such as amidation[2], diazonium reaction[3] and cycloaddition[4], can be achieved by DNA wrapping of the nanotubes. The ability to produce functionalised SWCNTs layers with a scalable, low-cost approach should take us a step closer to next-generation device applications.

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P030

CONTROLLED SYNTHESIS OF HIGH PACKING DENSITY SWCNT FIBER USING AEROSOL ROUTE FOR DEVELOPMENT OF HIGHLY EFFICIENT THERMOELECTRIC GENERATOR

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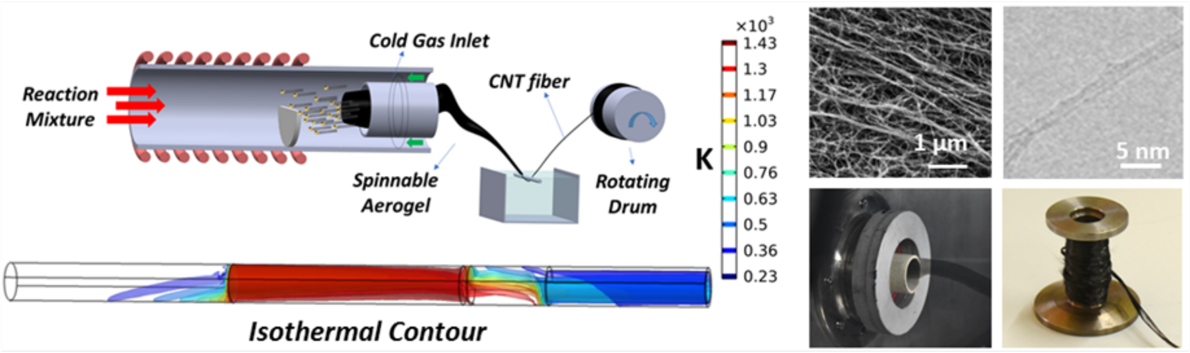
Despite numerous advantages, synthesis of amorphous carbon is a serious impediment for continuous synthesis of single wall carbon nanotube (SWCNT) fiber using floating catalyst chemical vapor deposition (FC-CVD). The removal of amorphous carbon post synthesis causes deterioration of properties of the SWCNT fiber synthesized in this process. There is a tradeoff between yield of SWCNT synthesis and amorphous formation. It was also observed that spinning of SWCNT aerogel into fiber is highly correlated with amorphous content. To overcome this issue, flow engineering has been used to control amorphous formation while maintaining the yield of SWCNT synthesis. This approach can improve the properties of the final product by reducing the amount of amorphous carbon and increasing the degree of alignment of the SWCNTs. The strategy used in this work also employs insitu densification of CNT aerogel resulted in synthesis of SWCNT with high electrical conductivity (4.5 MS/m) and lower defects (IG/ID >100). In this way, SWCNT fiber has been synthesized continuously for 12 hours using the optimized parameters with less than 1% amorphous carbon. Fabrication of thermoelectric generator with very high power factor ((20 mW m−1 K−2) was demonstrated using SWCNT fiber synthesized in FC-CVD process.



Schematic showing flow engineering in FC-CVD process for producing SWCNT fiber and isothermal contour at optimized condition in CFD study along with images of aerogel, fiber, TEM and SEM of SWCNT produced in this process (counter clockwise direction)

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P031

CONTROLLING EXCITON SIZE IN (6,5) CARBON NANOTUBES BY USING SOLVENT MIXTURES

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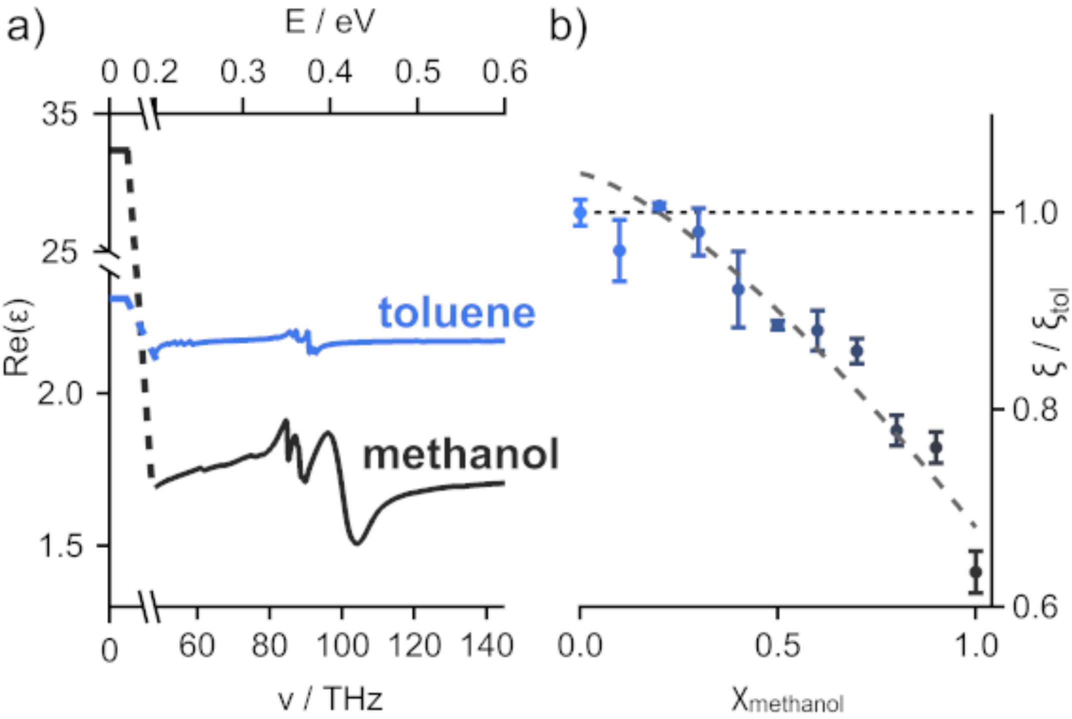
Size, mobility, and binding energy of excitons in low-dimensional semiconductors depend on the character of the environment, specifically its relative permittivity ε_r. However, it remains unclear which part of the spectrum of ε_r most significantly affects exciton character. Here, we investigate excitons with binding energies of several 100 meV [1,2] and a size ξ of several nanometers [3,4] in thin films of polymer-stabilized semiconducting (6,5) single-wall carbon nanotubes (s-SWNTs). We correlate changes in exciton size ξ with the character of the solvent environment by quantifying absorption-induced changes of exciton oscillator strengths using femtosecond time-resolved transient absorption spectroscopy and apply the phase space filling approach to determine exciton size [3,4,5]. Increasing the static relative permittivity $\varepsilon_{r,\ stat}$ by using toluene ($\varepsilon_{r,\ stat} = 2.4$) or methanol ($\varepsilon_{r,\ stat} = 33$) as solvent results in a decrease of exciton size by 36±2 % contrary to expectations, suggesting an increase at higher $\varepsilon_{r,\ stat}$ [6]. This indicates that the exciton character is controlled by higher frequency contributions of the dielectric function shown in Fig. 1.



Solvent dependent change in exciton size. a) Frequency dependence of the relative permittivity of methanol and toluene [7]. b) Change of exciton size in (6,5) s-SWNTs with methanol mole fraction.

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P032

CONTROLLING THE DIAMETER OF SINGLE-WALLED CARBON NANOTUBES USING NIW AND NIMO BIMETALLIC CATALYSTS

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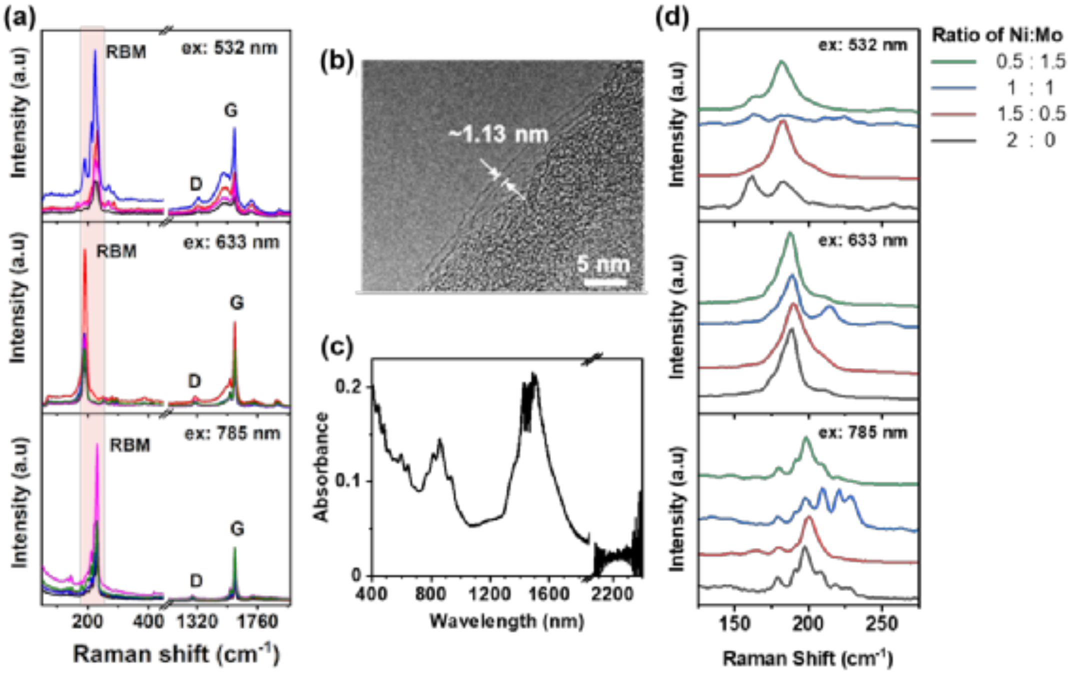
Using bimetallic catalysts is an important strategy to control the structure of single-walled carbon nanotubes (SWCNTs). In our previous studies,[1] we developed NiW bimetallic catalysts to grow SWCNTs with narrow diameter distribution on Si substrates. The W species played the role of dispersing and stabilizing Ni nanoparticles, thereby limiting the diameter of SWCNTs. A major feature of this catalyst is that it can effectively control the diameter distribution of SWCNTs in a wide growth window. Herein, we extended this catalyst system to the synthesis of bulk SWCNTs by chemical vapor deposition (CVD) and laser ablation. In CVD synthesis, we found that the diameter distribution of SWCNTs grown by NiW catalysts concentrated in the range of 1.05–1.28 nm, which was significantly narrower compared with those grown on monometallic Ni catalysts. The diameter distribution is greatly affected by the calcination and reduction processes of NiW catalysts, which may be due to the sublimation of WOx species at high temperature, which affects the formation of NiW catalysts. In the laser ablation method, we also found that the introduction of W or Mo can effectively reduce the diameter of SWCNTs, which indicates that W and Mo species may also play a role in limiting the size of Ni. Under optimized conditions, we have grown SWCNTs with diameters concentrated in the range of 1.10-1.35 nm using NiMo catalyst. Due to the suitable band gap and energy band position of these nanotubes, they are expected to be used as desirable channel materials in electronic devices.



SWCNTs with narrow diameter distribution grown by NiW catalyst in bulk CVD (a & b) and NiMo catalyst in laser ablation (c & d).

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P033

COVALENTLY BONDED GRAPHENE-CARBON NANOTUBE HYBRIDS

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The integration of carbon nanotubes (CNT) and graphene with covalently bonded junctions is of great significance to inherit the outstanding properties of each component and obtain additional advantages afforded by the multiscale structures. We fabricated covalently bonded graphene/CNT (G/CNT) structures by a facial thermal chemical vapor deposition (CVD) method. The defective carbon on the sidewall of CNTs can serve as nucleation sites for vertical growth of graphene to form a branch-leaf structure. Attributed to the advantage of the covalently bonded structure, the as-synthesized G/CNT structure exhibit high electrical conductivity, large specific surface area and excellent anti-agglomeration properties. G/CNT are expected as promising platform for electrocatalysis, in which electrons can be quickly transferred from the conductive network of CNTs to graphene through the covalently bonded junctions, and graphene increases the exposure of surface area for mass transport and charge transfer in electrolyte. As a proof of concept, G/CNT were applied as substrate to disperse iron species as oxygen electrocatalyst, which exhibited higher activity and durability than commercial noble-metal catalysts. These multiscale G/CNT structures are also highly promising for other energy and environmental applications.

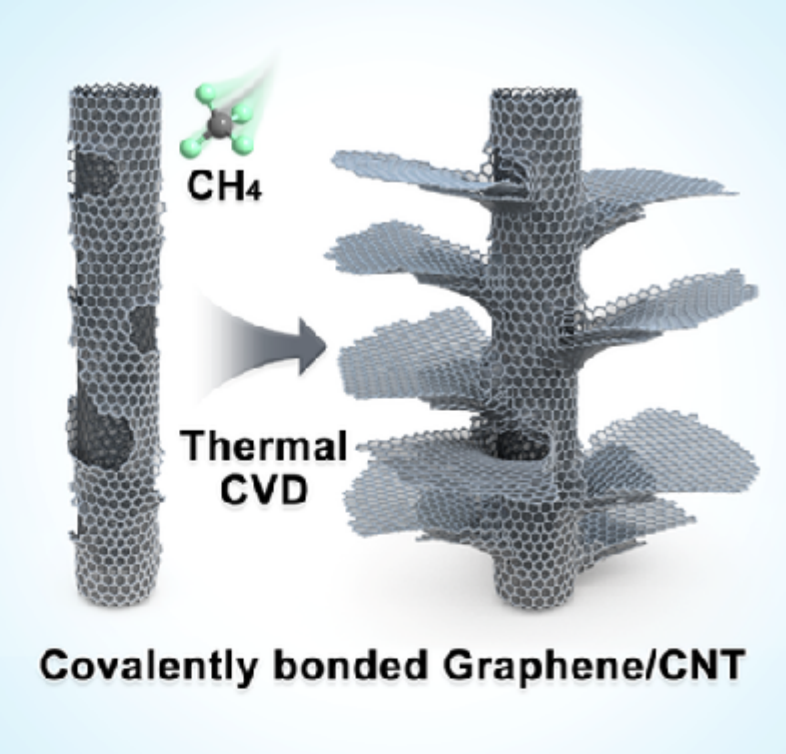

Fig.1. Schematic illustration for the synthesis of Covalently Bonded Graphene-Carbon Nanotube Hybrid

P034

CREATION OF STABLE BIOMIMETIC NANOPORES IN VIEW OF DESALINATION

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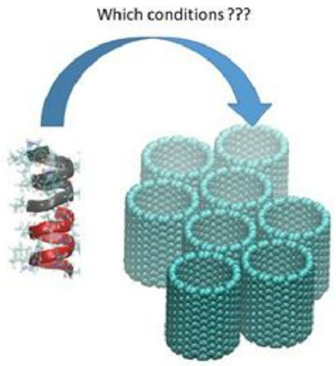
Due to climate change, developments in industrialization and increasing population growth are major factors that currently lead to the risk of water scarcity worrying the whole world. However, existing membrane technologies for water treatment suffer from inherent limitations in membrane materials and manufacturing techniques, which further diminish their performance in terms of permeability and selectivity as well as their excessive energy consumption.[1] To overcome the limitations of these membrane technologies, biomimetic approaches that mimic biological processes are considered promising solutions.[2]

The biomimetic membrane is composed of a biological channel confined inside a solid-state nanopore such as a carbon nanotube. Of all the existing ion channels, proteins such as gramicidin A are of particular interest. Indeed, they can organize themselves in biological membranes to spontaneously create nanochannels responsible for the selection of monovalent cations over divalent or anions. This is at the origin of their antibiotic actions due to the irregular distribution of ions within the host cell.

The transfer of biological entities into artificial nanopores such as carbon nanotubes requires several precautions because the environment of the protein will be different from lipid membranes.[3,] In this work, the effect of conformational stability of the protein inserted inside nanopores of different chiralities and the use of stapling strategies that allow the protein to retain its initial structure is studied using molecular dynamics simulations.

Our simulations results obtained demonstrate that the radius of the nanotube is a key factor and should be chosen with extreme care to stabilize proteins and let them work inside the carbon nanotube.



Membrane creation. Which conditions are necessary to insert the biological channel inside the carbon nanotube without perturbing the inherent properties of the polypeptide ?

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P035

CRYO RAMAN STUDY OF CONFINED CARBYNE

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Carbyne is a true one dimensional allotrope of carbon, consisting of an infinitely long chain of carbon atoms. Theoretical calculations predict outstanding mechanical, optical and electronic properties. It is highly unstable and has only ever been successfully synthesized inside carbon nanotubes, aptly named confined carbyne (CC). Based on our recent progress in the synthesis of CC regarding the yield and tailored properties [1-4] in combination with the huge resonance Raman cross section [5] there is a great application potential for thermometry via the temperature dependent line shape [6] and the Stokes/AntiStokes ratio [7].

We built a new in-situ Raman spectroscopy cryo-setup attached to our T64000 Horiba Triple monochromator system to unravel the temperature dependent response between 4-300 K in combination with laser annealing up to the synthesis temperature of confined carbyne. In this contribution we will show recent progress in unravelling the details of the temperature dependent carbyne response in the full temperature region accessing the full potential of contact free local thermometrical applications.

This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation program (MORE-TEM ERC-SYN project, grant agreement No 951215)

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P036

DEFECT ENGINEERING FOR HIGHLY ACTIVE TIO2 NANOTUBES PHOTOCATALYSTS

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The development of cost-competitive materials capable of producing fuels or electricity directly from the energy harvested from sunlight offers a desirable approach to fulfilling the need for clean, sustainable, and secure energy. Semiconductor metal oxide such as TiO2 in the morphology of self-organized nanotubes is abundant, photoactive, stable and cheap; and thus it has been among the most widely adopted materials for the conversion of solar energy into storable and transportable chemical energy such as e.g. hydrogen (H2). However, despite a huge scientific effort, its overall efficiency for solar-driven applications remains rather low due to several crucial limitations such as particularly fast recombination of photo-generated charges (electron-hole pairs) and sluggish kinetics of the redox surface reactions that hinder the practical application in this field. Defect engineering has become an attractive research direction for improving the optical and electronic properties of semiconductor photocatalysts towards boosting their photo(electro)chemical performance. For example, so-called non-stoichiometric black TiO2 (1) has demonstrated unexpectedly enhanced photo(electro)chemical activity, which has been attributed to the co-catalytic effect of unsaturated Ti3+ ion at the titania surface due to the presence of oxygen vacancies (VO). Additionally, these unsaturated defects/sites provide a strong affinity to tightly bond or anchor various species such as transition metals single atoms that can be used as even more effective co-catalysts. In this contribution, recent advancements regarding defect engineering toward significantly enhanced photocatalytic activity of TiO2 nanotubes will be summarized. (2-4)

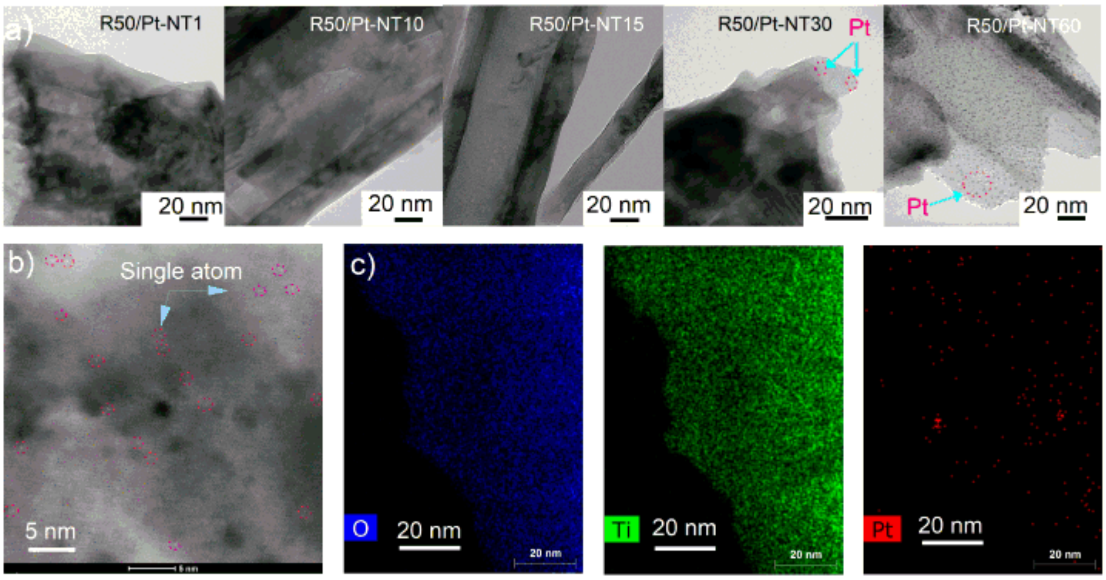

Figure 1. a) TEM images of treated samples at different impregnation time (ranging from 1 to 60 min) in hexachloroplatinic acid solution, b) HAADF-STEM image and c) EDS elemental mapping of R50/Pt-NT10 sample.

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P037

DEGRADATION BY-PRODUCTS OF FEW LAYERS BLACK PHOSPHORUS IN AIR

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As a layered semiconductor, black phosphorus (BP) has experienced increasing interest due to its thickness dependant bandgap and anisotropic physical properties. However, a thorough understanding of the reactivity and degradation of BP in air is still lacking, which limits the development of optoelectronic applications. Previous reports showed that black phosphorus flakes produce phosphoric acid at the surface when exposed to light, oxygen, and water [1]. In this work, we report the growth of micrometer-sized crystals on the surface of BP in air after few days. X-ray diffraction (XRD), Energy-dispersive X-ray spectroscopy (EDX) and Raman experiments reveal ammonium dihydrogen phosphate among the degradation products. To elucidate the origin of nitrogen in this compound, BP degradation process was investigated in highly controlled atmospheres. The conditions behind the formation of this product as well as its effect on degradation are here discussed. This work adds another piece to the puzzle of BP degradation.

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P038

DEVELOPING NEW CARBON FEEDSTOCKS FOR SWCNT GROWTH IN FC-CVD CONDITIONS

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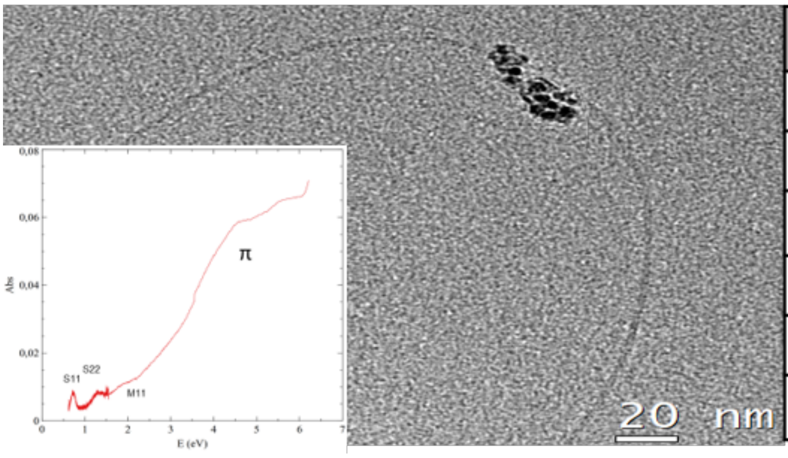
Despite intense research efforts for nearly 30 years, both experimentally and theoretically, the control of the atomic structure during the synthesis of single wall carbon nanotubes (SWCNTs) remains a major challenge. This is indeed a prerequisite to control electronic properties. Nature of carbon feedstocks is one of the control parameters one can play with as shown for instance by He et al. [1] and Liao et al. [2] for tailoring diameter and chirality of SWNTs. With this in mind, we aim at developing completely new carbon feedstocks such as 1,3-dioxolane and tert-butanol, or mixtures, for the growth of carbon nanotube films in FC-CVD conditions, using iron as a metallic catalyst precursor. These two carbon feedstocks, upon thermal decomposition, result in the formation of CO, CH_4 and C_2H_4 for tert-butanol and H_2, CO, CO_2 and C_2H_4 for 1,3-dioxolane in precise amounts. Routine synthesis conditions used in the FC-CVD reactor (880°C, 60 sccm of H_2 and 300 sccm of N_2 and ferrocene as a catalyst precursor) were applied in order to identify and compare the impact of these two feedstocks on the nature of the SWCNTs structure as inspected by optical absorption and TEM (Fig.1).



Product gas	%
H_2	30 - 50%
CO	20 - 25%
CO_2	10 – 20 %
CH_4	8 – 10%
C_2H_4	10 - 18%
C_2H_2/C_2H_6	2 – 5 %

a) Absorption spectra of a thin film of SWCNTs obtained with 1,3-dioxolane, b) TEM image of SWNT formed using 1-3 dioxolane and c) product gas composition of 1-3 dioxolane after a pyrolysis at atmospheric pressure between 963 and 1093K [3]

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P039

DEVELOPMENT AND STUDY OF LAMINATED COMPOSITE MATERIAL INTEGRATING CARBON NANOTUBES FOR LAUNCHER CRYOGENIC TANK APPLICATION

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Recent trends in the spatial fields require building low-cost and lightweight launchers, leading to the replacement of classical metal parts and components by composite materials. However, most of the weight in a launcher comes from its cryogenic storage vessels, and the materials used need to comply with mechanical, thermal, chemical, and fire-resistant specifications, due to the highly oxidative nature of liquid oxygen, and its temperature of -183°C. While carbon fiber/polymer (CF/P) composites are promising candidates, they develop micro-cracks when tested under cryogenic temperatures, leading to leaks [1]. Many research approaches tend to answer to this technological lock, but the potentialities of Carbon NanoTubes (CNTs) in terms of mechanical and physical properties, need to be explored deeper. In this context, our objective is to define the best way to process CNTs within a thermostable labo-grade cyanate ester matrix in layered composite materials for a launcher cryogenic tank. (i) Transfer of aligned CNTs mats or even of entangled CNTs on the carbon fiber fabric pre-impregnated with resin, or (ii) growth of nanotubes aligned directly on the dry ply [2]. The carbon nanotubes used in this study are obtained from an aerosol-assisted CVD (Chemical Vapor Deposition) synthesis technique, yielding vertically aligned carbon nanotube carpets [3-4]. The characteristics of VACNT carpets are tailored by modifying synthesis parameters, to lever on their length, diameter and density. For the transfer technique, nanotubes carpets on aluminum foil are then laid on raw pre impregnated carbon fiber cloth, and fused by hot pressing, then, after cooling, the aluminum foil is peeled off. The pre-impregnated obtained nanocomposite is ready to be stacked and cured through conventional approaches of infusion or hot molding. For the direct growth approach, another aerosol assisted CVD setup is used albeit the introduction of a layer of silica based material, enabling the growth of CNTs on the CF, yielding the same kind of carpets. Then those CNT-covered fibers can be layered and infused with the liquid resin, and cured to obtain the laminated composite material. Different nanotubes orientations and CNT volume content nanocomposites were elaborated and their influence on the mechanical, thermal and ignition resistance properties of the material were investigated. Samples were also observed by SEM after each step of the process, and their resistance against strain and delamination tested mechanically. Then their behavior while and after being at cryogenic temperatures will be characterized the same way in future studies.

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P040

DEVELOPMENT OF MULTI-MEDIA ENVIRONMENTAL SENSORS COUPLING GRAPHENE AND FIELD EFFECT TRANSISTOR

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European environmental standards in the field of water pollution require frequent chemical controls of waters at different sites. The currently used analysis techniques are costly, and do not allow to make the numerous analysis needed for a good monitoring. It is therefore essential to develop new devices, dedicated to micropollutants detection, portable and more adapted to on-site monitoring of aquatic environments. Sensors devices combining graphene with Field Effect Transistor configuration can give these specifications.

The objective is to make use of graphene's exceptional properties (high electrical conductivity, fast electron transfer rate, …) with FET configuration in order to develop micro-sensors.

First of all, the development of the FET based on CVD graphene (AS-One, Annealsys) will be presented with X-Ray Photoelectron Spectroscopy (XPS) and Raman spectroscopy. Characterizations are performed at each step of conception in order to follow surface chemistry and defect rate evolution induced by lithography steps. A fully electrical FET characterization highlighted a variation of the Dirac point position related to a doping of graphene surface induced by the adsorption of molecules, therefore showing the high sensibility of our sensor.

Then, a new design of Graphene FET sensor for metallic micropollutants detection using one droplet of water will be presented. This sensor has been tested and calibrated in water, in presence of a controlled amount of pollutant in order to evaluate the sensibility of the sensors.

The study used a combination of macroscopic characterization techniques (XPS, electrical measurement) and microscopic characterization techniques (AFM, Raman) in order to perform a global evaluation of the evolution of the surface chemistry, morphology, and crystallographic structure of the graphene layer. Overall, this study demonstrates the potential of using CVD graphene coupled with FET for fast, in-situ detection of micropollutants in water.

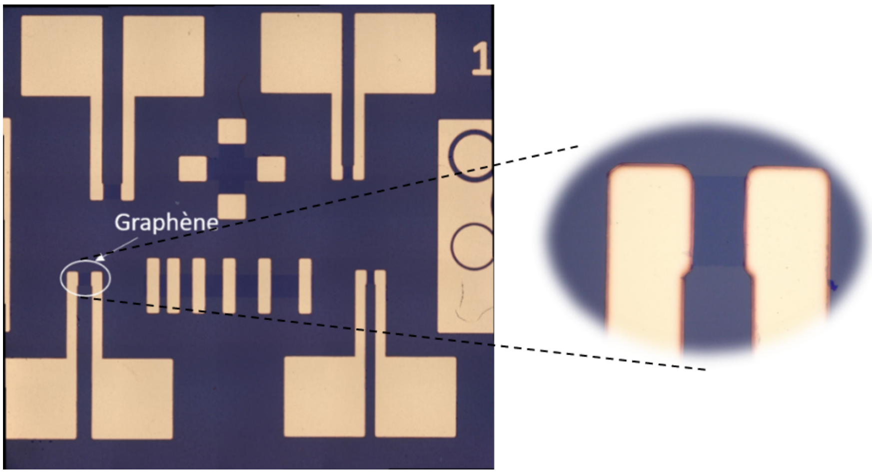

Figure 1. Graphene FET made on SiO2/Si substrates, Between the two surrounded electrodes is the active surface acting as the FET channel.

This work was supported by the region Centre-Val de Loire

P041

MEASUREMENTS OF THE SEEBECK COEFFICIENT AND ELECTRICAL RESISTANCE AT SINGLE NANOCONTACTS BETWEEN CARBON NANOTUBES

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Interface conductivity is a major factor that effects the transport properties of carbon nanotube (CNT)-based materials. CNT films have exhibited high-performance as the thermoelectric materials [1], and their power factors are strongly affected by the geometrical arrangement of CNTs [2]. The arrangements typically have numerous intertube boundaries with various configurations, such as parallel contacts in bundled CNTs and cross junctions of bundled CNTs. These can complicate our understanding of the contribution of each interfacial type to the conductivities when we conduct measurements using macroscale specimens. This study experimentally investigates the thermoelectric and electrical properties of CNTs at a nanometer scale individual interfaces using in situ transmission electron microscopy (TEM) with nanomanipulation techniques. First, a multi-walled CNT is suspended between two electrodes under TEM observation, where the temperature difference between these electrodes is set to 100–150 °C. The thermal electromotive force and two-terminal electrical resistance of the CNT are then simultaneously measured. The measured values of the thermoelectric power and electrical resistance depend on the tube diameters. This bridging CNT is then cut by applying Joule heat to obtain a pair of protruding CNTs, and the tips of each are contacted through Van der Waals interaction to form a single nanocontact [3]. By remeasuring the thermal electromotive force and two-terminal electrical resistance, we examine how these values decrease when a single van der Waals interface is induced on the conduction path. Here, we can arrange the morphological configuration of contacts between two CNTs. Measurements of thermal electromotive forces and two-terminal electrical resistances are conducted separately under several types of nanocontacts to understand experimentally how the contact morphologies affect the transport properties. These nanocontacts include parallel and cross contacts, in which the contact length [4] and junction angle are changed, respectively.

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P042

DICING NANOTUBES FOR FUNS

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We used quantum defects as spectral fingerprints to track defect-induced chemical cutting of semiconducting carbon nanotubes by hydrogen peroxide. Our results reveal that this oxidative reaction involves two distinct stages. In the first state, hydrogen peroxide attacks the defect sites and cuts the nanotube into shorter pieces, with the functional groups that induce the defect photoluminescence remaining at the ends of the cut segments. In the second stage (etching), the nanotubes are etched shorter from the ends, leading to a quick loss of the defect photoluminescence followed by decrease in carbon absorption at constant rates. This cut-then-etch selectivity provides direct molecular insights on the role of defects in carbon nanochemistry and may allow clocking the chemistry to attain fluorescent ultrashort nanotubes (FUNs) for bio-imaging, chemical sensing and quantum photonics.

P043

DIRECT GROWTH OF GLOBALLY ALIGNED GRAPHENE NANORIBBONS ON RECONSTRUCTED SAPPHIRE SUBSTRATE USING PECVD

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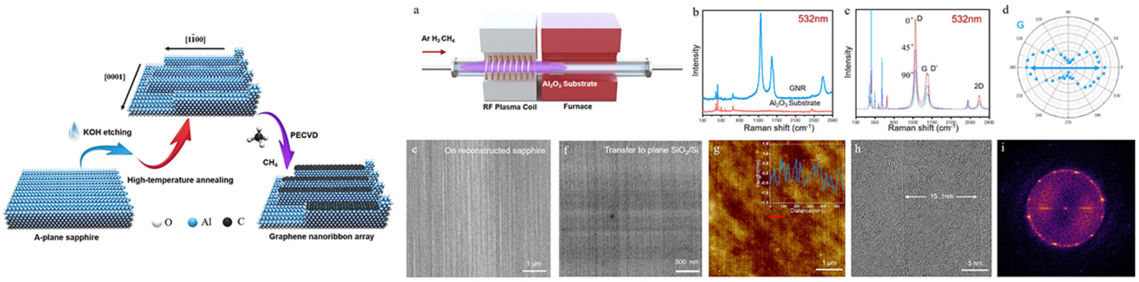
Graphene nanoribbons (GNRs) are regarded as an ideal candidate for beyond-silicon electronics. However, directly growing aligned GNRs with confined widths on insulating substrates has long been regard as a challenging problem. Most preparation strategies of GNRs apply metallic substrates with expensive organic molecules. There is still a lack of methods for the scalable synthesis of globally aligned GNR arrays on insulating substrates with high efficiency. In this work, we develop a facile approach, involving KOH pre-treatment and high-temperature annealing, to construct parallel atomic steps on the two-fold symmetry a-plane sapphire substrate. GNRs with global alignment across a region of 20 mm^2 are then grown on the step edge-enriched substrate through plasma enhanced chemical vapor deposition (PECVD) method. GNRs align well along the atomic steps on sapphire ([1-100]direction) with their widths and densities swiftly adjustable by step morphology modification on substrate surface. Polarized Raman characterization verifies the global alignment of as-grown GNRs on reconstructed sapphire. AFM characterizations demonstrate the high density of GNR arrays and TEM characterization proves the cramped width of GNRs (15.1nm). A step-edge confined growth mechanism is proposed, attributing the constraint on the nanoribbon broadening to a relatively low growth temperature in PECVD, which restrains the activation energy to suppress GNRs across step edges on sapphire and prevent detrimental nanoribbon widening. Our work filled the gap of research for directly growing aligned GNRs on insulating substrates, which provides a simple strategy to scalable synthesize high-density narrow GNR arrays on specific step edge-enriched substrates. We believe that this work would offer a new insight for scalable synthesizing well aligned nanoribbons of other two-dimensional materials.



Synthesis and characterizations of high-density aligned narrow horizontal GNRs. (a) Schematic illustration of synthesizing high-density aligned narrow GNRs with PECVD on reconstructed sapphire substrate. (b) The Raman spectra of bare sapphire and GNR arrays grown on reconstructed sapphire substrate. (c) Polarized Raman spectra of global aligned horizontal GNR arrays on reconstructed sapphire substrate. (d) Polar plot of the G peak intensities. (e) SEM image of high-density narrow GNR arrays grown on reconstructed sapphire substrate with parallel atomic step structures. (f) SEM image of high-density narrow GNR arrays which are transferred on plane SiO_2/Si substrate with the assistance of PMMA. (g) AFM image of high-density narrow GNR arrays which are transferred on plane SiO_2/Si substrate with the assistance of PMMA, inset is the height diagram of red line. (h) TEM image of GNR/graphene support membrane heterostructure on a holey SiN_x TEM grid. (i) FFT image of GNR in Fig. 1(h).

Direct growth of globally aligned graphene nanorib. Synthesis and characterizations of high-density aligned narrow horizontal Graphene Nanoribbons on reconstructed sapphire substrate.

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P044

DIRECT SYNTHESIS OF SEMICONDUCTING SINGLE-WALLED CARBON NANOTUBES TOWARD HIGH-PERFORMANCE ELECTRONICS

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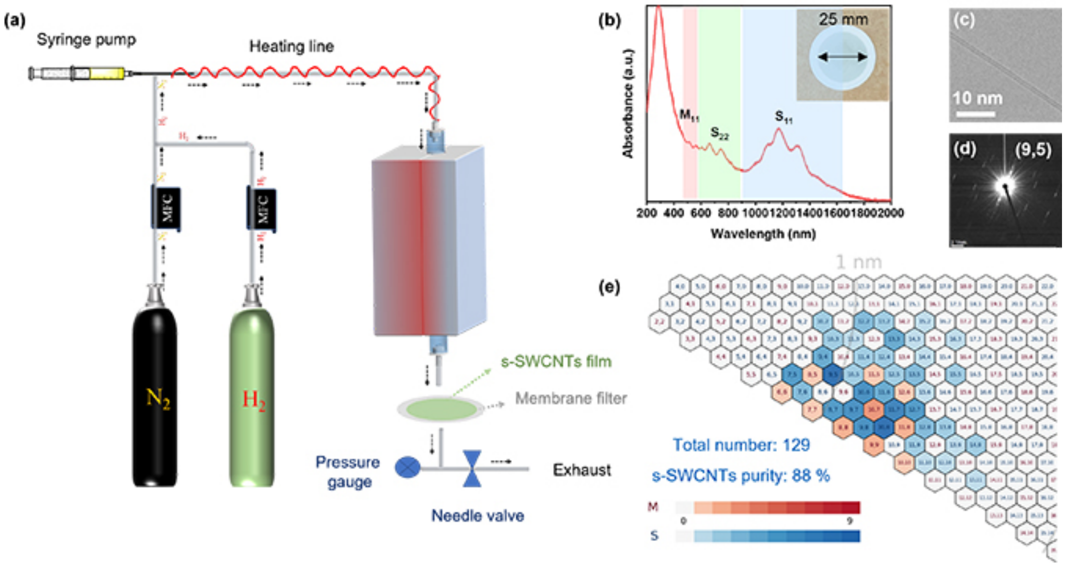
The large-scale synthesis of high-purity semiconducting single-walled carbon nanotubes (s-SWCNTs) is of crucial role in fabricating high-performance and multi-application-scenario electronics.[1,2] In this work, we develop a straightforward, continuous, and scalable method to synthesize s-SWCNTs on large scale. High-purity and individual s-SWCNTs of small-diameters distribution (ca. 1 nm) was synthesized with a high yield, through ingenious synthesis optimization. It is believed that the decomposition of isopropanol (IPA) produces both carbon monoxide (CO) and methane (CH_4) as carbon sources. Meanwhile, the water (H_2O) and carbon dioxide (CO_2) resulting from the decomposition are known to act as oxidizing agents and are selectively etching metallic-SWCNTs (m-SWCNTs), hence enhancing the production of s-SWCNTs. The performance of individual-SWCNTs field effect transistors (FETs) confirmed the high abundance of s-SWCNTs, presenting a mean mobility of 376 cm2 V^{-1} s^{-1} and a high mobility of 2725 cm^2 V^{-1} s^{-1} with an Ion/Ioff ratio as high as 2.51×10^7. Moreover, thin-film transistors (TFTs) based on the as-synthesized SWCNTs exhibited excellence in their performance with the mean mobility of 9.3 cm^2 V^{-1} s^{-1} and Ion/Ioff ratio of 1.3×10^5, respectively, verifying the enrichment of s-SWCNTs. Our work presents a simple and feasible route for the sustainable synthesis of high-quality s-SWCNTs for electronic devices.



Synthesis and characterization of s-SWCNTs. Figure 1. (a)The schematics of the floating catalyst chemical vapor deposition reactor for the synthesis of s-SWCNTs. (b)Absorption spectra of s-SWCNTs. Inset: s-SWCNTs film on filter. (c) A representative TEM micrograph of an individual SWCNT. (d) the corresponding electron diffraction pattern and the determined chirality index. (e) Chirality map of an as-synthesized SWCNT samples.

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P045

DOPING EFFECT OF MOS2 USING PERIODICALLY POLARIZATION-INVERSED SUBSTRATE

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As a typical Transitional Metal Dichalcogenide (TMD) material, MoS_2 has attracted much interest due to its intriguing opportunities for opto-electric device application. It has been known that the physical properties of TMDs are significantly affected by supporting substrates. Especially, ferroelectric substrates could affect the carrier density of TMD materials [1]. Therefore, periodically polarization-inverted structure which can be formed when spatially alternative external electric field is applied on ferroelectric materials, could be powerful tool to modulate carrier density geometrically without volatile or atomic displacement to TMDs. In this study, we demonstrated the carrier density of monolayer MoS_2 can be controlled by periodically polarization-inversed ferroelectric substrate.

We transferred an exfoliated monolayer (1L) MoS_2 flake onto a periodically polarization-inverted structure formed on a ferroelectric substrate MgO: $LiNbO_3$. Cross-sectional schematic of our sample is shown in Fig. 1(b). AFM and Piezo Force Microscopy (PFM) image of our sample is shown in Fig. 1 (a) and (b), respectively. 1L-MoS_2 has been successfully transferred onto pariodically polarization-inverted area. Photoluminescence (PL) intensity mapping was carried to investigate the distribution of carrier density of 1L-MoS_2. Figure 1 (c) shows the PL mapping image of exciton peak (1.88 eV), whose intensity changes according to the carrier density. It clearly shows that the PL intensity of 1L-MoS_2 is stronger on the down polarized domain of ferroelectric substrate. This result indicates that polarization induced electron doping and consequent negative trion formation occurs in up-domain region. On the other hand, polarization induced holes might compensate doped electrons in MoS_2 in down-domain region which brought the relatively strong exciton PL in this region. We also discuss the effects of h-BN inserted layer as a spacer layer between substrate and MoS_2.

This work was supported by JSPS KAKENHI grant number 22H05471, 21H01017, 21K18913, and “NEDO Intensive Support Program for Young Promising Researchers”

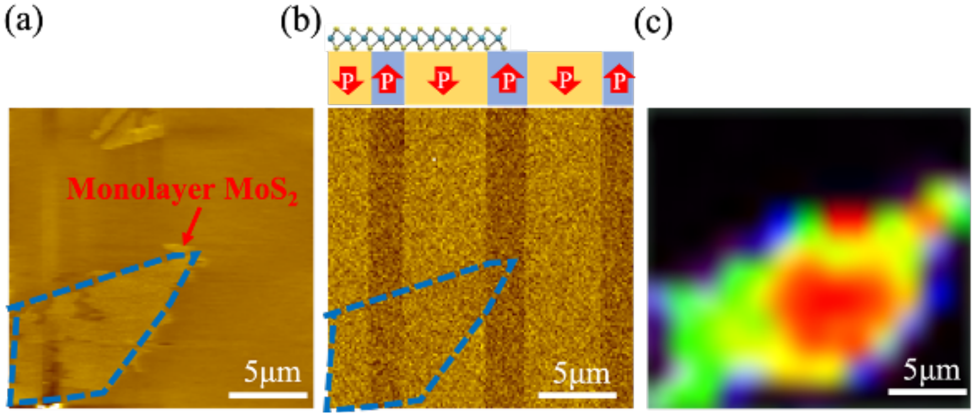

Fig.1. (a) AFM image and (b) PFM image of MoS2 on MgO: LiNbO3 substrate. (c) PL mapping of MoS2 on MgO: LiNbO3.

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P046

EFFECT OF SINGLE WALLED CARBON NANOTUBES AS ADHESIVE 1D CONDUCTIVE ADDITIVE ON SIOX/GRAPHITE LIBS ANODE.

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Silicon-based anodes have gained considerable attention in recent years as a potential solution to the limited energy density of conventional graphite anodes in lithium-ion batteries used in electric vehicles. However, silicon-based anodes still suffer from several drawbacks that huge volume expansion during lithiation/delithiation, the low conductivity nature of silicon and low initial coulombic efficiency[1]. Silicon oxide(SiOx) has emerged as an important alternative to silicon as the high capacity anode host to store lithium due to its smaller volume change upon lithiation[2]. In this study, we developed SiOx/Graphite composites(SGC) and employed SWCNT conductive additive to effectively suppress the volume expansion of SiOx, enhance the electrical conductivity. Also, the electrode containing SWCNTs showed that the interconnected networks between SWCNTs with SGC exhibits high adhesion strength on current collector. As the result, optimized SiOx/Graphite/SWCNT(SGSC) anode are evidenced to possess an excellent mechanical adhesion strength of ~0.7 kgf/20mm on Cu foil, Charge/Discharge stability of ~80% Columbic efficiency for 100 Cycles. The results show that SGSC are effectively designed to be applied to electric vehicles with long-term adhesive strength and high C-rate, while maintaining the stable and safe characteristics of silicon-based anode.

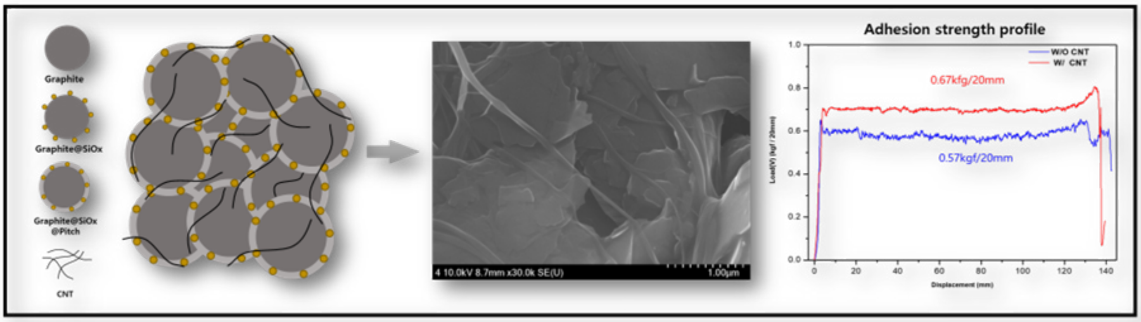

Fig.1. Schematics for SiOx/Graphite/CNT composites and enhanced adhesion strength profile with CNT networks.

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P047

EFFECT OF THE ORIENTATION OF A CARBON NANOTUBE ON ITS LOCALIZATION ACCURACY IN SINGLE-MOLECULE FLUORESCENCE MICROSCOPY

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Single wall carbon nanotubes (CNTs) are bright emitters in the SWIR domain which propelled them as unique nanostructures for applications in bioimaging or quantum sources. In particular, many applications are based on the possibility to control or detect CNT emission at the single molecule level. Interestingly, the emission dipole of CNTs is mostly linear along their backbones. According to theoretical calculation, when a 1D dipole with off-plane orientation is observed with a single molecule microscope, its 2D transverse localization will experience a systematic offset as a function of the position along the Z-axis. To verify this inference experimentally and quantify this effect in the case of 1D nanotubes, we compared the localization of CNTs and SWIR emitting Nanoparticles (NPs) when scanning their z-axial position at the single particle level. Unlike CNTs, because NPs have isotropic dipolar emission, their localization should not depend on their axial position. In practice, CNTs and NPs were immobilized in volumetric agarose, and the central position of their point spread function was obtained using Gaussian fitting to retrieve their nanoscale localization. We found that for CNTs, the center position varied linearly with the Z-axis position. We will present a quantitative discussion of this effect by comparing the results of the two samples, and its impact on applications where the localization accuracy is of importance.

P048

EFFICIENT SOLVENT-FREE PREPARATION OF BINDER-FREE ELECTRODES FOR LITHIUM-ION BATTERIES ENABLED BY AEROSOL SYNTHESIZED SINGLE-WALLED CARBON NANOTUBES

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Single-walled carbon nanotubes (SWCNTs) are a promising material that possesses excellent electrical conductivity, mechanical strength, flexibility and light weight. This opens a great potential for their application in energy storage devices with improved performance [1]. It has been shown that the addition of small amount of SWCNTs as a conductive additive to lithium battery electrodes can significantly enhance the electrochemical performance and mechanical stability [2]. Implementation of SWCNT additives has been shown to increase conductivity and cycling stability of the positive electrode [3]. However, conventional fabrication of the electrode by solution processing involves the mixing of SWCNTs and the active material, which is hampered by complications with proper blending of these two materials. In this work, we prepared self-standing NMC-based composite positive electrodes by two solvent-free methods, where hydrocarbon based aerosol chemical vapor deposition (CVD) synthesis of SWCNTs was employed. We employ two distinct methods for NMC fluidization: mechanical vibration with an aerosol flow of SWCNTs directed through the NMC powder and in situ gas-phase mixing of synthesized SWCNTs with aerosolized NMC material. We found samples produced by the second method to exhibit better performance in terms of higher specific capacity values, as shown in Figure 1. To conclude, this work can serve as a basis for future development of solvent-free electrode preparation methods, in particular to produce self-standing binder-free positive electrodes.

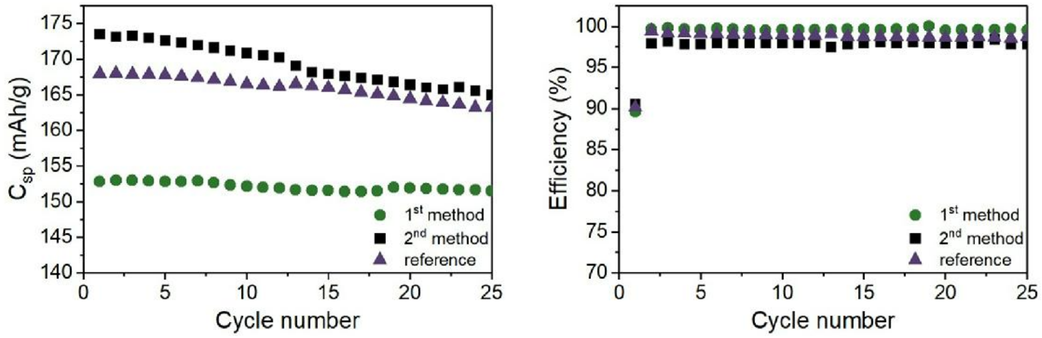

Figure 1. Specific capacity and Coulombic efficiency of the half-cell with self-standing SWCNTs/NMC622 cathode prepared by two methods and reference electrode (prepared by slurry method) during 25 charge discharge cycles at 1C.

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P049

EFFICIENTLY SYNTHESIS OF HIGHLY CRYSTALLINE ONE-DIMENSIONAL CRCL3 ATOMIC CHAINS WITH A SPIN GLASS STATE

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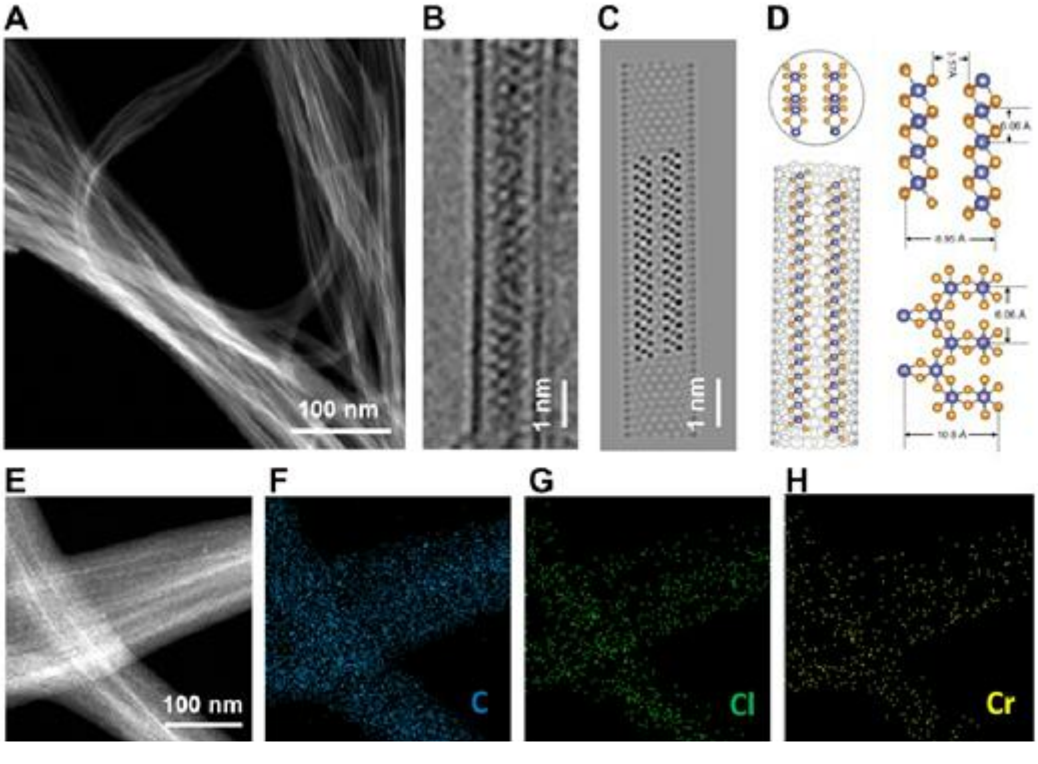
One-dimensional (1D) magnetic material systems have attracted widespread interest from researchers because of their peculiar physical properties and potential applications in spintronics devices. However, the synthesis of 1D magnetic atomic chains has seldom been investigated. Here, we developed an iodine-assisted vacuum chemical vapor-phase transport (I-VCVT) method, utilizing single-walled carbon nanotubes (SWCNTs) with 1D cavities as templates, high-quality and high-efficiency fabrication of 1D atomic chains of CrCl3 was achieved. Furthermore, the structure of CrCl3 atomic chains in the confined space of SWCNTs was analyzed in details and the charge transfer between the 1D atomic chains and SWCNTs was investigated through the spectroscopic characterization. A comprehensive study of the dynamic magnetic properties revealed the existence of spin glass states and freezing of the 1D CrCl3 atomic chains at around 3 K, which has never been seen in bulk CrCl3. Our work established an effective strategy for the control synthesis of 1D magnetic atomic chains, with promising potential applications in further magnetic-based spintronics devices.



Encapsulation of 1D CrCl3 atomic chains in SWCNTs. a-b, HAADF-STEM images of SWCNT bundles and single SWCNTs. c-d, The STEM simulation, and atomic structure of CrCl3@SWCNTs. e-h, EDX elemental mapping of CrCl3@SWCNTs.

P050

ELECTRICAL CONDUCTIVITY OF NANOCOMPOSITE THIN FILMS CONTAINING GRAPHENE AND PEDOT:PSS

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Conductive and flexible thin films made of nanoparticles dispersed in an insulating polymer matrix are particularly interesting to scientific and industrial communities. They have promising applications in various fields, such as energy storage, energy conversion, wearable electronics and sensors [1–3]. Until recently, metallic nanoparticles were the most commonly used material but a heavy thermal post-treatment is often required to reach a high conductivity. Graphene with its very high in-plane electric conductivity [4] is an attractive alternative for light-weight, flexible, easy-to-process and low-cost nanocomposites. Commercial graphene suspension comprising graphene nanoplatelets (GNP) are a ready-to-use solution. The graphene suspension can be mixed in a polyacrylic solution as a binder and then deposited on a flat substrate. In this configuration, the polyacrylic binder ensures the film adhesion to the substrate. The electrical conductivity of the film depends directly on the electrical percolation between the GNPs, as polyacrylic is known as insulating. The creation of a percolating conductive network along the GNPs remains a challenge, especially in the presence of an insulating polymeric matrix. The limiting factor to reach high conductivity levels is related to the presence of contact resistances between each GNP. The main objective of the study was to tackle this limitation. We introduced PEDOT:PSS into the GNP formulation as a conductive polymer that will restore electrical continuity. Although the intrinsic conductivity of the PEDOT:PSS is low compared to the intrinsic conductivity of GNPs, the addition of PEDOT:PSS in low concentration shows a significant synergistic effect by increasing the global conductivity of the film by two decades. The electrical resistivity of the film was measured by four-probe method and the surface morphology of the film was investigated at the nanoscale by atomic force microscopy (AFM) in conductive mode.

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P051

ELECTRICAL RESISTANCE AND MEMBRANE STRUCTURE OF BUCKY PAPERS IN WATER VAPOR

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A bucky paper (BP), which consists large amount of carbon nanotube (CNT), is a potential candidate for electrical devices due to its highly electrical conductivity and flexibility. Because BP devices are often used in the atmosphere, the effect of electrical properties of BP in water vapor is crucial for their applications. Although, the effect of water vapor on the resistivity of BPs have been observed, there is little agreement on its physical origin. [1, 2]. In this study, we measure the electrical resistivity of various types of BPs in a wide range of humidity and clarify physical origin. We prepared two types of BPs fabricated by super-growth (SG) methods under two different dispersion conditions [2]. One was dispersed by ethanol (SG-E) whereas the other was dispersed by water and surfactant (SG-S). We measured the resistivity by the four-terminal measurement method under controlled humidity at RH = 20, 40, 60, 80 % and at constant temperature $T \approx 24$°C. The resistivity of SG-E decreased, whereas SG-S increased. Thus, we found that different dispersion conditions exhibited opposite behavior of electrical resistivity in water vapor, even though BP was fabricated by the same method. Besides, we perform the measurement of contact angle of water drop on SG-E and SG-S surfaces and found the contact angle for the SG-S was much smaller than that for SG-E. In addition, we measured the expansion of BP in relative humidity. The expansion was observed only in SG-S. Thus, the SG-S could absorb water molecules and expand. We believe that the expansion may explain the increase in SG-S resistivity with increasing humidity. In the presentation, we explain the relation between humidity dependence of membrane structure and resistivity.

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P052

ELECTRON-PHONON COUPLING IN DOPED SINGLE-WALL CARBON NANOTUBES

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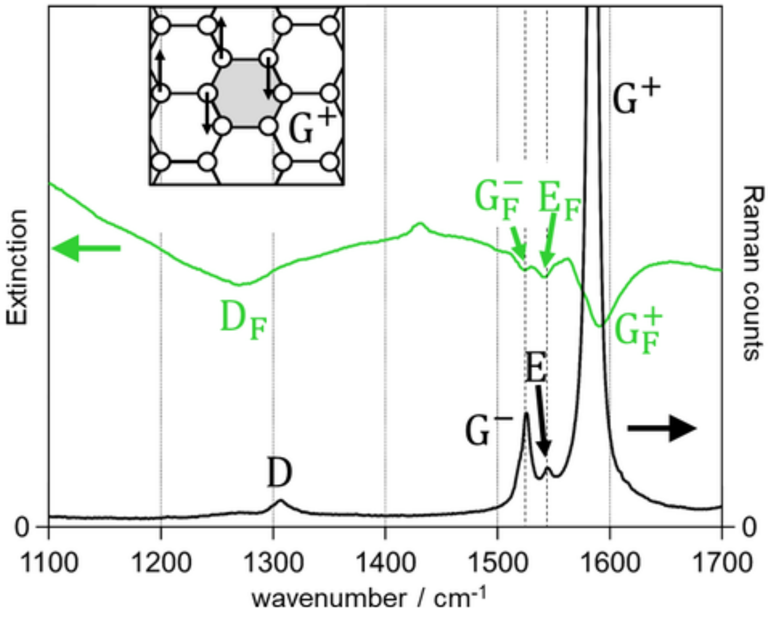
Electron-phonon (e-ph) coupling plays a key role for understanding physical phenomena such as electrical conductance, phonon-assisted optical absorption, superconductivity or the temperature-dependence of non-radiative decay [1]. Recent observations of infrared Fano anti-resonance signals in the range of vibrational modes of doped semiconducting carbon nanotubes (s-SWNTs) suggest that such features may be used for investigating e-ph interactions in these systems [2,3,4]. However, this requires a careful analysis of spectral lineshapes, intensities and widths as a function of doping level. Here, we present an investigation of one intra- and one inter-molecular Fano resonance in the 800 cm^{-1} wavenumber range of intrinsic and doped polymer-wrapped s-SWNT thin-films using high resolution infrared spectra. These modes and their respective e-ph coupling strengths are analyzed using a coherent superposition of coupled, harmonic oscillators. Fano-type resonance signals for the Raman active D- and G$^+$-phonons can also be observed because of their coupling to the Drude-like intraband absorption continuum in doped s-SWNTs [4]. The high spectral resolution also allows resolving IR bands associated with the Raman active G$^-$-and E-modes. The results shed new light on the e-ph coupling strength in s-SWNTs and help to better understand Fano resonances in low-dimensional doped semiconductors.



Raman and IR. Raman active vibrational modes (black) can be seen in IR spectra after doping (green).

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P053

ELECTRONIC STRUCTURE OF COVALENT NETWORKS OF TRIANGULAR GRAPHENE FLAKES EMBEDDED IN HBN

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Because of the structural similarity and small lattice mismatch between graphene and hBN, they can form an in- plane heterostructure in which all the bonds at the border are fully saturated. Chemical vapor deposition experiments have shown the in-plane heterostructure of hBN and graphene with zigzag borders. In such heterostructures, the border leads to peculiar localized states consisting of bonding and antibonding states of edge states of graphene and hBN strips. This border localized states are known to be border states those are localized at but extended along the borders. These facts imply that graphene nanonetworks embedded in hBN induce unique electronic properties by designing the border shapes and constituent domain structures. In this work, using density functional theory with generalized gradient approximation and ultrasoft pseudopotentials, we investigated the electronic structures of covalent frameworks of polymeric triangular graphene flakes ([n]triangulene where n is the number of hexagonal rings along one of the edges) embedded in hBN as potential candidates for in-plane heterostructures of graphene and hBN with unique electronic properties (Fig. 1). Our calculations demonstrated that the electronic structures of graphene nanonet- works embedded in hBN exhibited a small dispersion band near the Fermi level, even though the C atoms formed two- dimensional covalent networks. We also demonstrated that the detailed electronic structures of the heterostructures depend strongly on the size of the triangulene and constituent border elements. A honeycomb network of [3]triangulene in hBN was a semiconductor with a direct band gap of 0.7 eV at the K point. The other heterostructures exhibited ferrimagnetic spin polarization, in which the numbers of polarized electron spin depended on the constituent units.

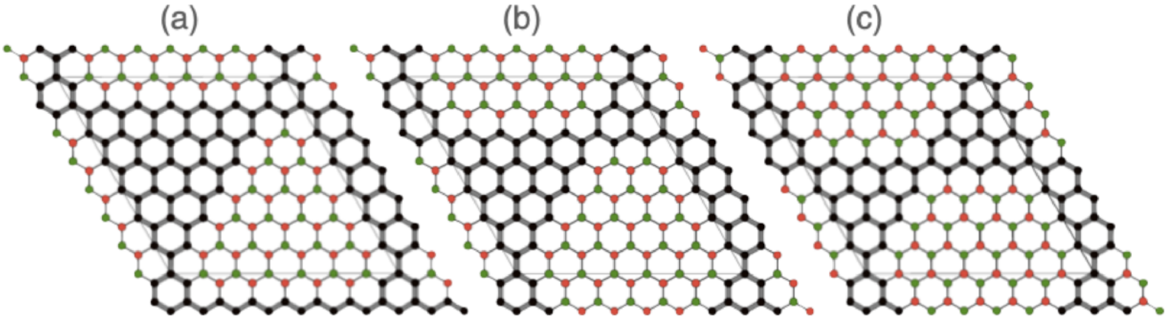

Fig.1. Geometric structures of covalent networks of (a) [5]triangulene and C6 ring, (b) [4]triangulene and [2]triangulene, and (c) [3]triangulenes embedded in hBN. Red, black and green balls indicate B, C and N atoms, respectively.

P054
ELECTRONIC TRANSPORT AND MAGNETIC PROPERTIES OF FIBERS FROM UNIAXIAL FULLERENE SUPRAMOLECULES ALIGNED WITH CARBON NANOTUBES

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We present a simple variation on the established carbon nanotube (CNT) chlorosulfonic acid (CSA) extrusion process that generates a fiber composed of uniaxial chains of aligned fullerene supramolecules, which self-assemble and align between the aligned few-walled CNT bundles. We present three varieties: high C60 loading CNT fiber (2% C60 and 2% CNT in 96% CSA by weight), low C60 loading CNT fiber (0.2% C60 and 2% CNT in 97.8% CSA by weight), and neat CNT fiber (2% CNT in 98% CSA weight) in the as-produced state, as well after a post process annealing (300 °C in Argon). As shown by TEM, XRD, and NanoCT characterization, the crystallinity and outer dimensions of the oriented fullerene supramolecules are dictated by processing conditions such as the fullerene/ CNT concentration and post-process annealing. We find that the initially insulating fullerenes do not impact the electrically conductivity of the CNT network itself and, relative to the neat CNT fiber, the fullerene addition can positively impact overall mechanical strength. Most importantly, this material provides a robust testbed for novel aligned fullerene wire transport. We present four probe electrical transport characterization, magnetization, and AC susceptibility measurements of the as produced, annealed, and doped material from room temperature down to 1.8 K, in magnetic fields up to 9 T. Tradeoffs between the percolative path, fullerene aspect ratio, crystallinity, and internal molecular pressure that are relevant for novel transport phenomena are discussed [1].

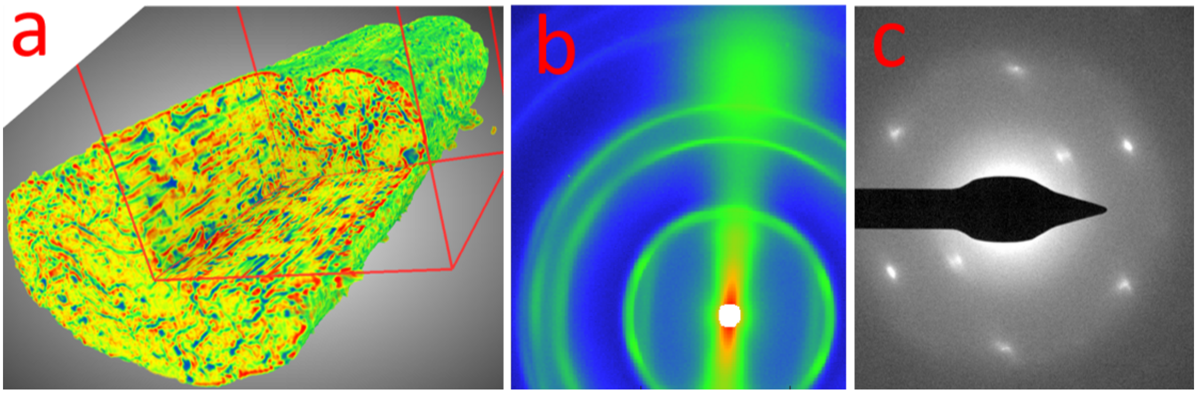

Figure 1. Structural characterization of the high C60 load CNT fiber: a, nanoCT scan showing interfaces between density variation. Cutway red box is 25 um x 25 um x 25 um ; b, transmission XRD showing alignment of C60 crystalline phases in the direction of CNTs; c, TEM electron diffraction showing the FCC crystalline nature of the C60 agglomeration.

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P055

ELECTRONIC-STRUCTURE TUNING OF MULTILAYER GRAPHENE BY PERPENDICULAR ELECTRIC FIELD AND STACKING ARRANGEMENT

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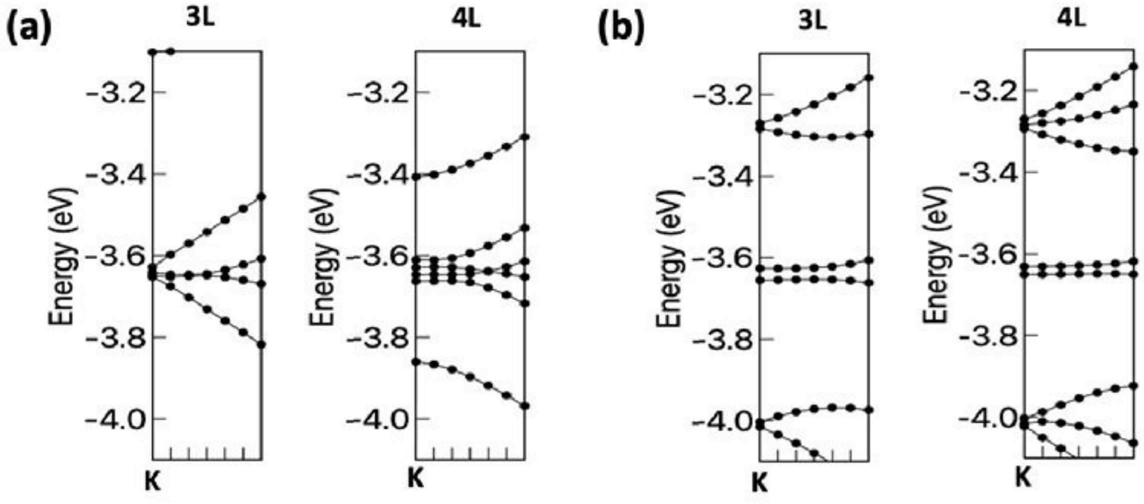
In recent year, graphene has gained significant interest in the wide areas of nanoscale sciences and technologies due to its excellent physical properties. The electronic structure of graphene is sensitive to the interlayer stacking arrangement and the number of layers [1]. Moreover, an external electric field modulates band dispersion spectra near the Fermi level of bilayer graphene [2]. However, the electronic properties of multilayer graphene under the electric field are uncertain in terms of their stacking arrangement and the number of layers. Therefore, in this work, we aim to elucidate the electronic structure of multilayer graphene under the perpendicular electric field using the density functional theory (DFT) combined with the effective screening medium method (ESM). DFT-ESM calculations revealed that the electronic structure of multilayer graphene with AB and ABC stacking under the perpendicular electric field strongly depends on the number of layers and their staking arrangement. Multilayer graphene with AB stacking under the electric field is a metal or a semimetal when the multilayer graphene consists of odd or even number layers, respectively. In contrast, the multilayer graphene with ABC stacking is a semiconductor which possesses flat band at the valence- and conduction-band edges, irrespective of the number of layers.



Electronic structure near the Fermi level and in the vicinity of the K point of multilayer graphene with (a) AB stacking and (b) ABC stacking arrangements under the perpendicular electric field.

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P056

ENCAPSULATION OF THIOPHENE DERIVATES IN BORON NITRIDE NANOTUBES (BNNT) AND THEIR OPTICAL PROPERTIES

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Boron nitride nanotubes (BNNTs) have gain special attention in the scientific community thanks to their small tubular structure, which is analogous to that of carbon nanotubes (CNTs). BNNTs are, however, good insulators with a wide bandgap (~5-6 eV) regardless of tube morphology, highly resistance against oxidation, up to 900ºC, and they are chemically stable and optically transparent from the UV down to the infrared regions of the electromagnetic spectrum.
Thiophene derivates are fluorescent dyes, which have received interest due to its potential applications in electroluminescent devices, such as OLED [1]. Previous works in our team studied the encapsulation mechanism of different dyes in SWCNT [2] and BNNT [3]. The focus of the present work is to explore the encapsulation process of a mixture of thiophenes: α-sexiothiophene (6T) and α-terthiophene (3T), which are optically active according to maximum absorption at λ_{max} = 354 nm and 436 nm, respectively. Using hyperspectral imaging, we characterize the encapsulation process of 6T/3T@BNNT according to different conditions of concentration and temperature. The distribution of the dyes inside BNNTs is determined on ensemble and individual BNNTs using a combination of techniques: fluorescence spectroscopy, AFM, TEM, hyperspectral Raman (RIMA ^{TM}) and FTIR.

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P057

ENERGY DISTRIBUTIONS OF ELECTRONS EMITTED FROM CLEAN GRAPHENE EDGES

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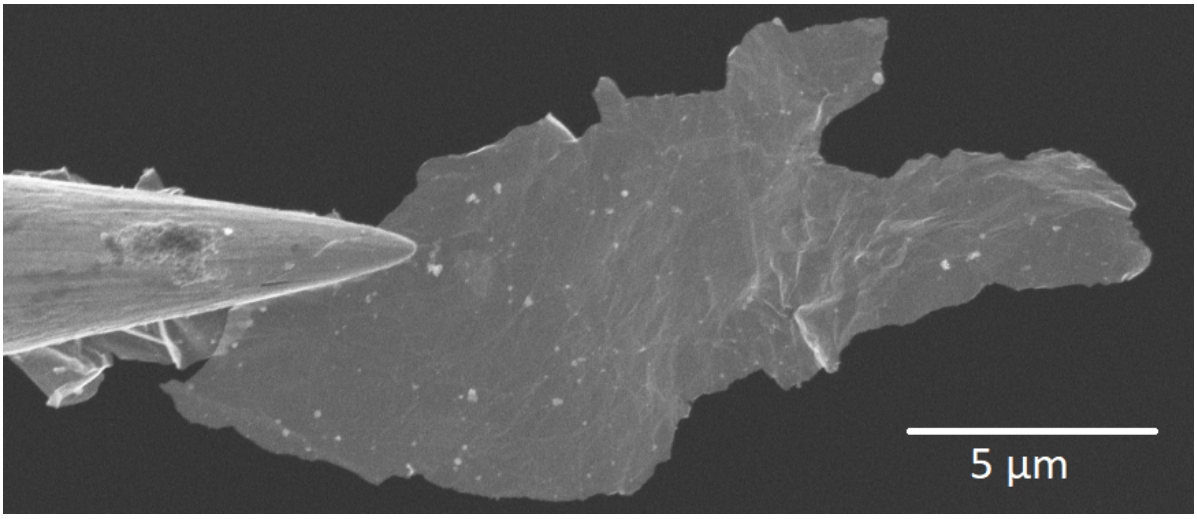
This poster presents a study on electron field emission (FE) into ultrahigh vacuum (UHV) from a single, cleaned, graphene sheet where its single sheet nature has been carefully characterized and the emission zones are unambiguously the sheet edges. This definitive approach is in contrast to almost all other studies in the literature and can now guide theoretical work and applications. Our sample characterization starts with transmission electron microcopy imaging, Raman characterization, controlled mounting of individual flakes in a scanning electron microscope followed by in situ high temperature and high field treatments. Detailed FE characterization was carried out including current-voltage plots, FE microscopy, and electron energy spectroscopy during subsequent stages of sample cleaning, at room and liquid air temperatures. The full width at half maximum (FWHM) of the energy peak as well as its relative shift versus current and voltage were explored. A notable result is that the energy spectra are very narrow, ten times less than previously reported [1,2].



Graphene flake. Graphene sample (produced by Chemical Vapor deposition with a drastic control of hydrogen etching) used for this Field Emission study. Before picking-up the graphene sheet at the apex of a tungsten tip as presented, we perform on the very same batch sample Raman spectroscopy and TEM diffraction to ensure the sample is indeed single layer graphene.

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P058

ENERGY TRANSFER FROM ENCAPSULATED SQUARAINE DYE MOLECULES TO CHIRALITY-SORTED SINGLE-WALL CARBON NANOTUBES

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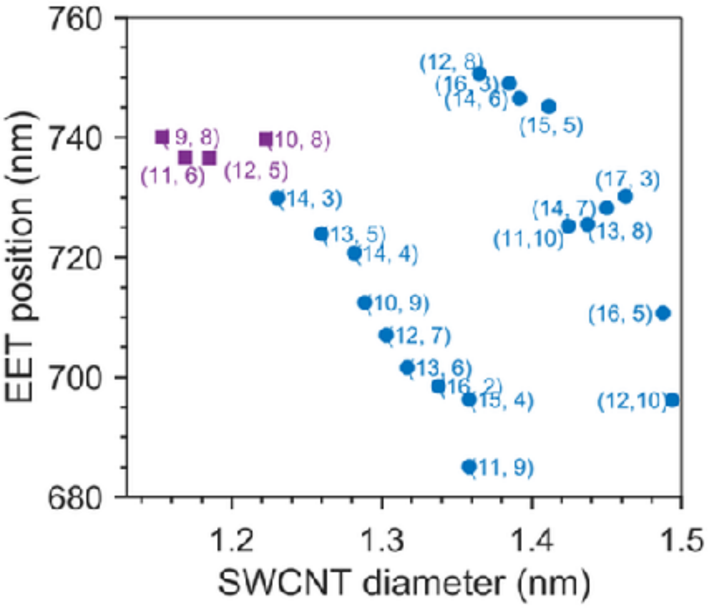
Single-wall carbon nanotubes (SWCNTs) are nanomaterials with a hollow core and a high aspect ratio combined with subatomic diameter variability. Therefore, they are unique channels able to encapsulate various molecules to form 1D hybrids. Dipolar dye molecules can be encapsulated and aligned, as previously demonstrated [1], and there is energy transfer (EET) from the dye molecules towards the SWCNTs [2]. The optical properties of dye molecules encapsulated in SWCNTs can be strongly modulated by the SWCNT diameter, indicating very specific diameter-dependent stacking and interactions of the molecules [2,3]. In this work we report this diameter-dependent dye absorption (see Fig. 1) of nearly single chirality dye-filled SWCNTs (obtained through extensive diameter sorting of the large-diameter tubes) by measuring and thoroughly fitting their unique photoluminescence-excitation maps [4]. Afterwards, we compare the results with a molecular model of these dye molecules inside a cylinder of a given diameter to predict the possible different stacking configurations of the dye molecules inside the hollow core of the SWCNTs. With it, we evidence that the SWCNT diameter is a parameter that can be used in order to tune optical properties of the 1D hybrids, and thus allowing forthcoming applications in optoelectronics. [4]



Encapsulated dye absorption wavelength from the EET for different (n,m) SWCNT as a function of their diameter. [4]

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P059

ENHANCED CARBON NANOTUBE PRODUCTION BY FLOATING CATALYST CVD VIA OVERHEATING OF CATALYST SOURCES

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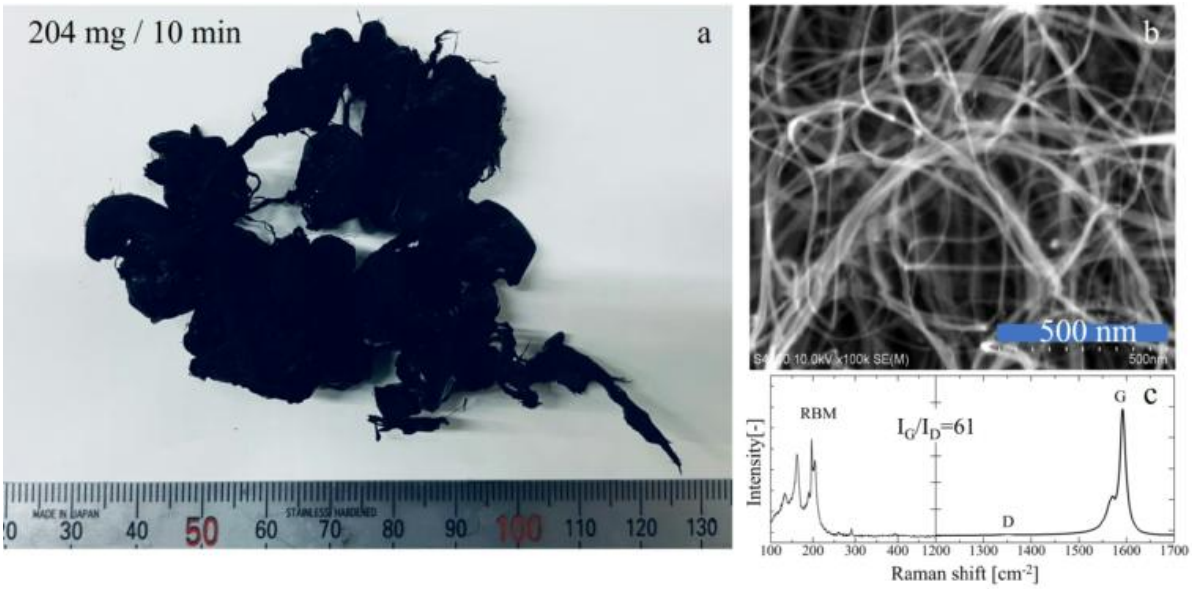
Single-wall carbon nanotubes (SWCNTs) have attracted extensive attention among researchers thanks to its unique chemical and physical properties. Floating catalyst chemical vapor deposition (FCCVD) is regarded as an essential technique for continuous production of high-quality SWCNTs [1]. However, the catalyst precursors gradually heated via heat transfer from the reactor wall yield catalyst nanoparticles with moderate density, resulting in productivity lower than that by supported catalyst CVD such as fluidized bed. If catalyst precursors are heated quickly with a time constant τ, catalyst density n can be enhanced following the equation $n = 1/L^3 = (D\tau)^{-3/2}$ (L: diffusion length, D: diffusion coefficient). Based on this concept, we previously developed the flame-assisted CVD method that used a premixed flame for τ as small as milliseconds and yielded SWCNTs with diameter of ~1 nm with narrow diameter distribution [2]. But the productivity was as small as ~0.3 mg/min because of the narrow window between oxidation and carbonization for catalyst activation.

In this report, we developed a FCCVD reactor with a microheater for instantaneous preheating of catalyst precursors. The catalyst precursors (ferrocene and sulfur) are rapidly overheated to a temperature (>1400 °C) higher than the CVD temperature (1100~1200 °C) in a narrow nozzle (Φ4 mm), and decomposed precursors are rapidly cooled to CVD temperature via mixing with CVD gas (e.g., CH_4, C_2H_4) to nucleate Fe/S particles and initiate CNT growth. This method produced CNTs at high yield (20~30 mg/min) with high quality (Raman G-band to D-band intensity ratio of ~50).



CNTs produced by FCCVD with overheating of catalyst precursors. (a) Digital images of 204 mg CNTs produced in 10 min. (b) SEM image. (c) Raman spectra (wavelength: 488 nm).

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P060

ENHANCED ELECTRICAL CONDUCTIVITY OF HIGHLY-ENRICHED GRAPHITIC-NITROGEN-DOPED SINGLE-WALL CARBON NANOTUBE FIBERS

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A chemical doping has offered a rich potential for tuning the electrical properties of carbon nanotubes (CNTs). Despite nitrogen-doped carbon nanotubes (N-CNTs) have been extensively studied [1], the precise control of the C-N doping properties (e.g., graphitic-N, pyridinic-N, and pyrrolic-N) and the electronic structure modifications are not yet understood. Furthermore, most of the literature reports so far have mostly devoted to the work on N-doped multi-walled carbon nanotubes, where the weak mechanical properties caused by a large number of defects limit their potential application. Moreover, the in-situ growth and doping mechanism of N-CNTs are still not well-understood, and some researchers have investigated the n-type graphitic-N doping of single-wall carbon nanotube (N-SWCNT) fibers by post-treatment such as plasma to enhance the electrical conductivity [2]. Here, we report a way to get high-quality N-SWCNTs with a highly-enriched graphitic-N, by varying the synthesis condition under a high flow rate of pure hydrogen with floating-catalyst chemical vapor deposition (FC-CVD) technique. We used ferrocene and thiophene as catalyst precursors and a promoter, respectively. Ethanol and pyridine were used as carbon and nitrogen sources. N-SWCNTs were further spun into homogeneous and stable fibers by solution spinning. We performed optical absorption measurement for the effect of N-doping, whereby the increased N content reduces the S_{11} peak (Fig. 1(a)). XPS spectrum showed our sample has rich graphitic-N amount, which have a stable sp2 structure (Fig. 1(b)). The N-SWCNT fiber shows mechanical properties up to 1.28 GPa and electrical conductivity up to 1.37 MS/m. In this presentation, the detailed effect of N doping on fiber strength and room temperature conductivity will be discussed. This work provides further insight for the future synthetic development and potential applications of N-CNTs.

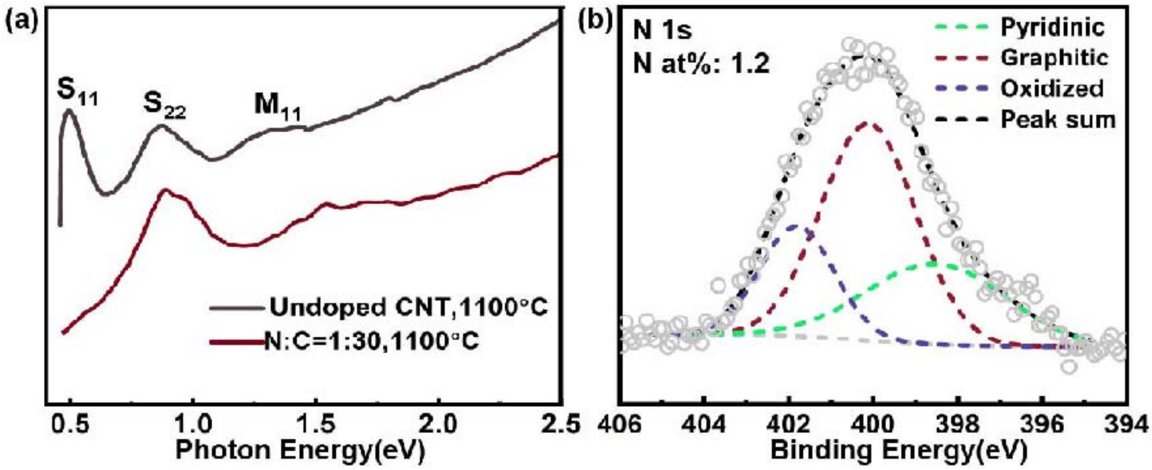

Figure 1. (a) UV-vis-NIR optical absorption spectra of N-SWCNTs and undoped SWCNTs. (b) XPS N1s spectra of N-SWCNTs (N:C=1:30,1100°C).

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P061

ENHANCEMENT OF LI INTERCALATION OF LIFEPO4 NANOPARTICLES WITH GRAPHENE

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Carbon-assisted energy storage in Li-ion battery (LIBs) is a crucial topic in the era of carbon neutral. Considering the power density of LIBs is always multi-factor dependent and most measures only effect affect in part, the authors report here a “three-in-one” effect as using simply adding graphene to LiFePO4 to fabricate the hybrid Li-ion battery-capacitors (LIBCs) cathode to enhance the performance of LiFePO4. The effects include the significant increase of electrical conductivity, accelerating ion diffusion rate, and an enhancement of capacitive performance owing to the larger mesopore ratio and larger electrolyte holding ratio of the cathode sheet. As a result, the graphene enhanced LIBCs exhibit much higher power density (with associated higher energy density), and longer life time. The simple but robust strategy would be useful to a practical battery solution at low cost.

P062
EXCITONIC TRANSITIONS OF QUASI-2D PEROVSKITES AT CRYOGENIC TEMPERATURES

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Due to their naturally formed quantum-well structure, two-dimensional (2D) perovskite semiconductors exhibit remarkable optoelectronic properties, attracting interest in a wide range of application fields including photovoltaics, light-emitting diodes (LEDs), photodetectors and lasers [1,2]. Understanding the origin of their photophysical recombination pathways is thus crucial. Recent investigations of 2D perovskite systems have revealed a variety of optically excited states such as direct and indirect excitonic transitions [3], self-trapped excitons [4,5] and biexcitons [6,7] at low temperatures. However, investigations that spectrally resolve the exciton fine structure in their quasi-2D analogues are still missing. Here, we report on a series of PL measurements between room temperature and 14 K on mechanically exfoliated 2D and quasi-2D lead iodide perovskites $(PEA)_2(MA)_{n-1}Pb_nI_{3n+1}$ (PEA, phenethylammonium; MA, methylammonium) with $n = 1$ and $n = 2$, 3 or 4, respectively. With decreasing temperature, the peaks shift to lower energies and the line-width decreases due to reduced thermal broadening. Therefore, the broad excitonic signals observed at high temperatures are found to break up into a multitude of individual transitions at cryogenic temperatures below 60 K. Additional evidence for the excitonic nature of these transitions is obtained from absorption and power-dependent PL measurements. Our investigations provide new insights into the exciton fine structure of quasi-2D perovskites and shed light onto the role of quantum confinement in this class of low-dimensional semiconductors.

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P063

EXFOLIATION, PHOTOPHYSICAL PROPERTIES AND FUNCTIONALIZATION OF NEAR INFRARED FLUORESCENT CACUSI4O10 NANOSHEETS

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Imaging in the near infrared (NIR) range of the spectrum is beneficial due to reduced light scattering, absorption, toxicity and autofluorescence. However, there are only few NIR fluorescent materials known and suitable for (biomedical) applications. Here, we exfoliate the near infrared fluorescent layered pigment CaCuSi4O10 (known as Egyptian Blue, EB) via different mechanical and surfactant-assisted approaches into 2D nanosheets (EB-NS) of high monodispersity. Dimensions of the nanosheets decrease with sonication time < 10 nm down to single EB layers (around 1 nm). The near infrared fluorescence of EB at 910 nm is retained in EB-NS and the total fluorescence intensity scales with size. Furthermore, we demonstrate that EB-NS display ultra-high photostability (no bleaching), are extremely bright compared to other NIR fluorophores and can be used for lifetime encoded imaging. We also show that the fluorescence lifetimes in the µs range depend on particle size and can be used to enhance contrast in imaging. Furthermore, we use silane chemistry to decorate the surface of the nanosheets with biomolecules. In summary, we introduce exfoliated 2D CaCuSi4O10 nanosheets as versatile NIR fluorescent material for photonics.

P064

FABRICATION OF CARBON NANOTUBE THIN FILMS ON BILAYER LIQUID INTERFACE WITH DIFFERENT DISPERSIBILITY

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One of the promising applications of carbon nanotubes (CNT) is transparent conductive thin films because of their flexibility and excellent thermal and electrical conductivity properties. CNT thin films can be fabricated by either a wet process, in which CNTs are dispersed in solution in advance or a dry process, in which CNTs are spun during or after synthesis. In the wet process, semiconducting and metallic single-walled carbon nanotubes (SWCNTs) can be separated after dispersion, and they can be applied to any CNT samples. However, there is concern that the electrical conductivity properties of the CNT thin film may deteriorate due to the shortening of the CNTs with intense ultrasonic treatment and/or contamination with surfactants during the dispersion process. On the other hand, in the dry process, there is no concern about contamination or shortening, but it is necessary to control the CNT thin films in the growth stage by the synthesis conditions. Forward the ideal CNT thin film fabrication, in this study, we attempted to fabricate CNT thin films by the wet process using dilute CNT dispersions. Vertically-aligned MWCNTs and vertically-aligned SWCNTs, which were synthesized in our laboratory, and commercially available CNT samples were dispersed in DMF by weak ultrasonication to prepare CNT-DMF solutions. Since no surfactant or strong ultrasonication (such as homogenizer) was used here, the CNT concentration in the DMF solution was dilute and no shortening was expected to have occurred. The CNT-DMF solution was gently poured onto the surface of water, which is a poor solvent for CNTs, and a layer of DMF was formed on the surface. The DMF layer quickly diffused into water and disappeared, but the CNTs remained on the surface and formed a thin CNT film. The CNT thin film was picked up by a hydrophobic membrane filter and transferred to various substrates such as silicon and glass. Using a dilute CNT solution, CNT thin films formed on the liquid surface can be very thin, and light transmittance of 95% (at 550 nm) was obtained.

P065

GAS-PHASE BUNDLING DYNAMICS OF HIGH-ASPECT-RATIO CARBON NANOTUBES: ATOMISTIC, MESOSCALE, AND ANALYTICAL MODELS

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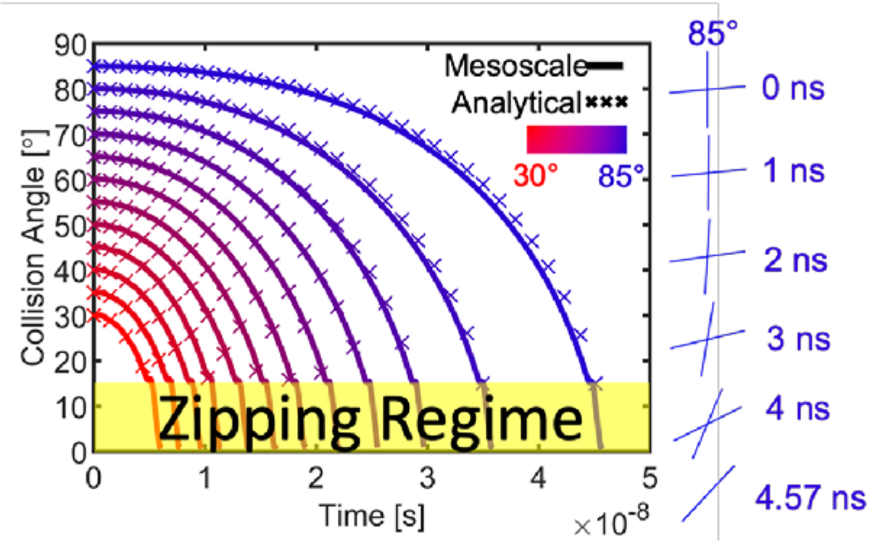
In floating catalyst chemical vapour deposition (FCCVD), the gas-phase aggregation and bundling of the nanostructures give rise to a CNT aerogel, which can then be extracted continuously from the reactor into fibre or mats. This makes FCCVD one of the most promising routes for high-volume production of carbon nanotubes (CNTs). The self-assembly behaviour between high-aspect-ratio CNTs dictates the resulting morphology at the nanoscale and subsequent properties of the bulk product. However, as the material spans across multiple length scales and its dynamics across multiple time scales, new models are needed to describe and understand the emergence of aerogel from CVD reactions. Previous work from our group provided the first known calculation of timescales on the agglomeration and bundling dynamics of individual CNT molecules in the gas phase [1,2], which is a prerequisite for aerogel formation. In this study, we advanced our analysis to meet the multi-scale challenge with mesoscale molecular dynamics (MD) models that are capable of predicting the reorientation time for CNTs of various types at 0.1% of the time cost compared to that of the atomistic MD models. This opens up timescales that would otherwise be impossible for atomistic MD models but still falls short for describing a population of 1D structures, i.e. an aerogel. We further developed an analytical model based on mechanics of rigid structures, which showed good agreement with results from the mesoscopic MD models. This multi-scale modelling capability would enable us to study not only aerogel formation from FCCVD reactors but also gas-phase 1D nanostructures in general.



Prediction of bundling time of two CNT molecules as a function of initial angle by mesoscale and analytical models

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P066

GRAPHENE DISPERSION IN WATER: FORMULATION AND STABILITY

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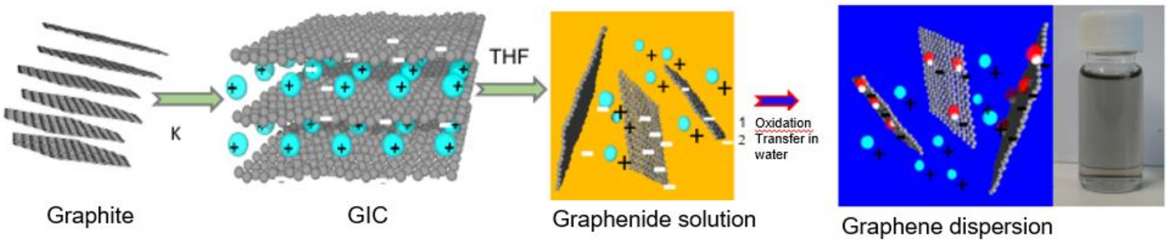
Graphene, a monolayer of graphite, is a hexagonal lattice of carbon with an atomic thickness. Formalized in the 1940s, it was first obtained by mechanical exfoliation of graphite by the so-called adhesive tape method in 2004 (1). As graphene is presenting outstanding mechanical, electrical, thermal and barrier properties (2), a lot of scientific research is channelled on its production. Some techniques such as the adhesive-tape method or the chemical vapour deposition produce good quality graphene but are not suitable for scaling-up to industrial quantities. For this reason, as for facilitating the incorporation of graphene into different final products, numerous research focus on the development of liquid formulations of graphene. The process that was developed by the CRPP (3) and adapted by the company Carbon Waters is based on the dissolution of graphite intercalated compounds (GIC) in an organic medium, leading to a graphenide solution. This solution is then oxidized and transferred into water where neutral graphene is dispersed and stabilized by adsorbed hydroxide ions. This dispersion is called "Eau de Graphène" (EdG) (Fig.1). The stabilization of graphene in water without surfactants is still not fully understood: other ions could preferably be adsorbed on the surface of the graphene, thus improving the stability and the concentration of the EdG. Through experimental work involving electrophoretic mobility, Atomic Force Microscopy and calorimetry, combined with molecular dynamic simulations (LAMMPS), the charge of the graphene in dispersion is investigated, thus allowing us to improve the understanding of the stabilization mecanisms of graphene in water.



Preparation of aqueous graphene dispersion. Preparation of aqueous graphene dispersion, adapted from Ref.3

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P067

GRAPHENE EPITAXY: FROM MISORIENTATION-FREE TO MISORIENTATION-ENGINEERED GRAPHENE FILMS

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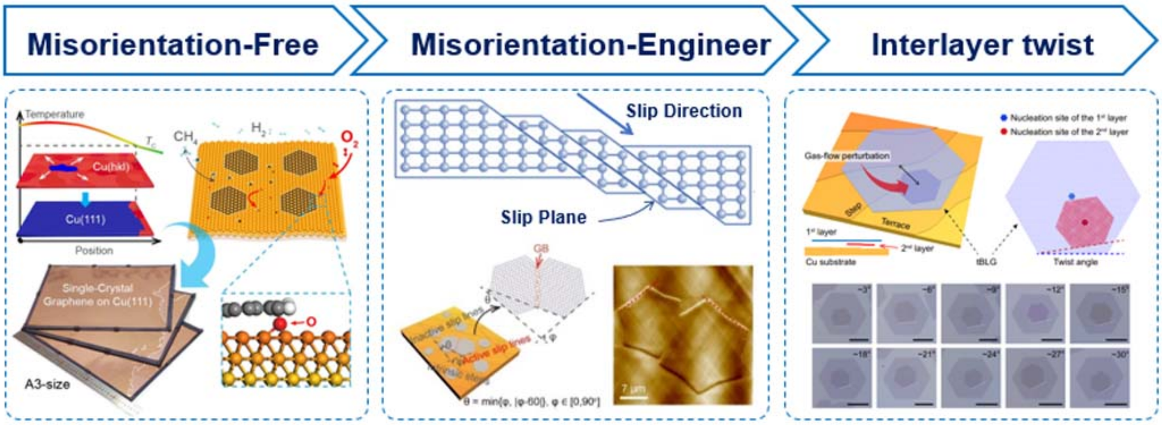
In this talk, I will introduce our recent works on controlled growth of high-quality graphene films via CVD approach, especially on controlling the crystallographic orientation of graphene. By designing and preparing single-crystal Cu(111) foils, we have opportunities in realizing the epitaxial growth of large-area single-crystal misorientation-free graphene film [1,2]. We designed and constructed a pilot-scale CVD system suitable for producing A3-size graphene films, which works well and output high-quality graphene films with high capacity [2]. To explore the possibility on controlling the layer number and stacking order, we developed a hetero-site nucleation method for growing twisted bilayer graphene (tBLG) [3]. Gas-flow perturbation and switching of the graphene edge termination play crucial roles in triggering the formation of interlayer twist. We also established a slip-line-guided growth principle to explain and predict the crystal orientation distribution of graphene on a variety of metal facets, further enabling the controllable synthesis of single-crystal graphene and grain boundary engineering of bi-crystal graphene on designed metal facets [4], which opens a new avenue for manipulating the crystal orientations, grain boundary structures, and even twisted angles of bilayer 2D materials in a bottom-up manner.



Pilot-scale misorientation-free graphene films; centimeter-scale misorientation-engineered Graphene Films; lab-level twisted bilayer graphene.

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P068

GRAPHITIC STRUCTURE ASSESSMENT OF CARBON NANOTUBES BY INFRARED C=C VIBRATIONAL MODES

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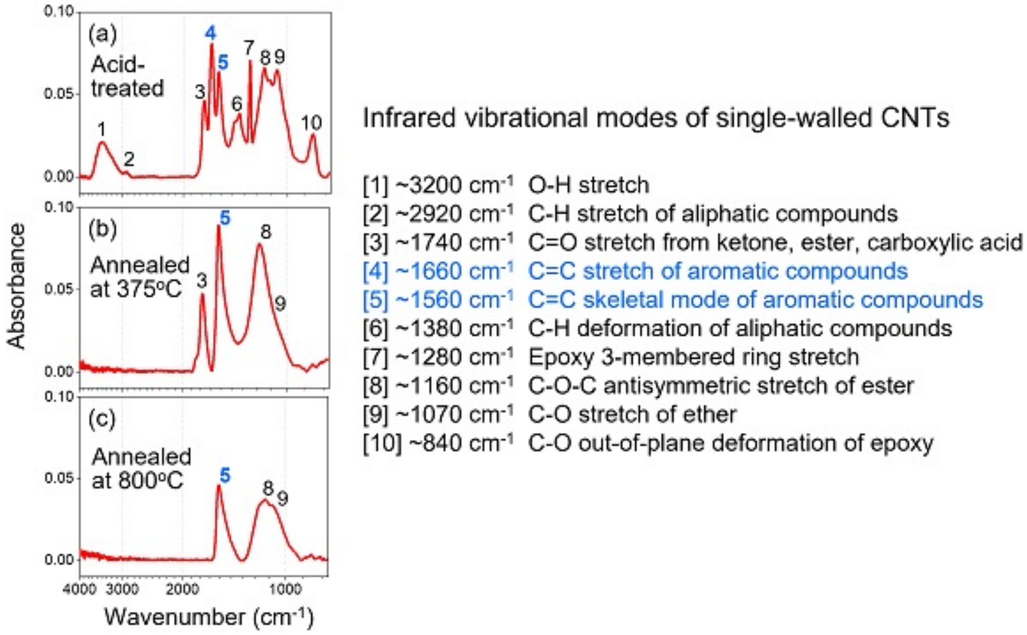
Quality control of nanocarbon materials such as carbon nanotubes (CNT) and graphene is necessary for the industrial applications. To assess the quality (graphitic structure), various analytical methods have been employed, e.g. Raman spectroscopy, X-ray diffraction, and thermogravimetric analysis. Infrared spectroscopy is semi-quantitative, but versatile, powerful tool to characterize the chemical bonds. Recently, we proposed the quantitative surface characterization of as-grown and acid-treated single-walled CNTs in a multifaceted approach, and successfully assigned the infrared vibrational modes [1]. In this study, infrared C=C vibrational modes were focused as a novel approach to assess graphitic structure of CNTs. We inspected the two kinds of skeletal and stretching modes of aromatic compounds around 1560 cm^{-1} and 1660 cm^{-1} (Figure). A comparison was made using the CNT films subjected to acid-treatment (introduction of functional groups), and further annealed under N_2 at 375°C and 800°C (removal of functional groups). Both the skeletal and stretching modes were detected in the spectrum of acid-treated CNT, while the stretching mode disappeared in the spectra of annealed CNTs, accompanied by the decrease in peak intensity of the functional groups. The skeletal mode is derived from the plural chemical bonds of aromatic rings in the graphitic sheet of CNT. On the other hand, the stretching mode stems from a single chemical bond of alkenyl group. Thus we demonstrated the C=C stretching mode of CNTs, which is indicative of a disordered graphitic structure brought by attachment of the functional groups to the CNT surfaces. The extensional study is in progress, and a peak intensity ratio of skeletal to stretching mode would be an asset to evaluate quality of CNTs.



Infrared vibrational modes of single-walled CNTs

[1]	~3200 cm^{-1}	O-H stretch
[2]	~2920 cm^{-1}	C-H stretch of aliphatic compounds
[3]	~1740 cm^{-1}	C=O stretch from ketone, ester, carboxylic acid
[4]	~1660 cm^{-1}	C=C stretch of aromatic compounds
[5]	~1560 cm^{-1}	C=C skeletal mode of aromatic compounds
[6]	~1380 cm^{-1}	C-H deformation of aliphatic compounds
[7]	~1280 cm^{-1}	Epoxy 3-membered ring stretch
[8]	~1160 cm^{-1}	C-O-C antisymmetric stretch of ester
[9]	~1070 cm^{-1}	C-O stretch of ether
[10]	~840 cm^{-1}	C-O out-of-plane deformation of epoxy

Figure. Infrared spectra and vibrational modes of single-walled CNT films, (a) acid-treated, further annealed under nitrogen at (b) 375 degree C and (c) 800 degree C.

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P069

GROWTH KINETICS OF SINGLE-WALLED CARBON NANOTUBES INSIDE METALLOCENE-FILLED SINGLE-WALLED CARBON NANOTUBES

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The applications of single-walled carbon nanotubes (SWCNTs) require nanotubes with defined properties [1,2]. The synthesis of carbon nanotubes should be controlled with all parameters, which regulate the growth kinetics of carbon nanotubes. The understanding of growth mechanism of carbon nanotubes is required to know growth parameters of nanotubes. There are three methods of synthesis of carbon nanotubes, arc-discharge, laser ablation, chemical vapour deposition (CVD). In the first two methods, it is impossible to study the growth kinetics, because the synthesis process is too fast. In the CVD method, the growth kinetics of forests of SWCNTs was studied. These forests consisted of SWCNTs with different diameter, chiral angle, conductivity type, chemical properties. In our work, we study the growth kinetics of individual chirality SWCNTs inside metallocene-filled SWCNTs. We reveal two stages of growth of carbon nanotubes on metal carbide, and metallic particle, which are formed as the result of decomposing of metallocenes. Both stages are characterized by growth rates, a and b, and activation energies, Ea, and Eb, accordingly. The first stage lasts for several minutes in the beginning of the growth process, and the second stage continues for many more hours until complete formation of inner SWCNTs inside metal-filled SWCNTs occurs. It is shown that the growth rates depend on the diameter of SWCNTs. The smaller diameter SWCNTs have larger growth rates. The activation energy is also dependent on the diameter of SWCNTs. The peculiarities of these dependencies are described in our works [3-5]. The activation energy is dependent on the chiral angle [6].

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P070

GROWTH OF HORIZONTALLY ALIGNED SEMICONDUCTING SINGLE-WALLED CARBON NANOTUBE ARRAYS USING CARBON MONOXIDE AS CARBON FEEDSTOCK

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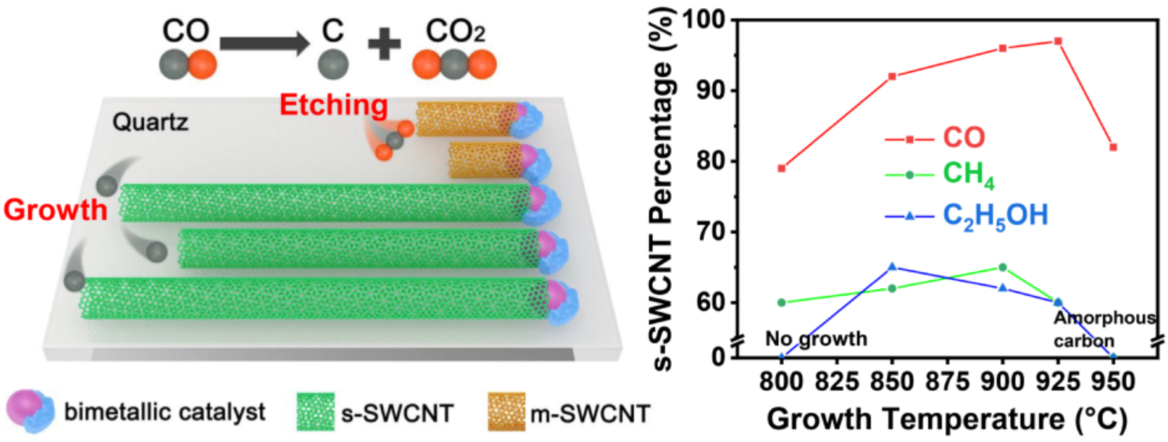
Horizontally aligned semiconducting single-walled carbon nanotube (s-SWCNT) arrays are good candidates for future nanoelectronics. Here, we developed a general approach to grow horizontally aligned s-SWCNT-enriched arrays on ST-cut quartz with bimetallic catalysts using carbon monoxide (CO) as carbon feedstock under atmospheric pressure. The disproportionation of CO produces not only carbon for SWCNT growth but also CO_2, which could act as an in-situ etchant to remove amorphous carbon and highly reactive metallic tubes. The use of bimetallic catalyst and quartz substrate facilitate the selective etching by narrowing the diameter distribution of as-grown SWCNTs to about 1.6 nm. At the optimized conditions, we realized the selective growth of horizontally aligned s-SWCNT arrays with the content of ~97% using CoCu catalysts, confirmed by Raman characterization together with electrical measurements of the field effect transistor devices. Compared to direct growth with ethanol or methane, higher selectivity can be obtained over a wider growth window with CO. The universality of s-SWCNTs synthesized from CO has been verified on various bimetallic catalysts, such as CoMn and FeCu. This work provides a feasible method for growing s-SWCNTs on substrates and demonstrates the practical potential for the scalable fabrication of CNT-based devices.



Growing s-SWCNT arrays using CO as feedstock. Schematic of the growth mechanism (left) and the comparison of the percentages of s-SWCNTs in the arrays grown from three carbon sources at different growth temperatures (right).

P071

GROWTH OF WAFER-SCALE HIGH-DENSITY HASAS WITH A TRIDENT STRATEGY AND THE HIGH THROUGHPUT CHARACTERIZATION

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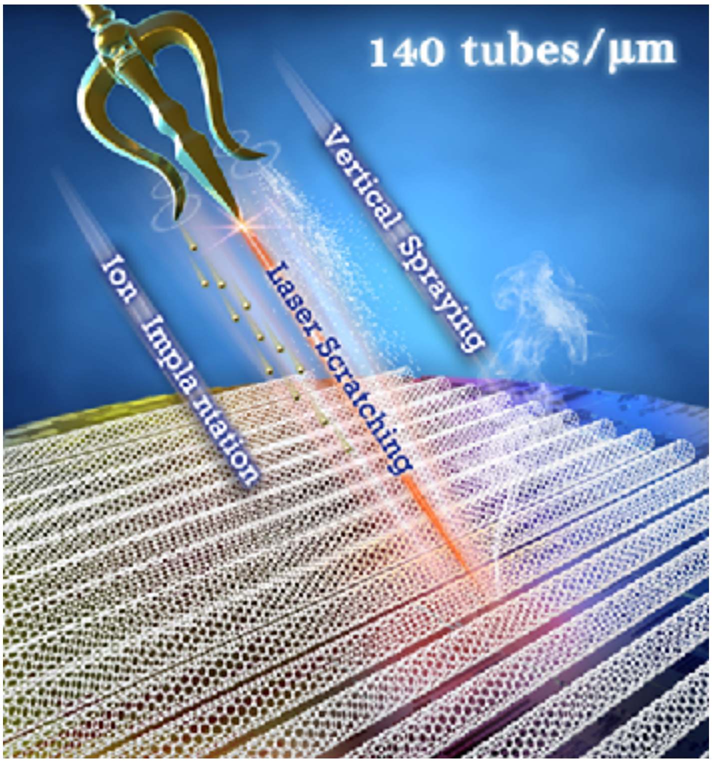
SWNT (single-walled carbon nanotube) horizontal arrays (HASAs) have been put on a very high pedestal in micro- and nano-electronics. However, after decades of study, HASAs still failed to live up to the expectation due to the trade-off between high density and large-area uniformity. Many post-processing methods have been developed to solve this problem, but mostly at the cost of the alignment and quality. Therefore, direct growth of HASAs with high-density and wafer-scale uniformity is highly desired, but remains a daunting task. Herein, we developed a "Trident strategy", synchronously optimizing the substrate surface morphology by laser scratching strategy, the catalyst distribution by ion implantation technique and the gas flow homogeneity by a "vertical spraying chemical vapor deposition" (VSCVD) system. With this three-pronged strategy, as-grown HASAs with the highest density of 140 tubes mm-1 could be uniformly distributed on a one-inch sapphire wafer. Besides, evaluating the wafer-scale uniformity of the as-prepared HASAs was needed. In this regard, we developed a "Three-leveled lever" characterization strategy with both high throughput and high precision. The breakthrough in the fabrication and characterization methods would help to accelerate the batch production and lab-to-fab transition of HASAs in the future.



The schematic of the Trident strategy. Growth of wafer-scale high-density HASAs with the Trident strategy, which composed of the laser scratching method to improve the uniformity of substrate morphology, the ion implantation technique to improve the uniformity of catalyst distribution, and the VSCVD system to improve the uniformity of gas flow.

P072

HEALTHY LIFE WITH CNT MATERIALS - MULTI-LEVEL MONITORING OF PHYSICAL ACTIVITY AND HEALTH

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The problem of heart diseases in the aging society of the Western world continuously increases. One of the possibilities to solve this problem is textronics - a combination clothes and advanced technical solutions based on nanotechnology.[1] Textronics can reduce mortality, improve recovery, monitor daily activity and ultimately reduce the healthcare costs. All of these goals can be achieved by observing functional parameters of heart, from a simple heart rate to a sophisticated multi-channel ECG. The recorded signals can be sent wirelessly (Wi-Fi/GSM) and initially analyzed by AI algorithms. Further, in the case of detecting health or life-threatening episodes, the remotely informed medical personnel will implement the necessary life-saving actions. The core of remote ECG systems is flexible electrical circuits conveniently implantable into textiles and electronics. The flexible electrical circuits could be easily printed or painted using electroconductive pastes based on various polyacrylic or polyurethane dispersions as prematrices and carbon nanotubes with the required characteristics.[2,3] Both the conductive paths and the electrodes are made of the same conductive paste. The insulations layers are made of a polymer base which is a matrix in the conductive element. Such an approach ensures compatibility and integrity of all elements. (Fig. 1).The system represents a versatile tool in remote medicine that can be easily utilized for applications such as monitoring and intervention for soldiers, firefighters, and other professionals or the in the cardiologic rehabilitation supervision, in which remote tracking of health is critical. **Acknowledgments:** The authors are very grateful for the financial support from the *National Science Center* (Poland), grant no. **2020/39/B/ST5/02562**, in the framework of the OPUS-20 program.

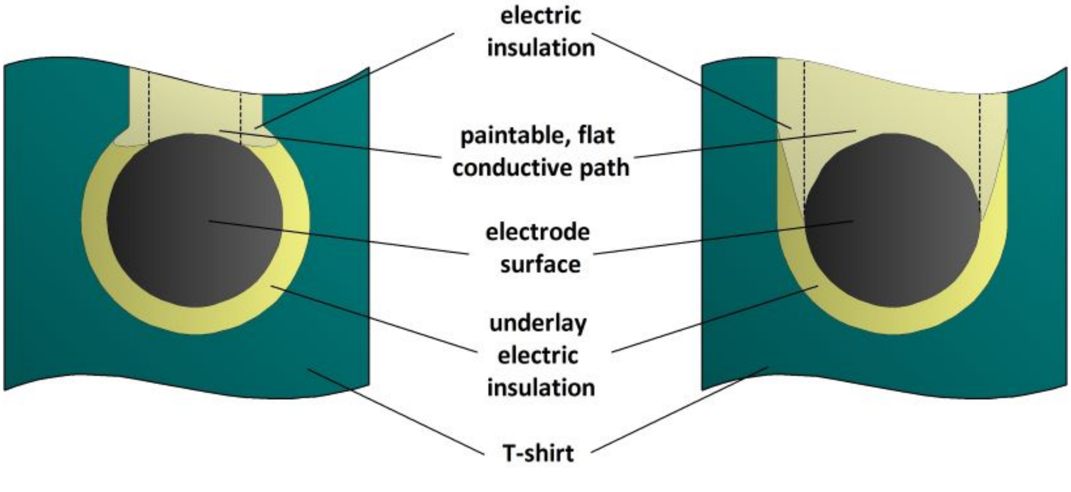

Fig. 1. Electrodes and paths

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P073

HIERARCHICAL STRUCTURE OPTIMIZATION STRATEGY FOR CARBON NANOTUBE FIBERS WITH ULTRAHIGH DYNAMIC STRENGTH

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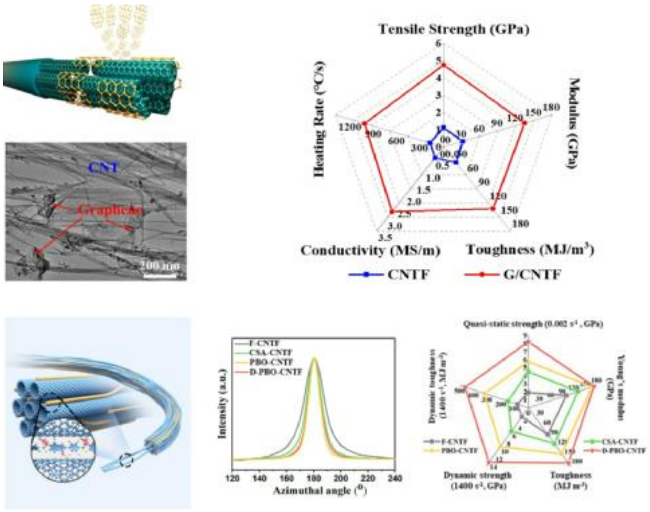
Carbon nanotube fibers (CNTFs) have been expected to inherit the striking mechanical properties of individual nanotubes, but their current performances are strongly impaired by imperfect assembly structures. Exploring methods for the controllable assembly and continuous preparation of high-performance CNTFs is still challenging. We developed a graphene/chlorosulfonic acid-assisted wet-stretching method to produce highly densified and well-aligned graphene/carbon nanotube fibers with excellent mechanical and electrical performances. Graphene with small size and high quality can bridge the adjacent CNTs to avoid the interfacial slippage under deformation, which facilitates the formation of a robust architecture with abundant conductive pathways. Their ordered structure and enhanced interfacial interactions endow the fibers with both high strength (4.7 GPa) and high electrical conductivity (more than 2 MS/m). Fiber-based lightweight wires show good flexibility and knittability, and the high-performance fiber heaters exhibit ultrafast electrothermal response over 1000 °C/s and a low operation voltage of 3 V. Furthermore, we propose a hierarchical structure optimization strategy for fabricating closely packed, well-aligned and highly interconnected fiber architectures through the combination of a bioinspired polymeric nanofibers-assisted mechanical training process and subsequent mechanical densification. This strategy enables to reinforce the intertube interactions at the nanoscale, improve the microscopic alignment and mechanically densifying macroscopic fibers. The resultant fibers exhibit ultrahigh dynamic strength of 14 GPa under high-strain-rate conditions and excellent energy dissipation capabilities, surpassing all other known macroscopic fibers. Our results provide insights into design and production of ultrastrong fibers with extremely high-strength and excellent impact-resistant performance.



High-performance carbon nanotube fibers. A hierarchical structure optimization strategy for fabricating highly packed and well-aligned carbon nanotube fibers with excellent quasi-static and dynamic strength.

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P074

HIGH CONDUCTANCE CARBON NANOTUBE ELECTRODE FABRICATION VIA PATTERNING FILTER

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Excellent electrical, optical, and mechanical properties make carbon nanotubes (CNTs) widely applied in the field of optoelectronics as transparent electrodes. However, the performance was limited by the finite absorbance of the CNTs, which brings about a trade-off between the conductance and transmittance. Patterning a thick CNT film was an effective method to overcome the trade-off. However, current techniques to pattern CNT films, such as lithography, solution printing and oxygen plasma etching, suffer from the disadvantages of contamination, complicated process, and limited conductivity improvement.

In this research, we developed a simple and quick laser-patterning filter technique for fabricating patterned CNT electrodes. Double-walled carbon nanotubes (DWCNTs) were synthesised by floating catalyst chemical vapour deposition (FC-CVD). By utilising the technique, high-performance patterned CNT electrodes can be fabricated directly and transferred onto a substrate by the dry pressing method. After doping with gold chloride, the CNT electrodes exhibit an equivalent sheet resistance of 1.3 $\Omega \cdot sq^{-1}$ at 90% transmittance, also with good mechanical properties. The patterned filter is not damaged or contaminated throughout the process, so it can be reused for fabricating CNT electrodes.

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P075

HIGH-PERFORMANCE AND POLARIZATION SHORTWAVE INFRARED PHOTODETECTOR BASED ON CARBON NANOTUBE FILMS

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Carbon Nanotube (CNT) is an ideal candidate material for shortwave infrared (SWIR) detectors due to its large bandgap tunability, strong infrared light absorption, and high mobility. We optimized the CNT film photodetector performance using multilayer CNT films and stacked contact electrode structure. The photodetector of multilayer CNT films exhibits maximum responsivity of 120 mA/W at 1800 nm wavelength, which is one order magnitude larger than a single-layer network CNT film with low density. Moreover, the dark current in the multilayer CNT films photodetector is also suppressed by a local n-type doping process. Finally, the optimization of our photodetectors with multilayer CNT films, stacked contact electrodes, and local n-type doping layer demonstrated a response spectral range of 1200-2100 nm, a peak D* of 3.94×10^9 Jones at room temperature, and a linear dynamic range over 118 dB. When the temperature decreases to 180 K, the D* of the photodetector can be improved up to 2.27×10^{11} Jones. Our work demonstrates the potential of CNT film for future SWIR imaging with a cut-off wavelength over 2100 nm.

The future direction of infrared photodetector technology development is the pursuit of multi-dimensional information detection, making the optical system planarization, and moving onto chip. Polarization detection can further obtain the polarization information of the detection target and background, which is characterized by the ability to achieve infrared target identification in complex environmental backgrounds. We have prepared a polarization photodetector using well-aligned CNT and investigated the performance in the SWIR band. Furthermore, an aligned CNT polarization photodetector with a 5×2 µm pixel size can image the laser spots with a radius of only 15 µm at 1.8 µm wavelength and shows polarization characteristics. Finally, a monolithic polarization integrated system (MPIS) based on the aligned CNT transistor, resistance, and photodetector was constructed to increase the anisotropic ratio of the photodetector. The amplified anisotropic ratio is the maximum reported in the SWIR band. Our work demonstrates the potential of aligned CNT for polarization detection applications as well as for monolithic polarization systems.

P076

HIGH-PURITY SORTING OF 1.2 NM-DIAMETER SINGLE-CHIRALITY SWCNTS WITH PYRIDINE-CONTAINING COPOLYMERS

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Single-chirality SWCNTs (sc-SWCNTs) are promising materials for upcoming electronics and optoelectronic applications in the post-Moore era. In particular, single-chirality SWCNTs with diameter distributed in a range of 1.2-1.4 nm have been regarded as ideal candidate for nanodevice development due to their unique bandgap and optoelectronic properties near 1.5 µm. However, the selective isolation ability of sc-SWCNTs becomes rather challenging when the nanotube diameter increases.

Herein, stepwise extraction strategy is introducing as an effective approach for the selective and precise separation of single-chirality SWCNTs. Two novel methods have been developed, namely enhanced ultracentrifugation (E-UCG), and stepwise extraction processing (STEP). With this methods, three monochiral species were successfully obtained. Three pyridine-containing copolymers with different copolymer unit or functional group, which successfully achieved isolation of (9,8) (10,8) and (12,5) SWCNTs with all the diameters around 1.2 nm at high single-chirality purity (82%, 92.3% and 95.6%). In summary, regulating the conjugated structure provides the basis for selectivity determination, and controlling the start materials at each step during separation is critical to the stepwise extraction strategy.

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P077

HIGH-THROUGHPUT CHARACTERIZATION OF HASAS SYNTHESIZED BY TRIDENT STRATEGY

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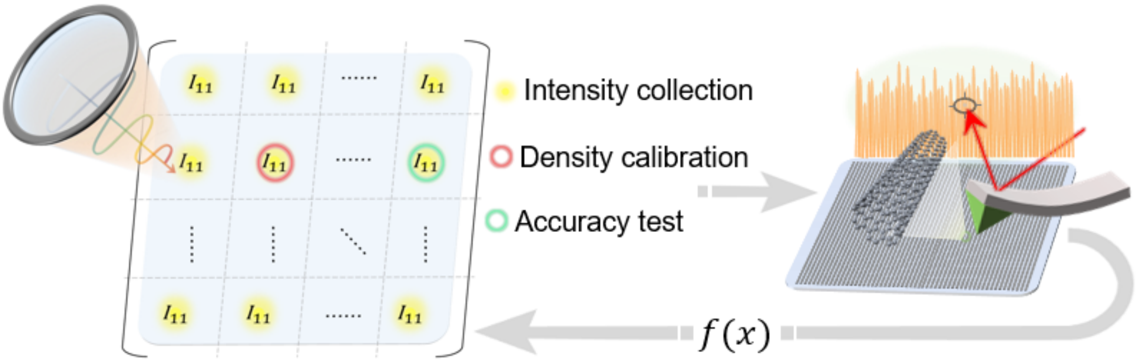
The synthesis of horizontally aligned single-walled carbon nanotube arrays (HASAs) have reached a wafer scale and brought higher request to the characterization techniques. Specifically, the rational evaluation of the HASAs density under wafer scale is highly desired for both the future development of synthesis and practical applications. The trade-off between the high-throughput and high-precision of the current characterization methods is the main limitation of the statistical and standard evaluation of HASAs density. To solve the problem, we developed a new technique by combining the Optical Imaging (high-throughput) and Atomic Force Microscope (high-precision), mainly based on "Three levers": the carbon nanotube (CNT) contrast of optical imaging was levered by the polarization control. The characterization scale of AFM was levered by AI programs. And finally, we bridged the enhanced optical signal of HASAs and the density data measured by "AFM+AI" under the same scale, and therefore levered the efficiency of density measurement by 4 orders of magnitude. This technique enables the statistical determination of the density of HASAs under wafer level. A standard characterization process was developed based on the as-synthesized 1-inch HASAs samples by Trident strategy. Moreover, we used a binary statistical indicator to evaluate the average density and uniformity of HASAs. This binary statistical indicator might be suitable to set a universal standard for density evaluation, which is meaningful for future development of HASAs.



"Three-leveled lever" Characterization. The schematic of "Three-leveled lever" characterization process.

P078

HIGHLY EFFICIENT DOPING OF CARBON NANOTUBE FILMS WITH CHLOROAURIC ACID BY DIP-COATING

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Single-walled carbon nanotube (SWCNT) based transparent and conductive films (TCFs) are one of the most prospective materials for novel flexible and stretchable electronic devices. Development of reproducible and scalable doping procedure is the key step towards the widespread implementation of SWCNT TCFs. Here, we thoroughly investigate a dip-coating technique for SWCNT doping as a promising approach for the practical manufacturing of SWCNT films with high performance. We examine the effect of dip-coating parameters on optical and electrical properties of the films using gold (III) chloride solution in isopropyl alcohol (IPA) and in situ investigate doping effects. This method appeared to easily fine-tune the optoelectronic parameters of SWCNT films and achieve a record sheet resistance value of 36 Ohm/sq. at the 90% transmittance in the middle of visible spectral range by increasing a work function value from 4.8 (for pristine SWCNTs) to 6.0 eV. The proposed approach allows efficient, uniform, and reproducible fabrication of highly conductive and transparent SWCNT films and opens an avenue for precise tailoring of SWCNT Fermi level for optoelectronic devices.

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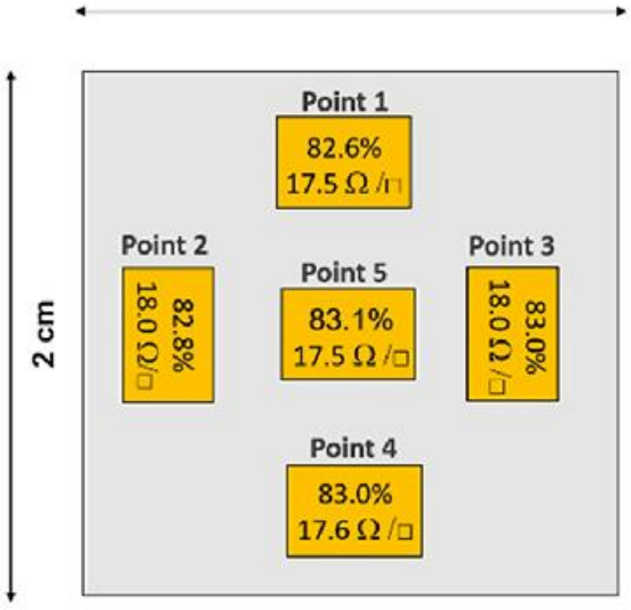

Figure. Transmittance and sheet resistance of SWCNT films measured in different points after dip-coating of SWCNT film into 30 mM HAuCl4 solution at 300 mm/min.

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P079

HOW TO MODEL OPTICAL PROPERTIES OF VERTICAL AND HORIZONTAL HETEROSTRUCTURES ?

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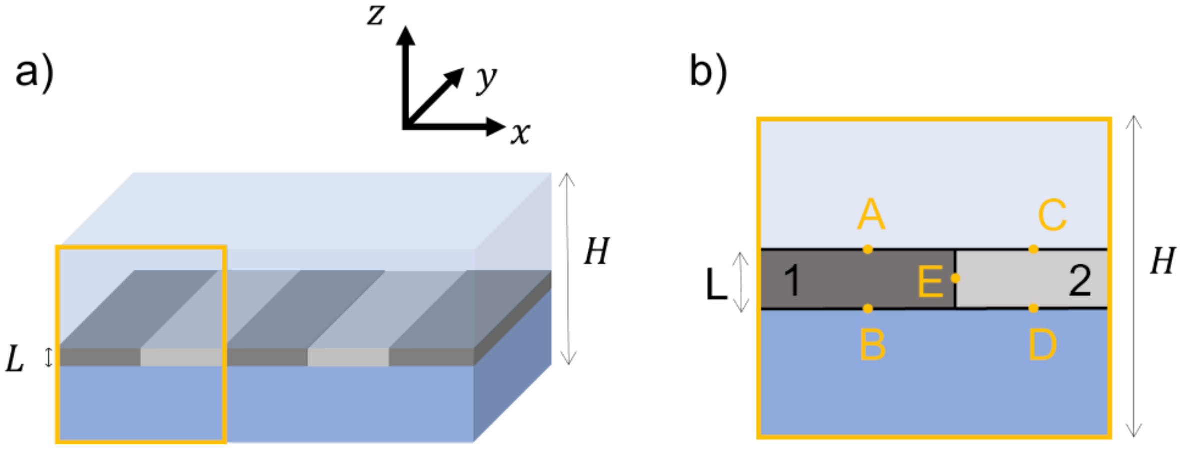
2D materials offer a large variety of electromagnetic properties that have been broadly investigated from visible light to microwaves. These properties can be tuned by nanostructuring as in nanodots or nanoribbons. Corrugation is also a manner to engineer the visible frequency response of graphene by an enhancement of the confinement of charge carriers and the excitation of plasmons, as evidenced by SERS measurements [1]

2D materials can also be combined to form heterostructures to expand the possibility to manipulate the interaction of light at the nanoscale. These heterostructures can be vertical (stacked 2D materials) or lateral (network of nanoribbons). In this work, starting from the microscopic description of the dielectric response function, we define effective medium surface susceptibilities to model the optical response of the vertical and horizontal hererostructures.

Vertical heterostructures effective response are based on a new model that reconcile the current sheet model and the thin film approach to account for single 2D layer. In our approach each layer is described by a kind of transfer matrix with intrinsic surface susceptibility that do not depend on the external medium [2]

For vertical heterostructures, we demonstrate the counter-intuitive result that very thin (compared to the wavelength) systems display an in-plane isotropy despite the ribbon-like structure where thick systems display the expected in-plane anistropy. [3]

For both vertical and horizontal heterostructures, our effective model is compared with ab-initio calculations and electromagnetic model that fully account of the nanoscale structure for graphene/BN heterostructures.



(a) Schematic view of the unit cell of a horizontal heterostructure of 2D materials b) unit cell

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P080

HYPERSPECTRAL MICROSCOPY DETECTION OF THE FLUORESCENCE SHIFT BETWEEN ENANTIOMERS OF EMPTY AND WATER-FILLED SINGLE-WALL CARBON NANOTUBES

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The remarkably chiral-structure-dependent properties of single-wall carbon nanotubes (SWCNTs) are also strongly influenced by their internal and external environment, which can therefore be investigated through optical spectroscopy.[1,2] In order to study this influence in detail, we developed a hyperspectral IR fluorescence imaging setup based on a microscope with a liquid crystal tunable filter. By resolving the spectra of individual SWCNTs, and even along the length of SWCNTs, the effect of inhomogeneous broadening is largely eliminated, and spectral details can be resolved which are inaccessible in bulk spectroscopy. An automated image processing scheme is used to obtain statistics on large numbers of individual SWCNTs. In particular, we show that not only the spectral shift in emission between empty and water-filled[1] chirality sorted SWCNTs can be resolved, but even separate emission peaks are observed for the left- and right-handed enantiomers, which interact slightly differently with the chiral surfactant with which they are coated. The approach is particularly promising for the quantification of enantio-selective separation results.

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P081

IDENTIFICATION OF PHONONIC PROPERTIES OF CONFINED CARBYNE BY RAMAN SPECTROSCOPY AND FIRST PRINCIPLE CALCULATIONS

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Carbyne is a true one dimensional allotrope of carbon, consisting of an ideally infinitely long chain. In theory, this material yields outstanding mechanical, optical and electronical properties. This one dimensional material is highly Raman active, and it is possible to synthesize it inside DWCNT [1][2] thus naming it confined carbyne (CC). Resonant Raman experiments reveal new features regarding an unusual specific line shape response of the G-Line from CC@CNT which is so far not understood. We aim to reproduce these features theoretically by ab initio methods [3][4] and consequently identify the interaction types ocurring in the framework of coupled modes. Experimentally, we utilize functionalizion [5] by altering the stepwise sythesis [6] of CC@CNT which allows us to isolate specific physical interactions occurring in this interface system. The parallel comparison of theory and experiament will allow us to fully uncover the phonoic spectrum of confined carbyne alongside with its interactions to the surrounding tubes.

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P082

IMPACT OF MOLECULAR DOPING ON SOLUTION-SYNTHESIZED GRAPHENE NANORIBBONS

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Graphene nanoribbons (GNRs) are graphene-based one-dimensional nanomaterials that exhibit unique optical and electronic properties depending on their width and edge type. Precise control over these structural parameters has been achieved in recent years by means of bottom-up synthesis. Yet, the investigation of their intrinsic optical and electronic properties, especially of solution-synthesized GNRs, has been limited by their poor dispersion stability and processability. Here we show that simple bath sonication of solution-synthesized 9-armchair GNRs with branched alkyl sidechains in organic solvents such as toluene and THF yields dispersions that are stable over several months. Liquid cascade centrifugation (LCC) of these dispersions gives several fractions corresponding to the applied relative centrifugal fields with slightly different optical and electronic properties. Here, we investigate the (transient) absorption and emission properties of individual GNRs (at cryogenic temperatures) as well as local and macroscopic charge carrier mobilities in dispersions and thin films depending on processing conditions, electrochemical and molecular doping. The interpretation of spectral shape and doping induced optical features is supported by time-dependent density-functional theory (TDDFT).

P083

IMPROVING THE MECHANICAL STRENGTH OF CARBON NANOTUBE FIBERS BY COMBINED TREATMENT OF HEATING AND ELECTRON BEAM IRRADIATED

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Carbon nanotube (CNT) fibers, which consists of a numerous number of CNTs, are expected to be applied to the light-weight structural materials due to its mechanical tolerance. Recently, high strong CNT fibers with high density and good alignment have been produced by wet-spinning method, and its density and alignment have almost reached to the theoretical limit [1]. Therefore, in order to fabricate stronger CNT fibers, it is necessary to develop methods to more finely control the structure among CNT bundles. In this study, we demonstrate an effective method to improve CNT fiber strength by combining the heat-treatment and electron beam (EB) irradiation. Commercially available pristine CNT fibers made by wet-spinning were purchased from DexMat (USA). Pristine CNT fibers are annealed at 1000-1800°C for 80 s in a nitrogen atmosphere, and at the same time, it is irradiated with an EB at an accelerate voltage of 400 kV and an irradiation dose of 10-200 kGy. Figure 1 shows the tensile strength of CNT fibers before and after treatments. Tensile strength of CNT fiber was increased by 1.2 times after 1200°C heat-treatment. Furthermore, the combined treatment of heating and EB irradiation increased the strength of CNT fiber to 3.1 GPa (approximately twice that of pristine). Raman spectroscopy suggested a relationship between fiber strength and the amount of sp2 carbon flakes generated in the CNT bundles, and it is clearly indicating the importance of interfacial modification among CNT bundles by post-treatment for improving macroscopic fiber strength. This work was supported by Innovative Science and Technology Initiative for Security, ATLA, Japan (Grant Number JPJ004596).

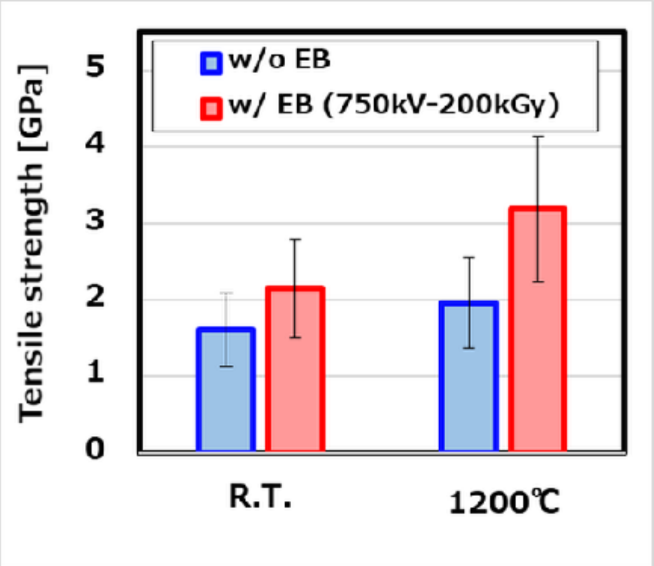

Figure 1. Tensile strength of CNT fibers before and after Joule-heating and/or EB irradiation.

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P084

COLLECTIVE RADIAL BREATHING VIBRATIONS IN HOMOGENEOUS CARBON NANOTUBE BUNDLES

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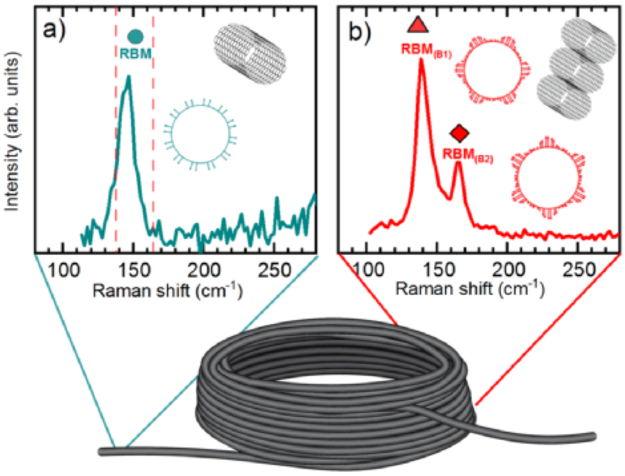
Carbon nanotubes (CNTs) are well known for being building blocks for films, ropes, and yarns with outstanding properties, where the degree of bundling plays a crucial role. The degree of bundling can be determined by the collective vibrational modes. When identical CNTs are arranged into two-dimensional hexagonal lattices, their vibrational properties are predicted to change and additional low-frequency modes are expected in the Raman spectrum [1]. Up to now, the experimental study of collective vibrations has been limited by a lack of pure homogeneous chirality bundles. We have established a self-coiling mechanism to produce such samples by CVD, where CNTs get arranged into coils and comprise perfectly aligned homologous bundles with a radial shape[2,3]. By characterizing and comparing the physical properties of the coil with respect to its tails, the bundling effects are clearly visible. In such structures, we observe two breathing-like modes RBM(B1) and RBM(B2) in contrast to the single radial breathing mode characteristic for isolated tubes. We investigate the exciton-phonon coupling for these modes with resonant Raman spectroscopy finding the same resonance energy for both BM peaks and confirming that both modes originate from the same chirality bundle. Additionally, we study the tube's diameter dependence of vibrational coupling by analyzing different tube diameter coils and other bundling geometries. We compare our experimental findings with a theoretical lattice-dynamical study of infinite bundles of identical tubes. These results provide an insight into intra-tube lattice dynamics in CNTs bundles for a better understanding of collective vibrational effects.



Raman spectroscopy of the RBM of carbon nanotube coil. a) Raman spectra for tail and b) coil (isolated-bundles effects). The peaks originating from collective vibrations are observed by RBM(B1) and RBM(B2).

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P085

IN-LINE BROADBAND PHARMA IMAGING WITH CARBON NANOTUBE SCANNERS

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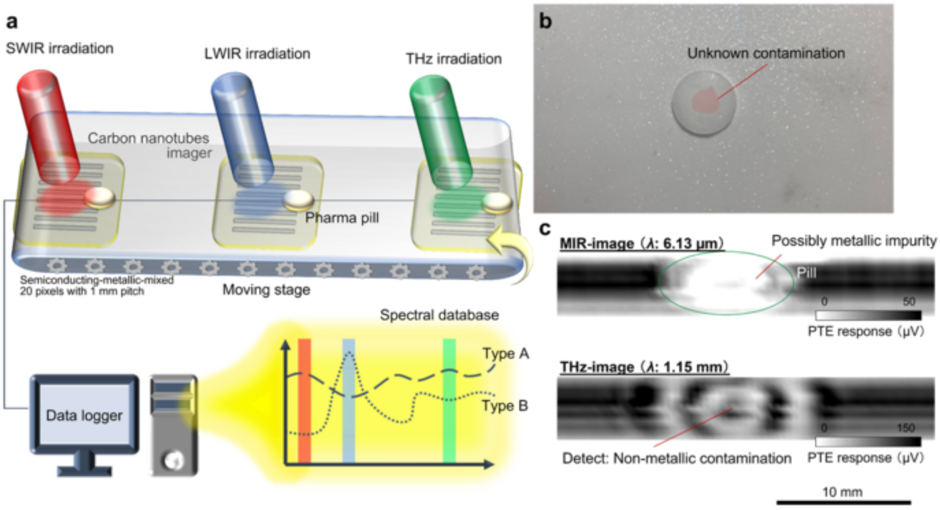
In recent years, the demand for nondestructive testing (NDT) is growing enormously, and one typical example is the testing of pharmaceuticals. Optical imaging is effective for pharmaceutical testing, especially the use of infrared (IR) and millimeter-wave (MMW) light, as each material exhibits different transmission properties [1]. In this study, a highly sensitive IR-MMW broadband imaging device [2] is used to perform basic NDT of pharmaceuticals by multi-wavelength measurement in these bands (Fig. 1a). In these bands, carbon nanotube (CNT) films are well known for their highly efficient absorption. Herein, multi-wavelength sensing in broad IR–MMW bands enables contamination testing and identification of non-metallic materials is now possible based on differences in transmittance.

Fig. 1b shows an example of the pill sample (100 mg sedative) used in this study. The pill contains a piece of plastic and is difficult to identify visually. In the figure, the location indicated in red is the contaminant. In contrast, Fig. 1c shows the results of dual-wavelength imaging at mid-infrared (MIR) and terahertz (THz) bands of the sample. In the MIR image, the contaminant was visualized. This is due to the lower MIR transmittance of the plastic pieces compared to the pill. On the other hand, in the THz image, the edge of the contaminant is visualized due to transmittance attenuation caused by scattering, but the contaminant itself is transmitted. This means that the MIR image alone indicates that the contaminant is potentially metallic. However, the contaminant can be identified as a non-metallic material by evaluation in combination with THz imaging. Therefore, the imaging device used in this study operates in the ultra-broadband from visible light to MMW and may further identify the composition of the pills.



a, Conceptional schematic. b, Photograph of a pharma pill to be inspected. The pill and contamination consist of potassium bromide and polytetrafluoroethylene. c, MIR and THz images, being obtained with 0.1 mm scan.

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P086

IN-SITU ELECTROSPUN NANOFIBER SEPARATOR ENABLING FOLDING-RESISTANT COAXIAL FIBER-SUPERCAPACITOR MODULE

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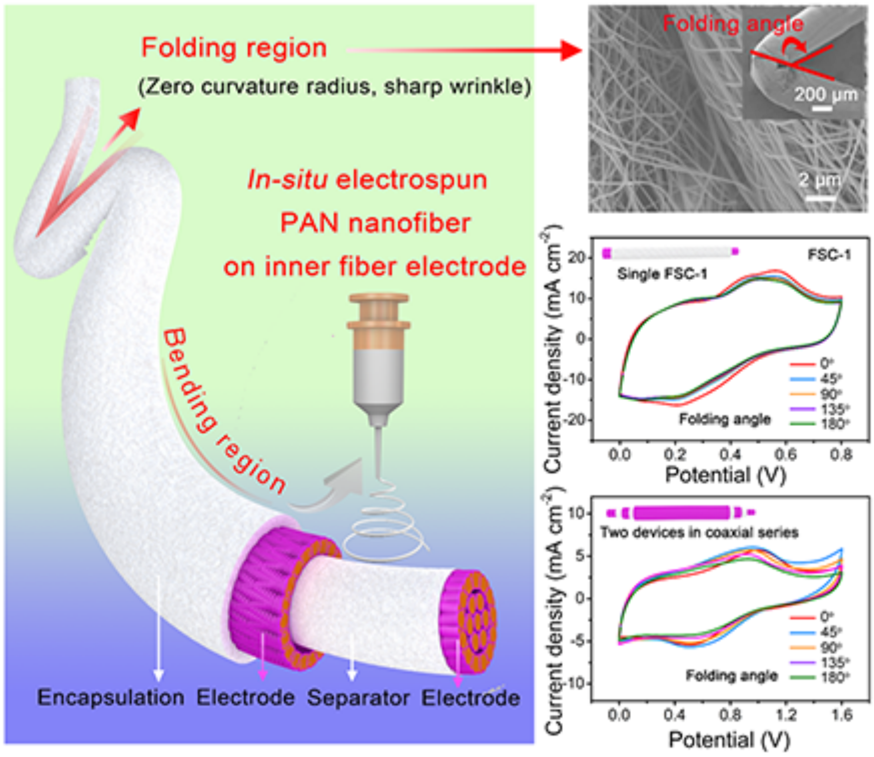
Mechanically strengthened fiber-supercapacitors (FSCs) are urgently needed in wearable electronics to adapt frequent severe deformations. However, current bendable FSCs using gel electrolyte as separator are easily short-circuited under harsh folding due to the limited stretchability of gel polymer. Herein, a folding-resistant coaxial FSC, for the first time, was fabricated through in-situ electrospinning polyacrylonitrile (PAN) nanofibers as separator on fiber electrode (Fig.1), thus effectively avoiding the short-circuit risk under highly localized stretching, compressing and folding. Moreover, such "epitaxial growth" ultrathin (~ 1 μm) PAN separator possesses high porosity, favorable strength and seamless contact with fiber electrode, enabling fast ion transport and decreased internal resistance of FSCs. Coupled with robust polyaniline/carbon nanotube (PANI/CNT) composite as model electrodes, our fabricated coaxial symmetric FSC exhibits outstanding structural folding-resistance without electrochemical failure. Amazingly, using such in-situ encapsulated separator, the as-assembled coaxial integrated series or parallel devices with higher output voltage and energy density still exhibit excellent foldable property, suggesting great practical potential.



Schematic illustration. Schematic illustration, structures and folding-resistance of the coaxial fiber-supercapacitors.

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P087

INDIVIDUAL CARBON NANOTUBE PHOTOTRANSISTORS AND BIONANOHYBRIDS VIA PHOTOCHEMICAL PATTERNING ON A CHIP

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Carbon nanotube (CNT)-based electronic circuits technology is actively developing using contemporary achievements in CVD growth and CMOS. Optical interconnection is considered as the next step in photonic integrated circuits. The CNT-based technology provides a new level of optoelectronic devices combining both the new chemistry of nanotubes and their unique properties to functionalization. The functionalization of carbon nanotubes is a promising way to increase the optical sensitivity of optoelectronic nanometer-scale devices. Utilized a unique lithography approach based on photochemical processing, a fast and easy technique for modification of single-walled carbon nanotubes (SWCNT) for novel optoelectronic devices was developed.

We have investigated two photochemical concepts of individual SWCNT modification: (i) based on ultrafast laser processing via two-photon local oxidation and (ii) engineered protein attachment based on phenyl azide photochemistry. It results in a novel approach of semiconducting single-walled carbon nanotubes conversion to different types of optoelectronic devices either through tuning laser irradiation dose or through the proper/specific adsorption site of a green fluorescent protein (GFP). The fabrication of optoelectronic junctions in the field-effect transistors based on individual SWCNT drastically increases the photoresponse of such devices. The selective wavelength photoresponsivity of the SWCNT/GFP structures reaches the value of more than 10^3A W^{-1} at 470 nm per single SWCNT at 1 V bias voltage [1]. For ultrafast laser processed nanotubes, we demonstrated the conversion of its type from quasi-metallic to semiconducting nanotube with an energy barrier of about 60 meV [2]. The photochemically tuned SWCNT-based transistors with induced optoelectronic response can be applied to detect extremely small light intensities with high spatial and spectral resolution in photovoltaics, integrated circuits, and telecommunication applications.

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P088

INDUSTRIAL APPROACHES FOR INCREASING THE PRODUCTION CAPACITY OF DIRECT-SPUN CARBON NANOTUBE FIBERS

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There have been many efforts to utilize carbon nanotube fibers (CNTFs) in various applications due to their high mechanical, electrical, and thermal properties. Among the fabrication methods, the floating catalyst chemical vapor deposition (FCCVD)-based direct spinning has been widely employed for continuous production of CNTF. However, this method allows for the formation of only a single CNTF from a reactor at a time, resulting in the limited productivity. In general, CNTFs with a large linear density (normally ranging from 6-8 tex) are regarded as favorable for improving production capacity in the direct spinning [1, 2]. However, despite the benefits in the production capacity, the thick CNTFs displayed relatively reduced intrinsic properties compared to thinner ones. Here, we explore a desirable approach to this issue by preparing CNTFs of various linear densities using the direct spinning method and comparing their characteristics. Further, we prepared braided yarns from thin CNTFs with a small linear density and compared their characteristics to a single CNTF with a large linear density. Taken together, we aim to derive a promising research direction for scale expansion in CNTF production.

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P089

INFLUENCE OF PHONON SCATTERING ON CURRENT FLUCTUATION IN CNTS

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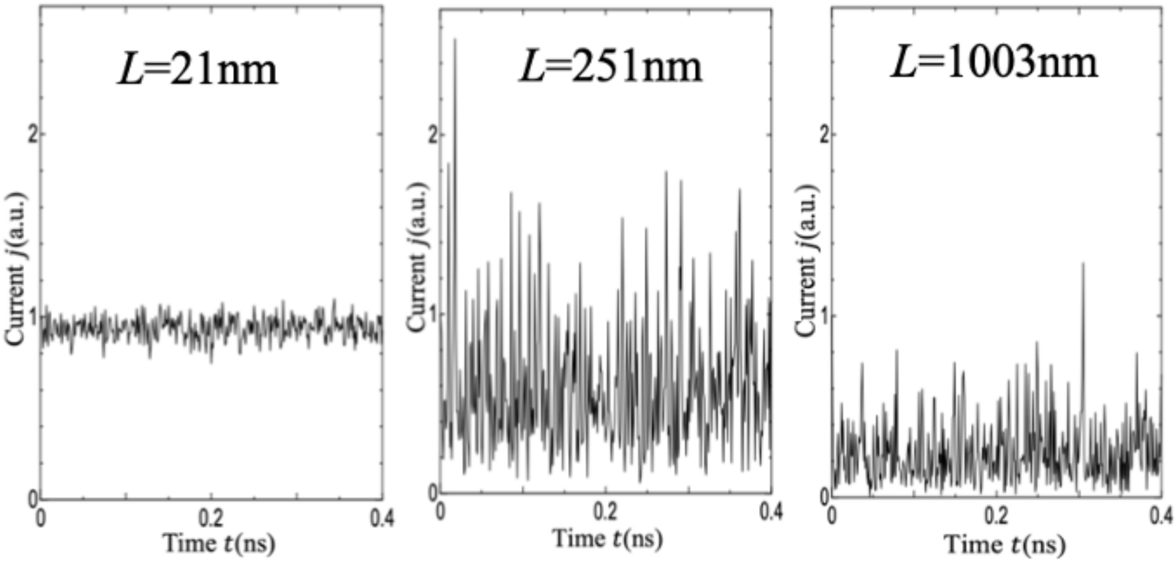
Carbon nanotubes (CNTs) are known to exhibit interesting quantum transport phenomena. Indeed, our recent theoretical study has shown that the electrical resistance of metallic CNTs exhibits a nonlinear behavior, neither the quantum resistance (R=h/4e^2) nor ohmic resistance ($R \propto L$) [1]. On the other hand, nonequilibrium current fluctuations in CNTs have not been studied thus far, and their understanding is important from the standpoint of basic science such as quantum transport physics and nonequilibrium statistical mechanics, not to mention their importance in applications. In this study, we develop a new simulation method to calculate time-dependent current and apply it to metallic CNTs. Figure 1 shows time-dependent current flowing through (5,5) CNTs with various lengths. We can see that the steady-state current (i.e., averaged current) decreases with increasing the tube length L, as the electron-phonon scattering events increase. From these time-dependent current data, we estimated the nonequilibrium current fluctuation of (5,5) CNTs with various length in terms of the variance of current defined by σ^2=$\langle (J\text{-}\langle J \rangle)^2 \rangle$. As a result, we found that σ^2 shows the maximum when L is closed to the mean free path, that is $L \approx L_\mathrm{m}$. In fact, the σ^2 at L=251nm near the mean free path is much larger than that at L=21nm (ballistic transport regime) and L=1,003nm (diffusive transport regime) as shown in Figure 1. In this presentation, we will explain the physical origin of appearance of the maximum current fluctuation around $L \approx L_\mathrm{m}$. In addition, we calculated the skewness (i.e., asymmetry) of current fluctuation defined by S=$\langle (J\text{-}\langle J \rangle)^3 \rangle / \sigma^3$. Interestingly, the skewness exhibits the maximum when L is several times the mean free path. Details will be discussed in the presentation.



Time-dependent current in (5,5) CNT

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P090

INFLUENCE OF WATER CONCENTRATION ON THE GROWTH KINETICS AND M/SC SELECTIVITY OF INDIVIDUAL SWCNTS FROM IN SITU OPTICAL MICROSCOPY

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Chiral selective synthesis of SWCNTs has been one of the main drawbacks that have hindered their application, specially in electronics, where high chiral purity is required. The control of chirality, length and density of synthesized CNTs has been studied by varying synthesis parameters, such as catalyst systems, temperature, pressure, carbon precursors and etchants [1]. Here, we studied the influence of pressure of the etchant (water) on the SWCNT growth kinetics during alcohol catalytic chemical vapor deposition (CVD). A water-assisted CVD coupled with an *in situ* optical imaging set-up was used. Homodyne polarization microscopy was used for imaging long aligned individual SWCNTs during their growth, as reported in [2]. To study the role of etching on the kinetics and M/SC selectivity of SWCNT growth, we performed a systematic study of the influence of water vapor concentration between 150 ppm and 1220 ppm. The influence of water concentration on the incubation time, the growth rate and the growth lifetime will be presented. We will also report on the influence of water concentration on the probability of etching events, the etching rate and the duration of etching.

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P091

INFRARED LUMINESCENCE OF BLACK PHOSPHORUS AT LOW TEMPERATURE: EFFECTS OF EXFOLIATION, CONFINEMENT AND ENVIRONMENTAL SCREENING

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Atomic layers of Black Phosphorus (BP) have been recently isolated, ten years after graphene. Among 2D materials, BP presents unique properties: atomic layers have a direct bandgap that can be tuned by the layer number. They interact with light in a wide range of wavelengths from visible (monolayer) to mid-infrared (bulk). This singularity makes it difficult to have an overview of the optical properties of the material, especially in the infrared range where luminescence is more difficult to investigate.

Here we present a photoluminescence study of BP starting from bulk crystal to thin layers. First the luminescence signal of the crystal is presented at 2K and the analysis of its fine structure allows us to highlight an intrinsic excitonic signature as well as to refine the a bandgap energy value at cryogenic temperature[1]. Then we show that after exfoliation, the crystal loses its fine structure in favor of a broad band, repeatedly observed in the recent literature[2,3], and probably correlated to the incorporation of defects during the process. The luminescence is then measured with respect to the thickness of the samples (4 nm to 1000 nm) and analyzed using a classical quantum well model. Finally, and by studying different heterostructures (BP/Al2O3, hBN/BP/hBN), we will establish the existence of an intermediate regime, between that of the atomic layers and the crystal, where the luminescence is dependent on quantum confinement effects and, at the same time, independent of the dielectric environment[4].

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P092

INFRARED SPECTROSCOPY AND MAPPING METHOD USING MULTILAYER-GRAPHENE MICROEMITTERS

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Infrared spectroscopy, such as Fourier transform infrared spectroscopy (FTIR), is an analysis used in various fields; however, the spatial resolution is limited by diffraction limits in analytical systems using focusing systems such as lenses and mirrors. In addition, the light sources used are millimeter-sized, and the modulation speed is slow (~10 Hz). We developed an IR spectroscopy system using multilayer graphene as a light source for FTIR. Carbon-based thermoluminescent devices, like the multilayer-graphene microemitters, have broadband spectra based on blackbody radiation [1-3]. Furthermore, we found that the multilayer-graphene microemitters have a modulation performance above 50 kHz and can be reduced in size to a few hundred nm [4]. Our spectroscopy method directly brings graphene and the material to be measured into proximity to each other, thus eliminating the need for lenses or mirrors between the emitter and the sample. We have demonstrated that this spectroscopy method can identify the location of organic compounds, such as polymer materials, by mapping measurements [4]. We demonstrated that the spatial resolution of the mapping measurement of ~1 µm is feasible [4]. This method is more straightforward than atomic force microscopy-IR (AFM-IR) or scattering scanning near-field optical microscopy (s-SNOM). This method will enable the development of analytical methods that significantly contribute to chemistry, drug discovery, and biology. This work was partially supported by Mirai Program (JPMJMI22G6), JST-Spring (JPMJSP2123) and A-STEP (JPMJTR20R4, JPMJTR221B) from JST, KAKENHI (23686055, 18K19025, and 20H02210) from JSPS, The Keio University Doctorate Student Grant-in-Aid Program from Ushioda Memorial Fund, Spintronics Research Network of Japan, the Core-to-Core program from JSPS, and NIMS Nanofabrication Platform in Nanotechnology Platform Project by MEXT.

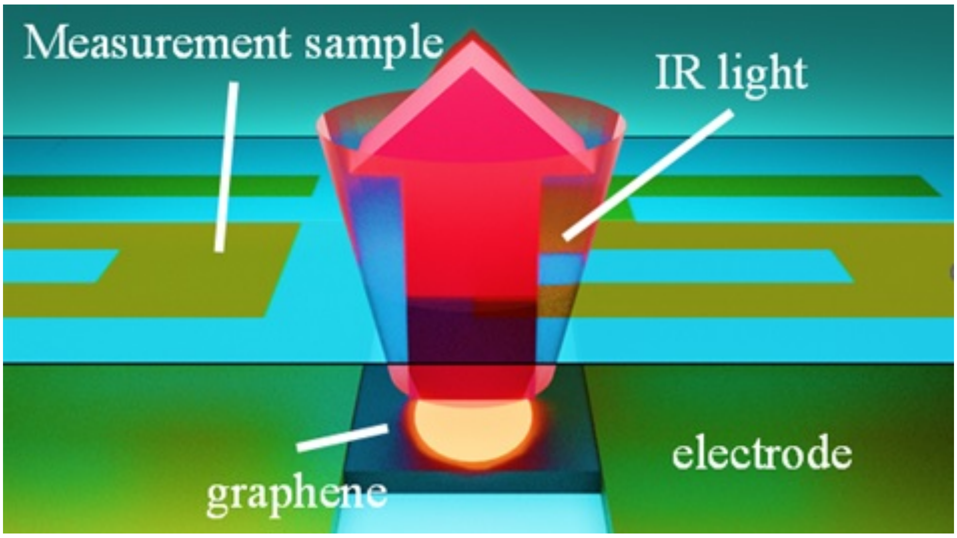

Fig 1. A schematic image of multilayer-graphene microemitters and the method of the IR analysis system.

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P093

INKJET-BASED BROADBAND CAMERA SHEETS WITH CARBON NANOTUBES

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CNTs-related materials have excellent physical and chemical properties and, can be adaptable for various applications including solar cells and capacitors. Furthermore, CNT films exhibit flexibility and broadband photo-absorption properties, making them suitable for stereoscopic imaging by employing CNT films as photo-thermoelectric imagers[1]. On the other hand, from the viewpoint of imaging usage, fine integration is essential to facilitate high-resolution visualization, video capturing applications, and so on. The viscosity of CNT solution varies depending on the CNT mass concentration in the liquid, and the drawing accuracy by inkjet printing differs accordingly (Fig. 1a). From the viewpoint of the electromagnetic wave absorption coefficient, the material exhibits broadband absorption characteristics regardless of the CNT solution concentration (Fig. 1b). In the THz region, in particular, absorption rate significantly increases with higher concentrations of the CNT solution, indicating the possibility of high-sensitive imaging device operations. Inkjet printing processes advantageously enable mechanical alignment of respective device materials. Simultaneously, this paper clarified that the use of higher viscosity CNT solution for printing maintains fundamental performances of the conventional flexible and broadband PTE imager[2].

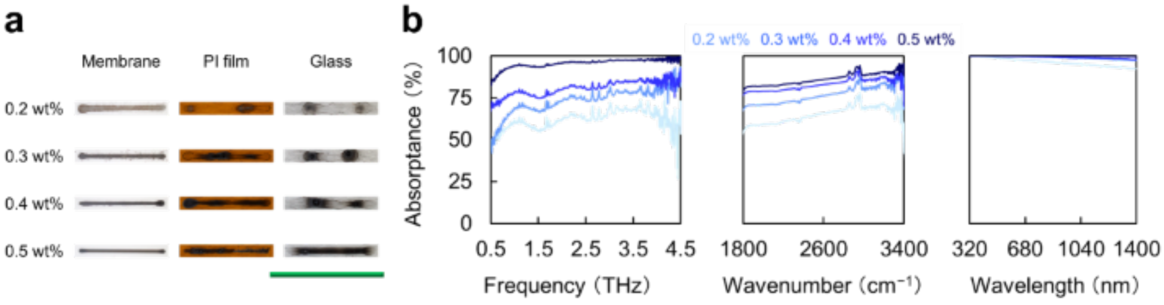

Fig. 1. a, Comparison of inkjet printing accuracy of devices by CNT solution concentration. The support substrates are membrane, PI film, and glass, respectively. Scale bar: 8 mm. b, Comparison of Electromagnetic wave absorption of CNT solution by Mass Concentration.

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P094

INTERCALATION OF DWCNT FIBERS WITH LONG-RANGE ORDERED BROMINE SPECIES

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Improvements in the control of alignment, packing, polydispersity, and metallicity of constituent CNTs in macroscopic films and fibers offer an attractive library of high property CNT-based materials [1]. The most gentle and efficient way of increasing electrical conductivity of carbon nanotubes is intercalation, consisting on adding dopants in the channels created by packed CNTs (similar to graphite intercalation compounds), which shifts the Fermi level without introducing structural modifications nor significant weight. An interesting result herein shown for the first time is that highly dense and aligned CNT fibers can be intercalated throughout the whole section and length of the fiber [2]. This achievement is demonstrated for vapor phase intercalation of bromine in DWCNT fibers, where a homogeneous distribution of dopant in the channels is accomplished (as shown in Figure 1.a) despite the difficulties for its entrance in bundles of such cross-sections (~50-1000 nanotubes) and length. Furthermore, long range order of Br species is found (as confirmed by WAXS patterns and DFT simulations), with neutral and anionic chains interacting among them and with the CNT walls (see Figures 1.b,c). The Br_2/Br_3^- intercalated CNT fibers present an increase of nearly one order of magnitude in room temperature conductivity, reaching ~10.7 MS/m, and which results stable in ambient conditions and upon annealing at relatively high temperatures (up to ~280°C). Through transport measurements down to cryogenic temperatures, the main contribution to the increase in electrical conductivity is attributed to a diminished barrier height for conduction between CNT junctions.

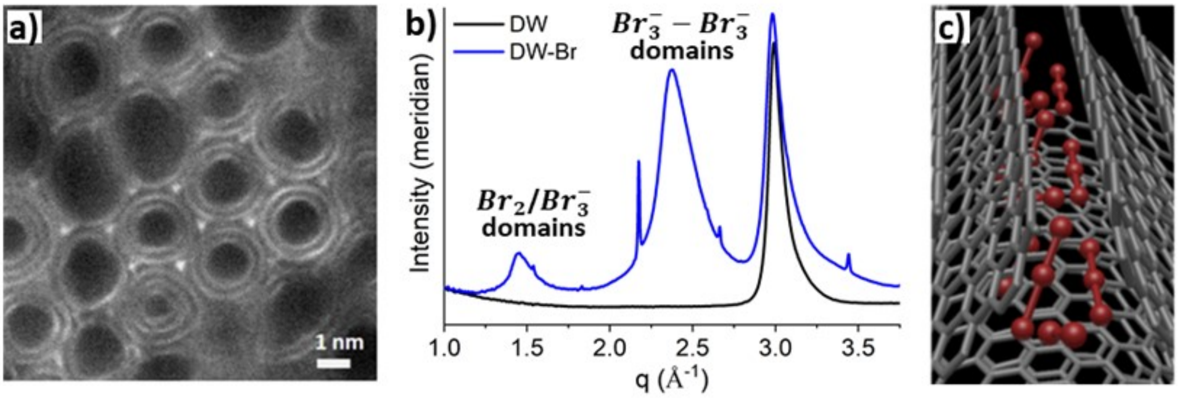

Figure 1. Structure of Br-intercalated DWCNT fibers. a) STEM micrograph in HAADF mode showing bromine intercalated in the channels, and with no encapsulated dopant. b) WAXS pattern showing ordered domains of bromine species. c) Detailed sideview of one of the ordered arrangements formed by Br species at a concentration of 26.1 wt% (close to the experimental value).

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P095

INVESTIGATION OF FIELD-EFFECT TRANSISTORS BASED ON INDIVIDUAL AND ALIGNED CARBON/BORON NITRIDE NANOTUBES

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Semiconducting single-walled carbon nanotubes (CNTs) can be used in ultrascaled field-effect transistors (FETs) without suffering from short-channel effects due to their thinness. For energy-efficient operation, subthreshold swing (SS) and hysteresis must be minimized, which can be improved by a large gate capacitance and a low interface state density. Considering the significant reduction of interface state densities in MoS_2 FETs through encapsulation by hexagonal boron nitride (hBN) [1], we expect that the wrapping of CNTs with hBN nanotubes (BNNTs) also leads to a superb switching and suppressed hysteresis in CNT-FETs. Here, we fabricate FETs using single or aligned CNT@BNNTs as channels to evaluate the potential of such heterostructures [2]. We synthesize isolated CNTs across micropillars, whereas the arrays of suspended CNTs are prepared by the anthracene-assisted dry transfer method. After growing BNNTs, we transfer the CNT@BNNTs onto flat Si/SiO_2 substrates for following fabrication steps. An AFM image of a typical CNT@BNNT array is shown in Fig. 1a. After an e-beam lithography process to define source and drain contacts, we etched surrounding BNNTs using XeF_2 gas [3], whereas CNTs were only fluorinated. Back-gate FETs were fabricated by the deposition of Ti/Au (insets of Fig. 1b,c). Figure 1b shows the transfer curve of a device with aligned CNT@BNNTs. Near-zero hysteresis is achieved as a result of thick BNNT coating (~7 nm). To explore the potential of such heterostructures in terms of switching behaviors, we also measure the transfer curves for a single CNT@BNNT as a channel (Fig. 1c). Despite the thick gate dielectric (~100 nm) with low dielectric constant, typical SS values are ~100 mV/dec, corresponding to the interface state capacitance of ~0.25 pF/cm.

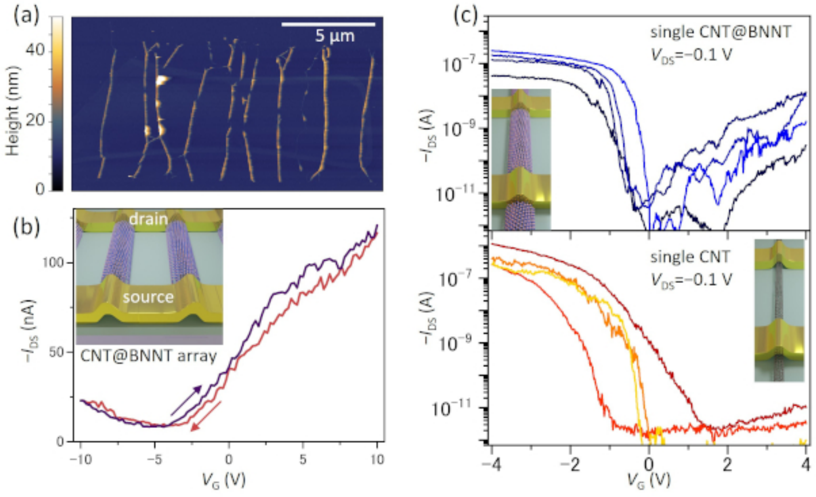

Figure 1. (a) AFM image of aligned CNT@BNNTs. (b) Hysteresis-free transfer curves of FETs with aligned CNT@BNNTs as channels. (c) Representative transfer curves of individual tube-based FETs with a CNT@BNNT (upper) and a CNT (lower).

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IONANOFLUIDS – MERGING IONIC LIQUID AND CARBON NANOMATERIALS TOWARD SUPERLUBRICITY

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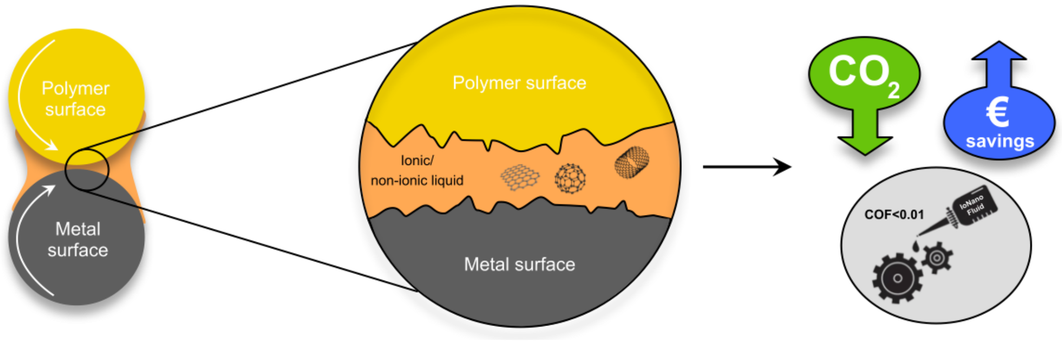
Lubricants from the beginning of civilization help us reducing energy consumption in the friction joints. The development of advanced tribology could reduce CO2 equivalent emissions by 1460 million tones and thus save EUR 450 billion. Different tribopairs such as metal-polymer or polymer-polymer require specific lubes dedicated to their construction.[1] With an excellent combination of properties, ionic liquids (ILs) emerge as promising candidates for the lubricants while their amalgamation with carbon nanomaterials – such as CNTs, graphene, CQDs etc. – yielding IoNanoFluids (INFs), can lead to superlubricity.[2] This phenomenon is a tribological regime described by a coefficient of friction (COF) <0.01. Here, we demonstrate that INFs based on ILs physicochemically compatible with CNTs (of a required morphology and surface chemistry) bring us closer to INFs displaying superlubricity in the metal-polymer tribopairs.[3]



Schematic representation of IoNanoFluids. Schematic representation of IoNanoFluid in tribology mechanism

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P097

JOULE HEATING: A UNIVERSAL PROCESSING ROUTE FOR NANOSTRUCTURED COMPOSITES

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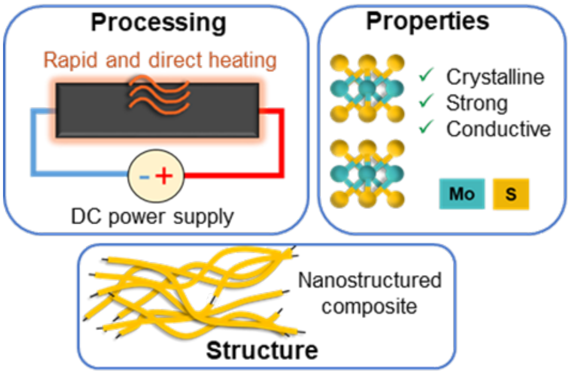
Carbon nanotubes (CNTs) are electrically conductive materials that heat up directly and rapidly in response to electric fields – an effect called Joule heating. Joule heating can be utilized to heat up nanocarbon composites from within, providing a targeted, controlled, and out-of-oven processing technique with applications in manufacturing, such as curing composites without molds, [1-3] recycling carbon fiber from spent composites, [4] bonding multi-material surfaces together, [5] and pyrolyzing waste into graphene. [6] In this work, we show a new processing route using Joule heating for a nanostructured network composite of carbon nanotube (CNT) fabrics and an inorganic phase (MoS_2), and then study the resulting structure and properties. [7] To this end, first, a unidirectional fabric of conductive CNT bundles is electrochemically coated with MoS_2. Afterward, the conformally coated inorganic phase is crystallized via heat generated by direct current passing through the CNT ensemble. The Joule heating process is rapid (heating rate up to 4000 °C/s), enables accurate temperature control, and takes as little as 2 seconds. The resulting composite material combines high electrical conductivity of up to $1.72\ (\pm 0.25) \times 10^5$ S/m, high tensile modulus as high as 8.82 ± 5.5 GPa/SG, and an axial tensile strength up to 200 ± 58 MPa/SG. The combined electrical and mechanical properties are orders of magnitude above granular composites and wet-processed nanocomposites of similar composition. The extraordinary longitudinal properties stem from the network of interconnected and highly aligned CNT bundles. Conductivity and modulus follow approximately a rule of mixtures, similar to a continuous fiber composite, whereas strength scales almost quadratically with the mass fraction of the inorganic phase due to the inorganic component constraining re-alignment of CNTs upon stretching. The Joule heating processing route can be applied to other CNT/inorganic composites, such as CNT/metal oxides, and the crystalline phase and morphology can be tuned by controlling the heating rate and target temperature. This leads to composites with specific strength above steel and electrical conductivity appropriate for use in electrochemical energy storage.



Joule heating of CNT/inorganic composites

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P098

LARGE SCALE SYNTHESIS OF VERTICALLY ALIGNED CARBON NANOTUBES ON METAL FOILS

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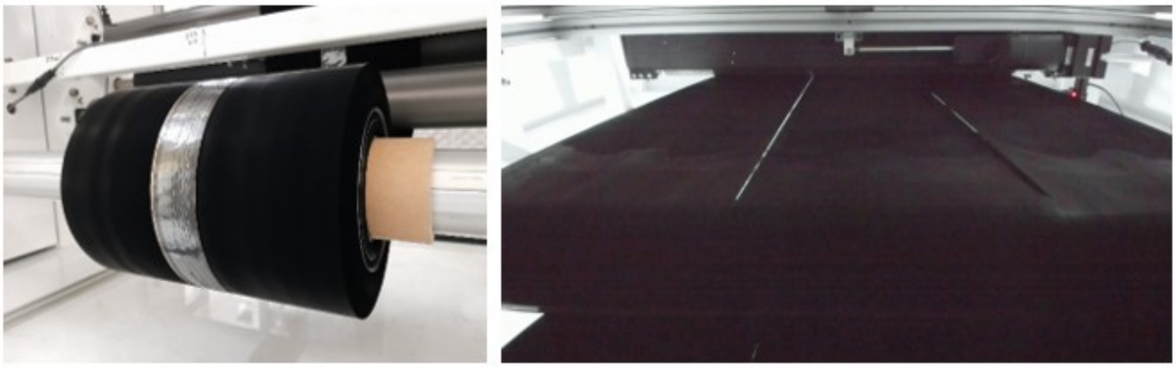
Thin and flexible metal foils coated with vertically aligned carbon nanotubes (VACNT) are efficient building blocks for various applications including:
- VACNT coated aluminum foil as active electrode of supercapacitors,
- VACNT coated copper foil as 3D current collector of lithium battery anodes,
- VACNT coated stainless steel foil as intermediate system for the interlaminar reinforcement of composite materials.

Though, growing VACNT on these substrates at industrial scale remains challenging while it is crucial to allow for the adoption of VACNT in commercial products.
Here we report our recent progress in the continuous manufacturing of VACNT by catalytic CVD on aluminum, copper and stainless-steel foils.
The specificities of each system and their advantages in the above-mentioned applications will be outlined and, for each case, the relevance of a single-step aerosol-assisted catalytic CVD process or a double-step process including a PVD catalyst deposition step will be discussed. The already demonstrated and further expected throughputs will be presented.
Finally, the added value of VACNT to the targeted applications will be highlighted, based on actual measurements and characterization of prototype devices.



Rolled 300mm wide and >100m long, double-side VACNT coated Al foil (left) and 3x300mm wide double-side VACNT coated stainless-steel foils (right)

P099

LONG AND DENSE VACNT GROWN AT LOW TEMPERATURE BY A ONE-STEP CCVD PROCESS

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This study focuses on the growth of vertically aligned carbon nanotubes (VACNT) by aerosol-assisted catalytic chemical vapor deposition (AACCVD). This one-step process operates at atmospheric pressure and leads to the continuous growth of VACNTs. It was initially developed at high temperature (800-850°C) [1,2,3] for the VACNT growth on quartz or silicon. The principle is based on the simultaneous injection of catalytic and carbonaceous precursors, in order to form in-situ the catalytic particles leading to the VACNT carpet growth. F. Nassoy et al. [4] adapted the process conditions to allow the growth of long and dense VACNT on aluminum at lower temperature (615°C) using dihydrogen and acetylene, and adjusting the Fe/C ratio that is important for the morphological quality control of VACNTs. The growth rates obtained (approximately 4µm/min) are similar to the state of the art referenced for growth using more complex CVD processes (multi-step). However, a phenomenon of carpet length limitation around 120µm, and therefore a progressive growth rate reduction, has been observed for long synthesis durations (beyond 40min) [4], as also reported in different works of the literature studying CVD methods in 2 steps [5,6]. The hypothesis adopted to explain this limitation is poisoning of the catalytic particle [4,5,7] by disordered carbon resulting from an overly efficient decomposition of acetylene.

This work explores more precisely the role of the carbon source content, the Fe/C ratio and CO2 addition on the synthesis of VACNTs on aluminum substrates [8] with the main objective to overcome the limitations of VACNT growth, constituting a drawback for applications requiring long and dense VACNTs. By using acetylene as carbon feedstock and ferrocene as catalyst precursor, we demonstrate that when acetylene content is reduced to 1.5vol%, it is possible to grow dense VACNT carpets up to 700 µm length while maintaining constant the VACNT growth for long synthesis duration (up to 160min) and improving the carbon conversion yield. An optimum Fe/C ratio of 0.8 coupled with a low acetylene content gives the highest growth rate (5.4µm/min) ever reported for a thermal AACCVD process operated at such a low temperature. The CNT number density can be controlled by varying the Fe/C ratio, enabling high density forests (e.g., 1.3x10^11CNT/cm2). Moreover we demonstrated that CO2 addition clearly prevents the phenomena of saturation and degradation and allows to get forests as long as 800µm for long synthesis duration (up to 320min).

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P100

SWCNT-BASED NANOCOMPOSITES WITH ULTRA-LOW PERCOLATION THRESHOLD FOR ELECTRONIC APPLICATIONS

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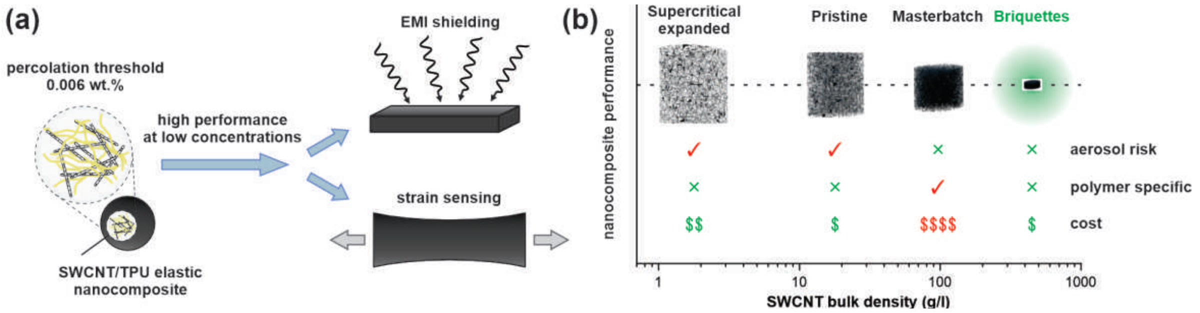
CNT/polymer nanocomposites are one of the most important fields in CNT-based applications. Meanwhile, despite the fact the SWCNT-based ones often demonstrate superior properties, the vast majority of the works are devoted to nanocomposites based on MWCNTs which is mainly due to their wider prevalence and easier processing procedures. Motivated by the recent drop in SWCNT price, we have focused on the elastic SWCNT/thermoplastic polyurethane (TPU) nanocomposites with low concentrations of SWCNTs. Manufactured by coagulation (antisolvent) precipitation technique, SWCNT/TPU nanocomposites have appeared to possess ultra-low percolation threshold of 0.006 wt% and state-of-the-art performance in soft electronic applications at low SWCNT concentrations – strain sensing and EMI shielding [1]. We attribute these results to the high nanotube dispersion degree achieved by appropriate fabrication technique and moderate SWCNT length – golden middle between high dispersibility and high conductivity. Moreover, in our next project, we have proposed an approach to simplification of handling with SWCNT powders by using pre-consolidated briquettes of SWCNTs with high bulk density [2]. We have demonstrated that SWCNT/thermoset nanocomposites fabricated from such briquettes are not inferior in SWCNT dispersion within polymer as well as in electrical and thermal properties to those prepared from pristine SWCNT powders, aerosolized ones, and even to those manufactured from commercial masterbatches with pre-dispersed SWCNTs. The simple and cheap technique of pre-consolidation compresses large-scale voids in SWCNT powders not affecting its structural properties (surface area and defectiveness) and dispersion in polymer, meanwhile, it allows avoiding high powder aerosolization, specificity to certain polymer matrices (what masterbatches have) and is considered as a safe solution for large-scale SWCNT-based nanocomposite production. This work is supported by the Council on grants of the President of the Russian Federation (grant НШ-1330.2022.1.3).



(a) Schematic representation of SWCNT/elastomer nanocomposites with high performance at low SWCNT concentrations; (b) Schematic diagram demonstrating same nanocomposite performance at higher SWCNT bulk density with highlighted advantages [1,2]

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P101
METAL STACKS AS CNTFET CONTACTS

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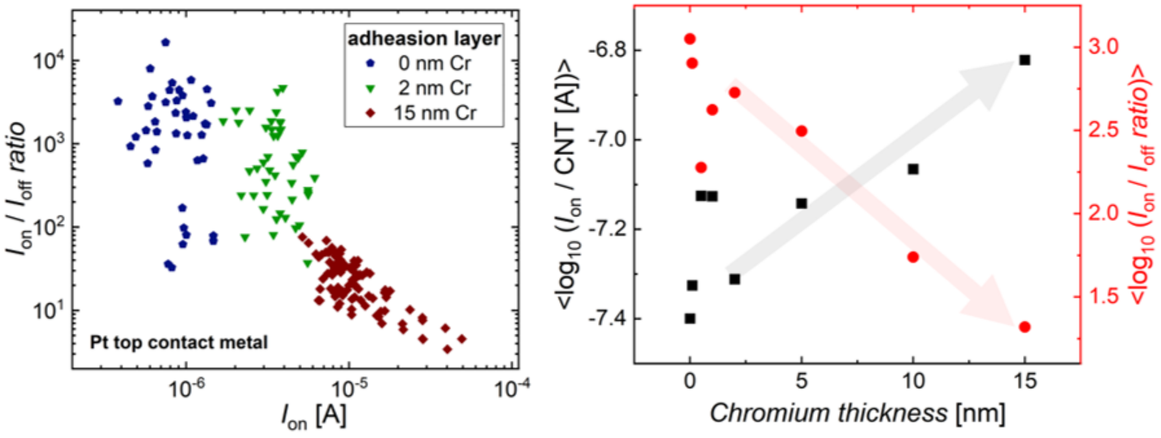
Excellent metal to nanomaterial contacts are essential in nanomaterial-based devices to exploit their unique properties. A low Schottky barrier and a low contact resistance are of high importance for single-walled carbon nanotube-based field-effect transistors (CNTFETs) to increase the current per tube. Accompanying effects like improved noise performance and an increased device transconductance would in particular push the operation frequency of high frequency CNTFETs. However, experimental data still reveals a lack between the theoretically predicted contact resistances per tube approaching the quantum resistance [1] and achieved values [2] for a statistically relevant amount of devices prepared under scalable fabrication compatible conditions. Several aspects such as contamination at the metal-CNT interface, the contact geometry as well as the choice of the contact metal have a major impact. Pd and Pt are known as good contact metals for p-type CNTFETs. However, their adhesion on oxides is weak and hence typically thin Cr and Ti adhesion layers, which are known to form contacts with larger contact resistances, are deposited in advance resulting in a heterogeneous metal contact. We present the impact of different Cr and Ti thicknesses in combination with a Pt top contact onto CNTFET performances with and without a device passivation as exemplary shown in the figure below. Not passivated devices with increasing Cr thickness feature an increasing on current but a decreasing on/off current ratio. To understand this behavior comprehensive electrical, AFM and Raman measurements will be presented.



CNTFETs transfer characteristics analysis. Overview of on current and on/off current ratios of not passivated CNTFETs with Pt top contacts and Cr adhesion layers with different thicknesses on the left side; corresponding mean values of the logarithm of the on currents per CNT in black and on/off current ratios in red for the different chromium thicknesses calculated from over 40 devices for each shown data point on the right side.

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P102

MICRO-SCALE METAL PLATING ON CARBON NANOTUBES

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Metal plating on carbon nanotube at micro-scale was carried out by using a home-made instrument. It is found that a variety of metals can be deposited on the surface of carbon nanotubes. Compared with traditional plating method, the current approach enables accurate electroplating within a few microns, which is very helpful for fabricating metallic micro stripes precisely. It was also used to weld carbon nanotubes to electrodes to get better electrical contact and less contact resistance. This approach might also be utilized in other nanomaterials, such as 2D materials to directly printing electrodes on them.

P103

MICROWAVE OPTOMECHANICS OF THE TRANSVERSAL CARBON NANOTUBE VIBRATION

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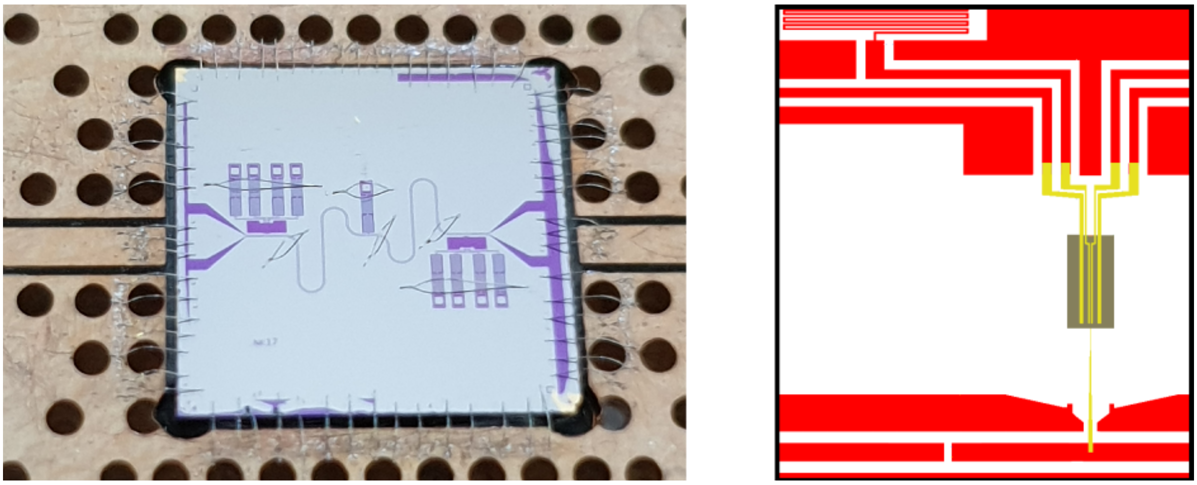
We have demonstrated optomechanical coupling of a carbon nanotube and a coplanar microwave resonator at millikelvin temperatures [1,2]. In the measured device, the nanotube acts both as a mechanical resonator and as a quantum dot. The nonlinear electronic response of Coulomb blockade enhances the microwave optomechanical coupling by several orders of magnitude, overcoming the mismatch of scales between microwave and mechanical subsystem and reaching a single photon coupling of up to g_0~100Hz. This novel optomechanical system presents several interesting features, least of all a widely tunable coupling parameter. For optimized parameters, e.g., strong optomechanical coupling (with hybridization of vibrons and photons) and the quantum coherent limit (where manipulation is faster than thermal decoherence) is within reach. Since the publication of [1], we have achieved significant improvements of our microwave resonators integrating the nanotube transfer areas and electrodes. Ongoing work aims at optimizing the carbon nanotube growth and the transfer of the nanotubes onto the resonator chip, as well as the cryogenic millikelvin setup for the measurements. We present the current state of our work, towards quantum control of the carbon nanotube vibration.



(left) Test device for integration of a vibrating carbon nanotube with a coplanar waveguide resonator. (right) Detail drawing of the nanotube transfer area.

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P104

MOLECULAR DYNAMICS SIMULATION OF CARBON NANOTUBE GROWTH UNDER TENSILE STRAIN

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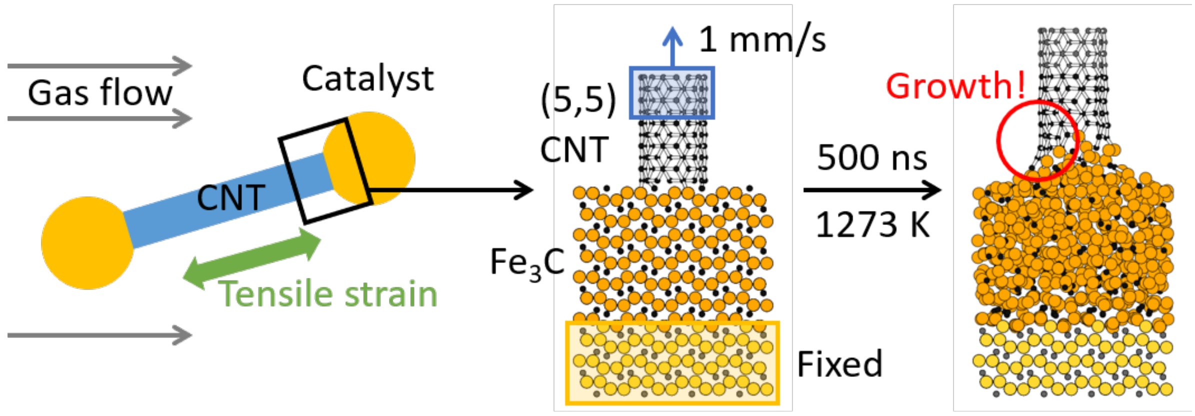
Floating-catalyst chemical vapor deposition is attracting much attention not only as the continuous and scalable production methods of carbon nanotube (CNT), but also due to its possibility to product long CNT [1, 2]. Because of the difficulty of direct observation of floating catalyst in experiment, molecular dynamics (MD) simulations are useful to understand the growth processes of CNT at atomic level.

In this work, we focused on the tensile strain between two catalyst that are bridged by single CNT. CNT-catalyst contact point was modeled to short CNT on cementite Fe_3C. The bottom of the cementite was fixed and the top of the CNT was lifted by constant velocity during simulations to introduce tensile strain. All calculations were performed by using LAMMPS package [3]. NVT ensemble was used with the Nosé–Hoover method to control the temperature of the systems [4, 5, 6]. The bond-order-type potential was used to describe the interaction of atoms in cementite and CNT at once [7].

Our simulations showed that CNT can grow up under appropriate temperature even if the CNT lifting speed is high (1 mm/s). We will discuss the effect of temperature, CNT chirality, carbon supply on CNT growth under tensile strain.



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P105

MOLECULAR EVOLUTIONARY GROWTH OF ULTRALONG SEMICONDUCTING DOUBLE-WALLED CARBON NANOTUBES

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The self-assembling synthesis accompanied with template auto-catalysis loop and the ability to gather energy, induces the appearance of chirality and entropy reduction in biotic systems, being related with the origins of life and evolutionary behaviors. However, an abiotic system with biotic characteristics is of great significance but still missing. Here, we demonstrate the molecular evolution is characteristic of ultralong carbon nanotube growth, revealing the advantage of chiral assembly through template auto-catalysis growth, stepwise-enriched chirality distribution with decreasing entropy, and environmental effects on the evolutionary growth. Specifically, the defective and metallic nanotubes perform inferiority to semiconducting counterparts, among of which the ones with double walls and specific chirality (n, m) are more predominant due to molecular coevolution. An explicit evolutionary trend for tailoring certain layer chirality is presented toward perfect near-($2n$, n)-containing semiconducting double-walled nanotubes, as shown in Figure 1. These findings extend our conceptual understanding for the template auto-catalysis assembly of abiotic carbon nanotubes, and provide an inspiration for synthesizing chiral materials with kinetic stability by evolutionary growth.

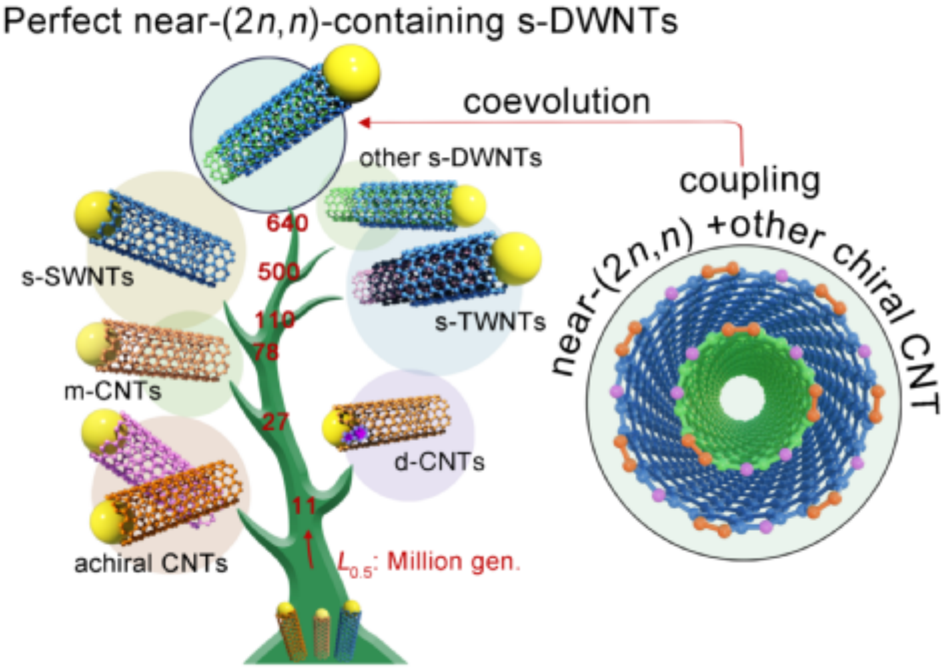

Figure 1. Schematic summarizing the stepwise evolution toward perfect near-(2n, n)-containing semiconducting DWNTs.

P106

MOLECULAR EVOLUTIONARY GROWTH OF ULTRALONG SEMICONDUCTING DOUBLE-WALLED CARBON NANOTUBES

J. Gao [1*], Y. Jiang [1], S. Chen [1], H. Yue [1], H. Ren [1], Z. Zhu [1], F. Wei [1]

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The self-assembling synthesis accompanied with template auto-catalysis loop and the ability to gather energy, induces the appearance of chirality and entropy reduction in biotic systems, being related with the origins of life and evolutionary behaviors. However, an abiotic system with biotic characteristics is of great significance but still missing. Here, we demonstrate the molecular evolution is characteristic of ultralong carbon nanotube growth, revealing the advantage of chiral assembly through template auto-catalysis growth, stepwise-enriched chirality distribution with decreasing entropy, and environmental effects on the evolutionary growth. Specifically, the defective and metallic nanotubes perform inferiority to semiconducting counterparts, among of which the ones with double walls and specific chirality (n, m) are more predominant due to molecular coevolution. An explicit evolutionary trend for tailoring certain layer chirality is presented toward perfect near-($2n$, n)-containing semiconducting double-walled nanotubes, as shown in Figure 1. These findings extend our conceptual understanding for the template auto-catalysis assembly of abiotic carbon nanotubes, and provide an inspiration for synthesizing chiral materials with kinetic stability by evolutionary growth.

Figure 1. Schematic summarizing the stepwise evolution toward perfect near-(2n, n)-containing semiconducting DWNTs.

P107
MOLECULAR SIMULATIONS OF ICOSAHEDRAL ALLOY NANOPARTICLES WITH EXTRAORDINARY THERMAL STABILITY

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As demonstrated by W-Co alloy-catalyzed single-walled carbon nanotube (SWCNT) growth [1], the *solid* catalyst is essential for chirality control. However, we cannot imagine nano-meter scale solid alloy at elevated temperatures. In this study, we discovered high symmetric icosahedral Co13Fe42 and Ni13Ti42 clusters (Mackay clusters [2], Fig. 1 (a-b)) by molecular dynamics (MD) simulations using Tersoff-type [3] and modified embedded atom method (MEAM) [4] potentials. The clusters had much higher melting temperatures than pure 55-mer cluster of each element. There can be two origins of the high thermal stability. First, these clusters had rotational vibration modes of the inner shell against the outer shell, and those modes might prevent the structure from collapsing even if the magnitude was high. Second, this structure had high cohesive energy, which required high energy to cause phase transition. Co13Fe42 also had a characteristic that it became most stable when the inner shell formed an angle of 15 degree against the outer shell (Fig. 1 (c)). We call the rotated clusters Super Mackay to distinguish from regular Mackay clusters. Super Mackay cluster successfully catalyzed SWCNT growth in MD simulations under a wide range of temperature conditions, and it kept the structure during the simulation despite the high temperature and the existence of carbon atoms (Fig. 1 (d-e)). Due to the stability and the catalysis, these kinds of clusters can be anticipated as chirality-controllable catalysts for SWCNTs as well as multi-purpose nanocatalysts.

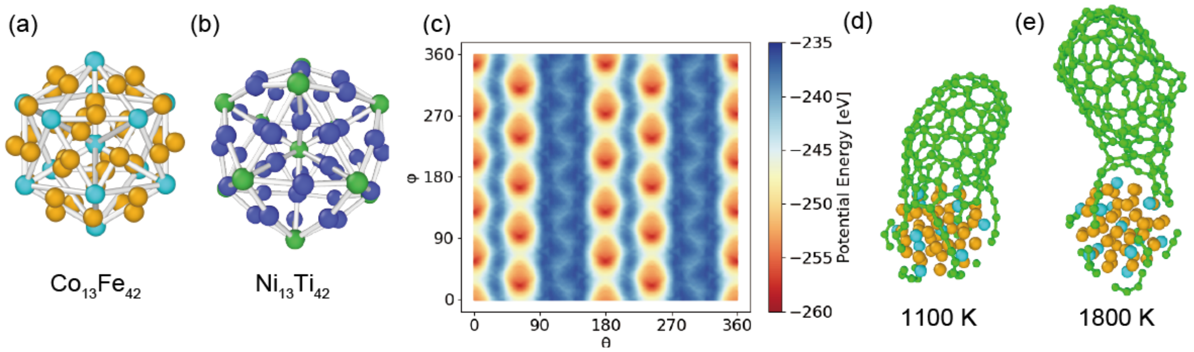

Fig. 1. Super Mackay clusters. (a) Structure of Co13Fe42 cluster. Cyan and orange balls represent Co and Fe atoms, respectively. (b) Structure of Ni13Ti42 cluster. Green and blue balls represent Ni and Ti atoms, respectively. (c) Potential energy of Co13Fe42 cluster depending on the angle between inner and outer shells. (d-e) SWCNT growth from Co13Fe42 cluster at 1100 K and 1800 K, respectively.

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P108

MOLECULE SUPER-TRANSPORT THROUGH MACROSCOPIC LENGTH OF INDIVIDUAL CARBON NANOTUBE

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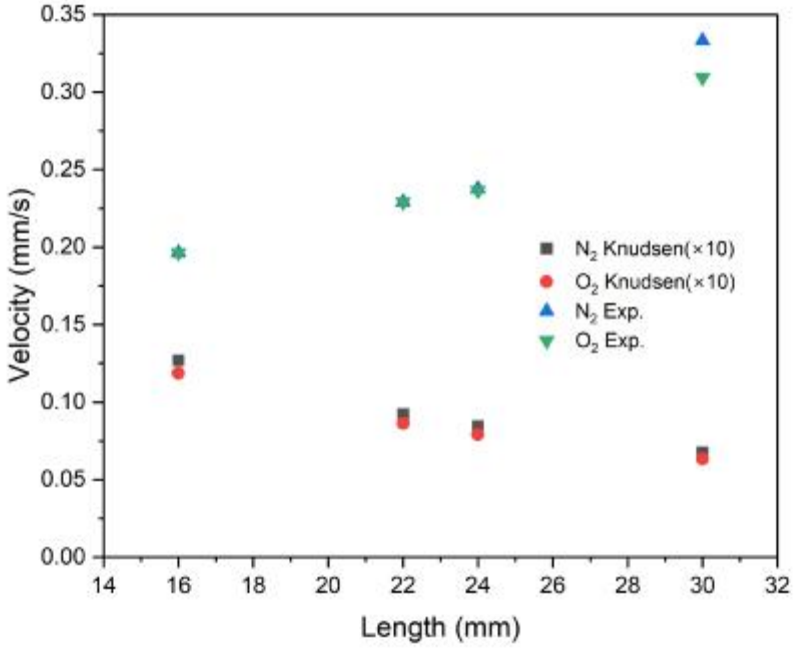
The recent emerging nanofluidics promotes the exploration of special hydrodynamic behaviors in nanoconfined flow. Due to the pore size in nanofluidic field usually being smaller than the mean free path of gas molecules, Knudsen equation conventionally describes the gas flow. By contrast, some researchers demonstrated that gas permeation in angstrom-scale channel with several micrometers' length exhibited ballistic transport that was orders of magnitude faster than Knudsen flow [1]. However, there are few experimental evidences that demonstrate this super-transport is still valid under macroscopic scale. Herein, we establish a mass spectroscopy system to research the gas permeation in single ultra-long carbon nanotube and the gas diffusion is one order of magnitude faster than expected from Knudsen theory. It indicates that the physics behind gas super-transport is still efficient at the macroscopic length scales, reflecting a frictionless gas-carbon interface. This work provides a new insight for super-transport of macroscopic length and exhibits the possibility of the low energy-consumed process.



Dependence of gas permeation on length of individu. Dependence of gas permeation on length of individual carbon nanotube

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P109

MULTI-FUNCTIONAL CARBON NANOTUBE SPONGE-LIKE PAPER THAT HOLDS LITHIUM POLYSULFIDE AND SUPPORTING SALTS FOR SIMPLE FABRICATION OF STABLE AND HIGH ENERGY-DENSITY LI-S BATTERY

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Lithium-sulfur (Li-S) battery has attracted great interest due to its huge theoretical capacity of 2510 Wh/kgLi$_2$S. However, in reality, most of them are inferior to the commercialized Li-ion batteries in terms of cell-based energy density because the sulfur positive electrode is often made of small amount of sulfur with large amounts of metal current collector, polymeric binder, and conductive filler, and because electrolyte is used at excessive amount in the cells. We have developed a Li_2S_x-CNT electrode [1] using sub-millimeter-long few-wall carbon nanotubes (CNTs) produced by fluidized bed [2]. The positive electrode of Li_2S_x held in a sponge-like freestanding CNT paper worked with an electrolyte/sulfur (E/S) ratio as low as 4 µL/mg, and realized a high energy density of 400-500 Wh/kg$_{cell}$ on an interior cell mass basis (electrode, separator, and electrolyte) [1]. The Li_2S_x-CNT positive electrode showed excellent performance, however, the cycle life of the full cell was limited because of the degradation and dendrite formation of the Li negative electrode. This time, we changed the supporting salt of the electrolyte from LiTFSI (lithium bis(trifluoromethanesulfonyl)imide), which is popular for sulfur positive electrode [3], to LiFSI (lithium bis(fluorosulfonyl)imide), which is known to form stable solid electrolyte interphase (SEI) layer on Li negative electrode. The composite positive electrode was fabricated by impregnating Li_2S_8 and supporting salts onto a self-supporting CNT paper. A full cell was then fabricated by wetting the stack of Li negative electrode | polypropylene separator | Li_2S_8-Salt-CNT positive electrode with solvent DOL(1,3-dioxolane) & DME(1,2-dimethoxyethane). The full cell made using LiFSI showed improved capacity retention (93% at the 40th cycle) and Coulombic efficiency (~99%) compared to that made using LiTFSI (85% at the 40th cycle and 95–98%, respectively) (Fig. 1).

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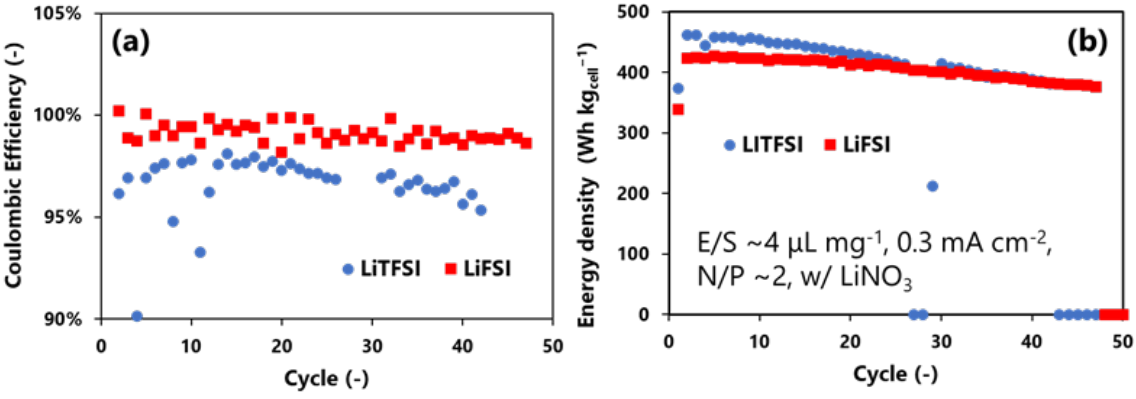

Cycle performance of Li||Li2Sx-Salt-CNT full cells

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P110

MULTI-WAVELENGTH COMPUTED TOMOGRAPHY WITH CARBON NANOTUBES BROADBAND IMAGERS

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I. Introduction: Carbon nanotube (CNT) films have potential applications in a variety of technologies. One such application is a broadband electromagnetic wave imaging device[1], which enables non-destructive inspection including material identification and structural restoration by multi-wavelength measurement in the near-infrared (NIR) to terahertz (THz) and millimeter wave (MMW) bands. Although the integration of image information engineering is indispensable in restoring the internal structure of subjects, these efforts are still insufficient. In this study, we have combined wideband, multi-wavelength measurement using a CNT film-based photo-thermoelectric imaging device array with Computed Tomography (CT) measurement, which is a representative example of image information engineering. We report on the nondestructive material identification and reconstruction of structures composed of multiple layers and composite materials.

II. Results: Fig.1b shows semiconducting-metallic-mixed single-walled CNT (SWCNT) dispersion (0.5 wt%) and SWCNT film-based photo thermoelectric imaging device array. This device can efficiently absorb ultra-broadband electromagnetic waves in NIR to MMW range and detect them as electrical signals through the photo-thermoelectric effect (PTE)[1] (Fig.1c). Fig.1d represents the NIR-CT results for a structure with a 1 mm diameter metal bar installed inside a 10 mm wide glass outer wall. CT restored the whole structure by transmitting the NIR through the glass. Because of the reflection of NIR by the metal surface, a reconstructed image followed the shape of the metal bar. By using the ultra-broadband absorbance characteristics of this device, it is possible to detect the change in transmittance of respective material in each band for subjects consisting of more complex materials and layers. The material identification and structural reconstruction of multi-layered and composite material structures by wide-band, multi-wavelength CT imaging utilizing these techniques will be presented at the conference.

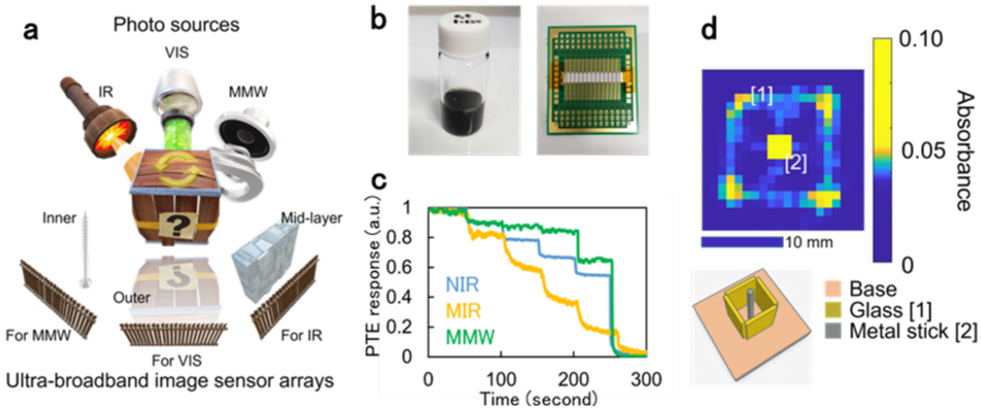

Figure1. a, Conceptual diagram. b, CNT dispersion and SWCNT film-based PTE imager arrays. c, Changes in the device's responses for controlling output powers of broad sources. d, NIR-CT demonstrations. The imager comprises a 20-pixels-array with 1-mm-pitch. Scan resolution: 1°-step rotation.

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P111

N-INCORPORATION IN MONOLAYER CVD GRAPHENE BY AN ATMOSPHERIC PRESSURE N_2 DIELECTRIC BARRIER DISCHARGE

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Nitrogen doped graphene, or N-graphene, is a promising material for a wide range of applications such as supercapacitors, optoelectronic devices, and biosensors [1,2]. Nitrogen plasmas have been proved to be an excellent path to generate N-graphene [3,4] from polycrystalline monolayer graphene films grown by chemical vapor deposition (CVD). In this study, CVD graphene has been exposed to low-frequency Townsend dielectric barrier discharge operated in nitrogen at atmospheric pressure. In such conditions, the discharge is weakly ionized, and the neutral gas temperature is close to 300 K. In addition, plasma-graphene interactions are dominated by plasma-generated N atoms and metastable N2(A) states, with the latter acting as a 6 eV energy reservoir. To investigate the mechanisms of nitrogen incorporation by the plasma-based process, Hyperspectral Raman IMAging (RIMA) and X-ray Photoelectron Spectroscopy (XPS) have been performed over different processing time. A clear defects generation is observed from the Raman signature with a transition towards amorphization for longer discharge exposure times. From the high spatial resolution of RIMA, different Raman dynamics can be seen at the grain domains (GD) versus at the boundaries (GB) of CVD graphene [5]. It is found that there is a selective nitrogen incorporation at GDs, a feature linked to preferential healing of plasma-generated defects near GB [6]. N-uptake is further discussed using the model proposed by Robert-Bigras et al. [7] in which defects generation plays a critical role in the N-incorporation kinetics.

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NANOPORE STRUCTURE OF HIGHLY ENRICHED DOUBLE-WALLED CARBON NANOTUBES BASED ON FE-MO/MGO CATALYST

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We report nanopore structures of highly enriched double-walled carbon nanotubes (DWCNTs) synthesized with yields of over 70% via catalytic chemical vapor deposition using Fe-Mo/MgO catalysts. The carbon yield, tube diameter and crystallinity of the synthesized DWCNTs were characterized by high-resolution transmission electron microscopy, field emission scanning electron microscopy, thermogravimetric analysis, and Raman spectroscopy. The nanopore structure and adsorption characteristics of the purified DWCNTs, obtained by removing the support and catalyst, were analyzed through the N2 adsorption at 77K. A significant advantage of the highly enriched DWCNTs with small bundle network structures is that the guest molecules can easily access the outer (or external) surface of the DWCNTs, resulting in a high specific surface area (SSA) of over 700 m2/g-1 and pore volume of 2.30 mLg-1. Additionally, the SSA of DWCNTs increased by more than 30% after purification with various acid solutions, which is due to the change in the distribution of micropores and mesopores. These results suggest that highly enriched DWCNTs with SSA and high pore volume can be used as CNT-based structures for applications such as high-performance energy storage through a facile solution-based process.

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NEAR-INTRINSIC PHOTO- AND ELECTROLUMINESCENCE FROM NETWORKS OF SINGLE-WALLED CARBON NANOTUBES ON BCB-PASSIVATED SURFACES

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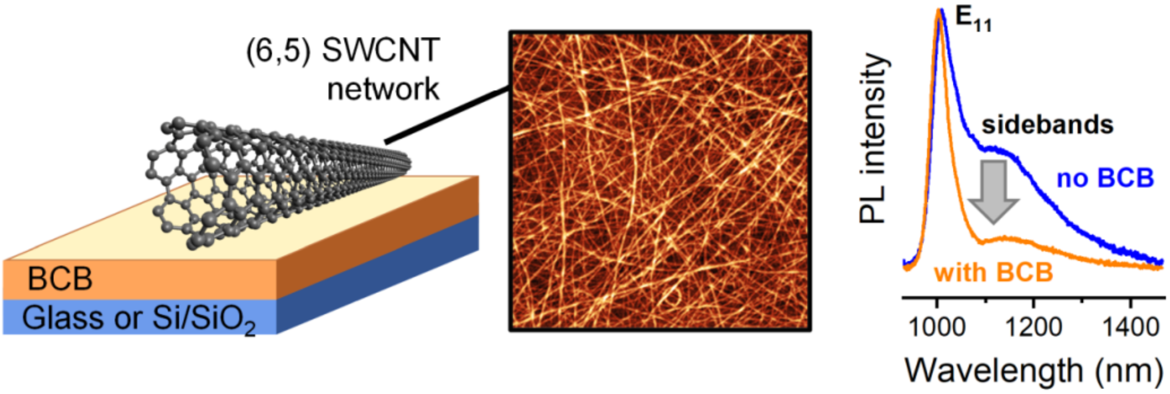
The photo- and electroluminescence spectra of semiconducting single-walled carbon nanotube (SWCNT) thin films on commonly used glass and Si/SiO2 substrates are often compromised by broadening of the main excitonic emission peak and unwanted low-energy sidebands [1]. Here, we show that surface passivation with the commercially available, low dielectric constant, cross-linked polymer BCB significantly enhances the emission properties of (6,5) SWCNTs to the same level as hexagonal boron nitride (*h*-BN) flakes do. The presence of BCB suppresses sideband emission, especially from the Y_1 band, which we attribute to defects introduced by interaction of the nanotube lattice with oxygen-containing terminal groups of the glass or silica surface. The simple and reproducible deposition of homogeneous BCB films over large areas combined with their resistance against common solvents and chemicals employed during photolithography make them compatible with standard semiconductor device fabrication processes. Utilizing this approach, we demonstrate light-emitting (6,5) SWCNT network field-effect transistors on BCB-treated glass substrates with excellent electrical characteristics and near-intrinsic electroluminescence spectra. Consequently, passivation with BCB could become a standard surface treatment for spectroscopy of and optoelectronic devices with SWCNTs and other low-dimensional emitters.



Photoluminescence spectra from dense networks of (6,5) SWCNTs on a glass substrate with or without BCB passivation layer.

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P114

NEW SPECTROSCOPIC SIGNATURES OF PRESSURE INDUCED REVERSIBLE COLLAPSE IN SINGLE-WALLED CARBON NANOTUBES

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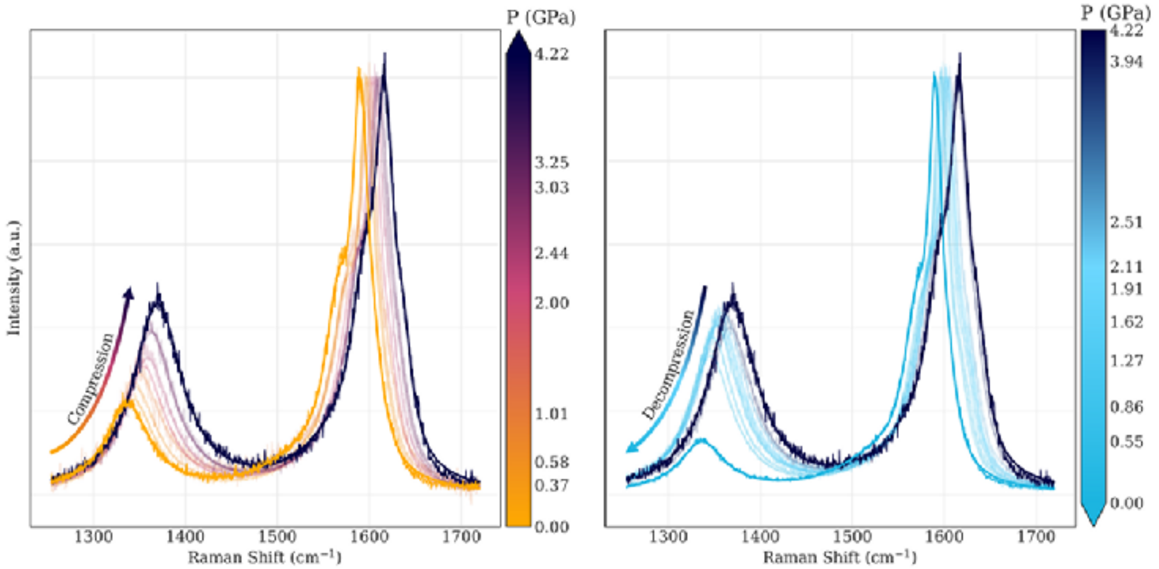
The radially collapsed structure of carbon nano-tubes [1] constitutes an intermediate geometry between the 1D-tube and 2D ribbon-like structure which offers opportunities in the optimization of electrically conductive composites [2] or reinforcing fibers [3] for instance. The pressure induced radial collapse of carbon nanotubes [4] has been shown to exhibit characteristic signatures in the Raman spectrum as changes in the evolution of the G-mode associated to the attenuation of the associated radial breathing mode (RBM) [5,6]. Recent studies show that the symmetry reduction introduced by the radial collapse leads to the formation of a characteristic D-band in the Raman spectrum without disorder [7]. In this work, we have successfully shown the use of this signature as a probe for the high-pressure evolution between the circular and the collapsed structure of single-walled carbon nanotubes. The study of the D-band is not possible in Raman high-pressure experiments using the diamond anvil cell pressure apparatus at pressures below ~10 GPa [8]. In fact, diamond most intense Raman peak overlaps the D-band, hence preventing its detection. In order to avoid such problem, we used a sapphire anvil cell, which provides an optical window for the detection of both the D-band and the G-band. Our study allowed us to observe the D-band development at the expected nanotube collapse pressure as well as its reduction after pressure release, confirming its link to the collapse process.



In situ Raman signature of the pressure evolution of SWCNTs using a sapphire anvil cell.

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P115

NON-DESTRUCTIVE LOW-TEMPERATURE CONTACTS TO MoS_2 NANORIBBON AND NANOTUBE QUANTUM DOTS

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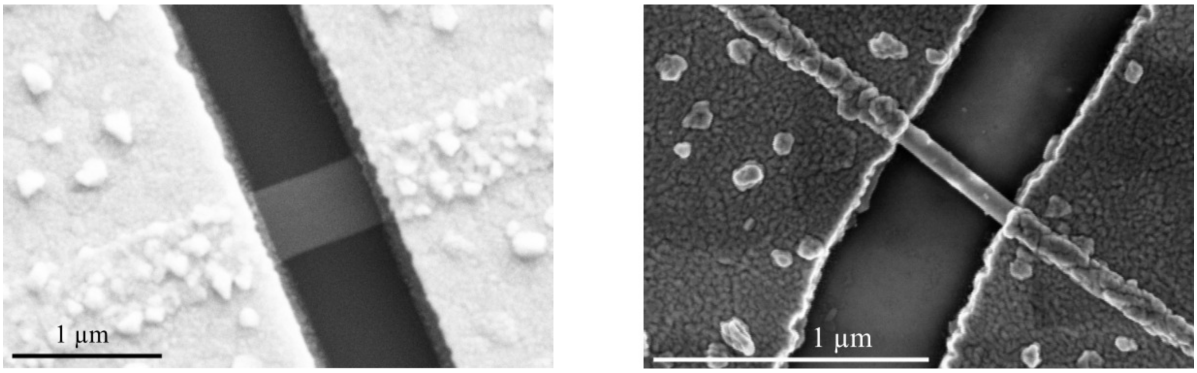
Planar TMDCs are at the center of manifold research efforts due to their intrinsic two dimensional nature and their outstanding electronic and optical properties. Despite detailed studies of their optical parameters, worldwide efforts to reach single electronic level transport in lithographically designed quantum dots at low temperatures - towards spin, valley, or charge qubits - have so far been mostly unsuccessful. This is due to the requirement for very small confinement potentials as well as disorder from dangling bonds at the edges of nanoflakes. Both issues can be circumvented by using clean, as-grown MoS_2 nanotubes and nanoribbons. First Coulomb blockade measurements were recently performed on a MoS_2 nanotube grown from vapour phase [1,2], and were so far limited by disorder below the metallic scandium contacts. Here, we present low temperature measurements on MoS_2 nanotubes and nanoribbons contacted using bismuth [3]. Bismuth is less reactive and has a vanishing density of states at the Fermi edge, suppressing metal-induced gap states. Our data clearly shows the non-destructive and transparent nature of these contacts to our quantum dots and indicates quantum confinement [4].



SEM images of devices incorporating a MoS_2 nanoribbon (left) and a nanotube (right).

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P116

OBTAINING MECHANISTIC UNDERSTANDING OF CNT SYNTHESIS VIA FCCVD BY INDEPENDENTLY DECOUPLING FLOATING CATALYST AND PRECURSOR AVAILABILITY

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Traditionally, the synthesis of CNTs has been achieved by utilizing ferrocene and thiophene as catalyst and precursor, respectively. This approach has been convenient for simplifying instrumental requirements FCCVD reactors but has the limitation of intertwined kinetics of precursor decomposition and Fe and S catalyst and promoter availability. Any attempt to study the reaction mechanism based on such precursors for the catalyst and promoter of CNT is subjected to such difficulty, significantly limiting the mapping of a more general reaction mechanism. For this reason, we have developed a methodology to sublimate readily available elemental sulfur(Fig.1a) and synthesize nanoparticles of desirable sizes by utilizing a spark discharge generator (SDG)[1](Fig.1b). With this, a more thorough reaction window could be scanned,(Fig.1c). In the past, the minimum amount of sulfur (S) necessary for achieving CNT aerogelation was about 10 mg/hr producing a mixture of SW and MWCNTs[2]. By using a sublimator, SWCNTs from toluene were obtained with as little as 0.22mg/hrS, 50 times less than using thiophene[2], and showing the promise of this approach. In addition, the position of sulfur injection in an FCCVD reactor substantially affects the iron catalyst evolution and, therefore, the consequent CNT diameter obtained[3]. Thus, the standard deviation for the lognormal fit of the size distribution of CNTs can be linked to track the point at which the natural aerosol evolution of the catalyst stops as the carbon precursor becomes available and CNTs are synthesized, preventing further catalyst agglomeration. On the other hand, the utilization of Fe catalyst from SDG was reported for the synthesis of CNTs, but spinning was reportedly not possible[4]. Our preliminary results show that spinning with an SDG catalyst is easier using thiophene than sublimed sulfur. This is studied by a complete decoupling and mechanistic study on the effect of both.

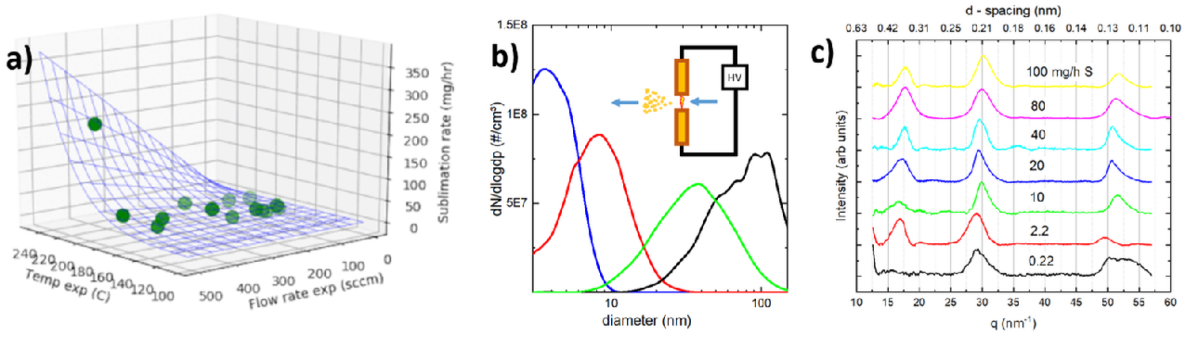

Fig 1. a) A sublimator allows accurate control of readily available elemental sulfur b) Specific size distributions are achievable via spark discharge generator (SDG) c), d-spacing from electron diffraction indicates differences in CNTs synthesized as a function of sublimated sulfur.

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ON-CHIP TORSION BALANCES WITH FEMTONEWTON FORCE RESOLUTION AT ROOM TEMPERATURE ENABLED BY CARBON NANOTUBE AND GRAPHENE

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The torsion balance, consisting of a rigid balance beam suspended by a fine thread, is an ancient scientific instrument, yet it is still a very sensitive force sensor to date. As the force sensitivity is proportional to the lengths of the beam and thread, but inversely proportional to the fourth power of the diameter of the thread, nanomaterials should be ideal building blocks for torsion balances. Here, we report a torsional balance array on a chip with the highest sensitivity level enabled by using a carbon nanotube as the thread and a monolayer graphene coated with Al nanofilms as the beam and mirror. It is demonstrated that the femtonewton force exerted by a weak laser can be easily measured. The balances on the chip should serve as an ideal platform for investigating fundamental interactions up to zeptonewton in accuracy in the near future.

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P118

ONE-DIMENSIONAL HBN/CNT VAN DER WAALS HETEROSTRUCTURES FABRICATED BY ATOMIC LAYER DEPOSITION

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Graphene's isolation has led to a strong interest in two-dimensional (2D) materials and the ability to stack them into van der Waals (VdW) heterostructures has opened up a wide field of applications based on these new materials. Neither too weak nor too strong, VdW coupling allows connecting two different materials to combine their intrinsic properties and/or to create new ones. The interest in this coupling is currently extending beyond 2D materials, with 1D VdW heterostructures that consist of coaxial stacking of two or more distinct materials. The two-dimensional electron confinement associated with VdW stacking is expected to improve/modify the physical and chemical properties of the final material compared to the initial ones. In particular, Hexagonal Boron Nitride (hBN) is generating much interest as it is isostructural to graphene with a large bandgap, excellent thermal stability, and photoluminescence intensity in the visible or UV spectral regions; thus, coaxial stacking of hBN onto carbon nanotubes (CNTs) can enrich optoelectronic properties of the initial structures [1]. Fabricating these high-quality hBN/CNT heterostructures requires a synthesis approach capable of precisely controlling the epitaxial deposition onto supports at the atomic scale. Based on self-limiting gas-surface reactions, Atomic Layer Deposition (ALD) has proven to be ideally suited for fabricating functional hetero-nanostructures, such as carbon nanotube-based materials [2]. Herein, a two-step ALD process of hBN is utilized for fabricating hBN/CNT heterostructures based on polymer-derived ceramics chemistry [3]. Briefly, a pre-ceramic layer of polyborazine is successfully deposited on single-wall or multi-wall CNTs within the first ALD step and then annealed at high temperatures in the second step to convert the polyborazine into crystalline hBN. The resulting BN-coated CNTs are thoroughly investigated employing advanced characterization techniques. Specifically, high-resolution transmission electron microscopy exhibits the fabrication of highly crystalline hBN/CNT heterostructures, and electron energy loss spectroscopy permits us to observe a conformal and homogeneous coating of hBN layers onto single-wall and multi-wall CNTs. The influence of the ALD parameters and post-annealing treatment on BN growth (thickness, number of layers, homogeneity) and structure (amorphous, turbostratic, hexagonal phase) is explored in detail as well as the impact of the starting carbon material on the final heterostructures in terms of morphology and crystallinity. Particular attention is paid to the successful fabrication of 1D VdW heterostructures made of few-layer hBN coated-single wall carbon nanotubes. The Raman and photoluminescence spectroscopies are performed to evaluate the structural and optical properties of the obtained heterostructures.

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ONE-DIMENSIONAL SEMIMETAL CONTACTS TO TWO-DIMENSIONAL SEMICONDUCTORS

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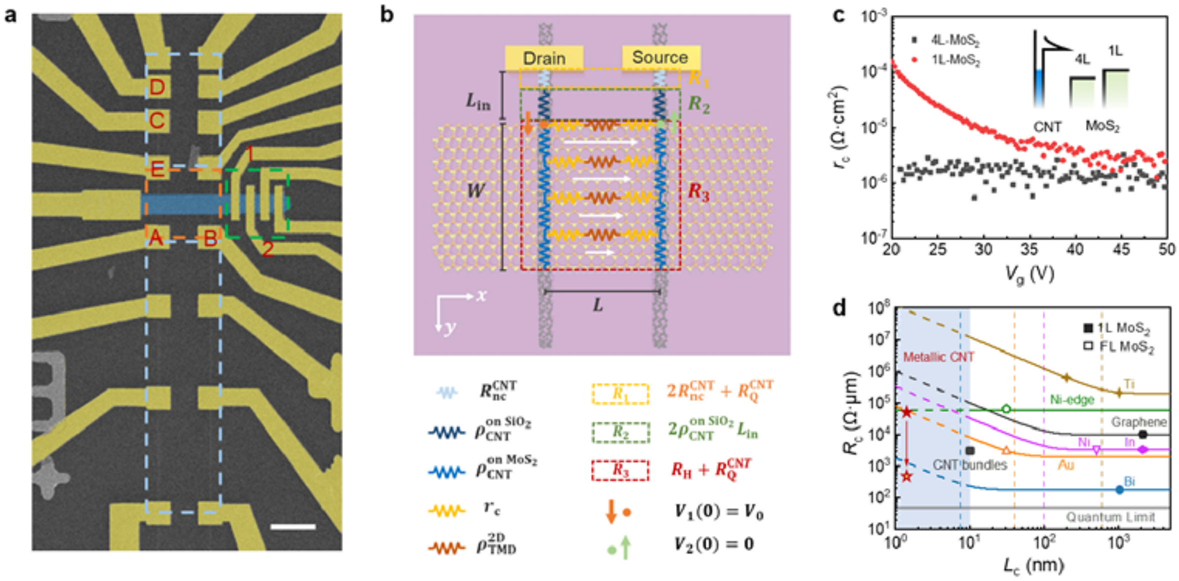
Two-dimensional (2D) semiconductors are promising in channel length scaling of field-effect transistors (FETs) due to their excellent gate electrostatics. However, scaling of their contact length still remains a significant challenge because of the sharply raised contact resistance and the deteriorated metal conductivity at nanoscale. Here, we construct a 1D semimetal-2D semiconductor contact by employing single-walled carbon nanotube electrodes, that can push the contact length into the sub-2 nm region.[1] Such 1D-2D heterostructures exhibit smaller van der Waals gaps than the 2D-2D ones, while the Schottky barrier height can be effectively tuned via gate potential to achieve Ohmic contact. We propose a longitudinal transmission line model for analyzing the potential and current distribution of devices in short contact limit, and use it to extract the 1D-2D contact resistivity which is as low as 10^{-6} Ω·cm^2 for the ultra-short contacts. We further demonstrate that the semimetal nanotubes with gate-tunable work function could form good contacts to various 2D semiconductors including MoS_2, WS_2 and WSe_2. The study on 1D semimetal contact provides a basis for further miniaturization of nanoelectronics in the future.



One-Dimensional Semimetal Contacts to Two-Dimensio. Fig.1 a, False-colored SEM image of the back-gate MoS2 (blue) FET with SWCNT contacts (white). b, Schematic diagram and equivalent circuit of the CNT-contacted MoS2 FET. c, Extracted interface contact resistivity of the CNT/1L-MoS2 and CNT/4L-MoS2 heterojunction. d, State-of-the-art contact technology for MoS2 transistors plotted as a function of contact length.

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ONE-DIMENSIONAL VAN DER WAALS (HETERO)^{2}STRUCTURE

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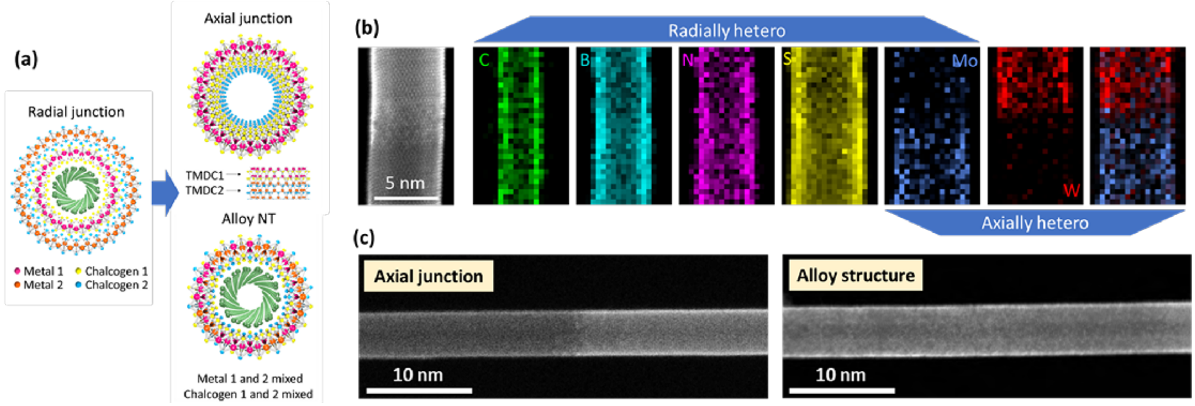
The first demonstration of high quality one-dimensional (1D) van der Waals (vdW) heterostructure - single-walled carbon nanotubes (SWCNTs), boron nitride nanotubes (BNNTs), and molybdenum disulfide (MoS_2) sequentially wrapped as radial junction - has been achieved by chemical vapor deposition in 2020, which suggests the high potential of common 2D vdW heterostructures being rolled into their 1D counterparts [1-3]. A considerable literature has grown up around the theme of 1D vdW heterostructures since then, but much of the research up to now has been restricted to the limited types of 1D vdW heterostructure.

In this work, we take a further step and broaden the concept of 1D vdW heterostructure. For starters, tubular tungsten disulfide (WS_2) was achieved in SWCNT-BNNT-WS_2 heterostructures as the outermost layer. Furthermore, this WS_2 can be axially combined with the previous tubular MoS_2 to form a 1D MoS_2 - WS_2 axial junction. Such nanotube structure is proven to be both radially and axially hetero, and the whole structure is only confined to a width of 5 nm (Fig1b). Besides 1D MoS_2 - WS_2 axial junction, 1D MoS_2 - WS_2 alloy nanotube can also be materialized as the outermost layer (Fig1c). This “double hetero” structure not only has extended our knowledge of the current 1D vdW heterostructure, but also lays the groundwork for future research into the newly developed 1D vdW heterostructures as the next generation electronics or optoelectronics.



(a) Broadening the concept of 1D vdW heterostructure to axial direction [3]. (b) ADF image and chemical distribution of a 5 nm width nanotube which has both radial and axial junction. (c) ADF images showing the outermost layer of MoS2 and WS2 can be combined to form the axial junction and alloy nanotube.

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OPTICAL PROPERTIES OF MANY-BODY EXCITONIC TRANSITIONS OBSERVED IN ANTIFERROMAGNETIC FEW-LAYER NIPS3

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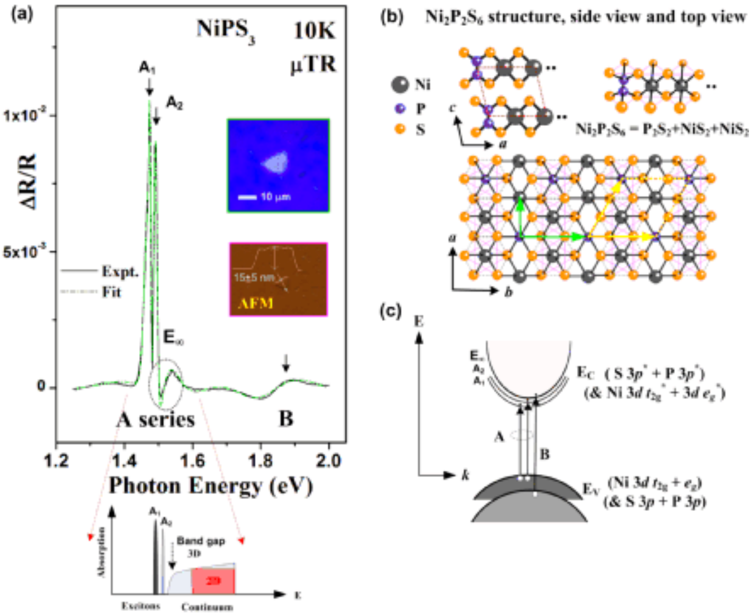
$NiPS_3$ is an antiferromagnetic 2D semiconductor with a Néel temperature (TN) for antiferromagnetic to paramagnetic transition at about 150 K. In this work, band-edge excitons of few-layer $NiPS_3$ are characterized via micro-thermal-modulated reflectance (µTR) measurements from 10 to 300 K. Prominent µTR features of the A exciton series and B are simultaneously detected near the band edge of NiPS3. The A exciton series contains two sharp A1 and A2 levels and one threshold-energy-related transition (direct gap, E_g), which are simultaneously detected at the lower energy side of $NiPS_3$. Moreover, one broadened B feature is present at the higher energy side of the few-layer NiPS3. The A series excitons may correlate with a majorly d-to-d transition in the Rydberg series with a threshold energy of E_g=1.511 eV at 10 K. The binding energy of A1 is about 36 meV, and the transition energy is A1~1.366 eV at 300 K. The transition energy of B measured by µTR is about 1.894 eV at 10 K. The excitonic series A may directly transit from the top of valence band to the conduction band of $NiPS_3$, while the B feature might originate from the spin-split-off valence band to the conduction band edge. The direct optical gap of $NiPS_3$ is ~1.402 eV at 300 K, which can be confirmed by µTR and the transmittance experiments. Based on the experimental analysis, the band-edge nature of layered nickel phosphorus trisulfide is thus realized.



Low-temperature excitonic series in NiPS3. (a) Band-edge excitons of the A series and B transition in few-layer NiPS3 observed via µTR measurements at 10 K. Insets show the microscopic image and AFM results of the few-layer sample on an SiO2/Si substrate. The lower inset depicts the representative scheme of Rydberg series absorption for contrast. (b) Atomic arrangements of the side and top views for the layered Ni2P2S6 structure. (c) Representative band-edge scheme for the A series exciton and B transition in NiPS3.

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P122

OPTICAL PROPERTIES OF METALLIC CARBON NANOTUBES: BEYOND THE STANDARD SEMI-EMPIRICAL MODEL FOR PLASMONIC PREDICTIONS

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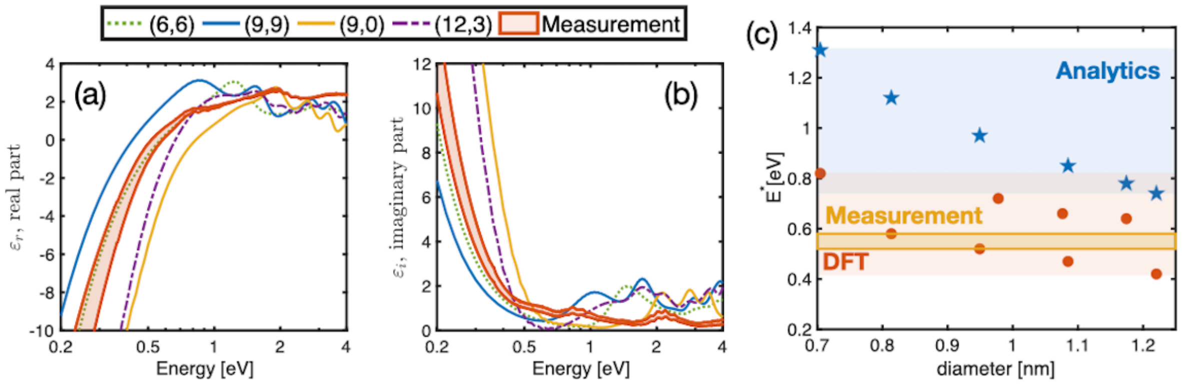
In recent years, plasmonics has become a rapidly growing area of research with the potential to bring advancements in various fields such as sensing[1] and highly integrated photonic devices[2]. In an effort of miniaturization, metallic Single-Wall Carbon NanoTubes (m-SWCNT) could be envisioned as the smallest metallic wire, a building block for plasmonic devices at the nanoscale. In order to engineer such practical nanotube-based optical devices, the knowledge of m-SWCNT complex dielectric constant is fundamental. However, experimental measurements are mostly limited to unsorted samples[3] or focused only on a narrow frequency range[4]. Furthermore, most theoretical calculations have focused on the optical properties of semiconducting SWCNT or missed the intraband-transitions contribution of m-SWCNT. An analytical model, known as the surface conductivity model[5], has also been developed but has not been confronted with experiments. Therefore, we investigate the intraband-transitions contribution to the optical properties of metallic carbon nanotubes both experimentally and theoretically[6]. The experimental dielectric constant for m-SWCNT samples is derived from reflectance measurements through electromagnetic modeling and Kramers-Kronig relations (figure a-b). It is found in remarkable agreement with the predictions from ab initio calculations but demonstrates a failure of the standard semi-empirical model[5] (figure c), widely used in various fields of physics especially for predicting the optical properties of many 2D materials. We report new theoretical predictions for the plasma frequency of m-SWCNT unambiguously validated by experimental observations.



m-SWCNT experimental complex dielectric constant (a) real and (b) imaginary part compared with DFT calculations. (c) Cut-off energy as a function of the diameter from analytics (blue stars), DFT (red dots) and measurement (yellow area).

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OPTICAL PROPERTIES OF SORTED SINGLE WALL CARBON NANOTUBES THIN FILMS

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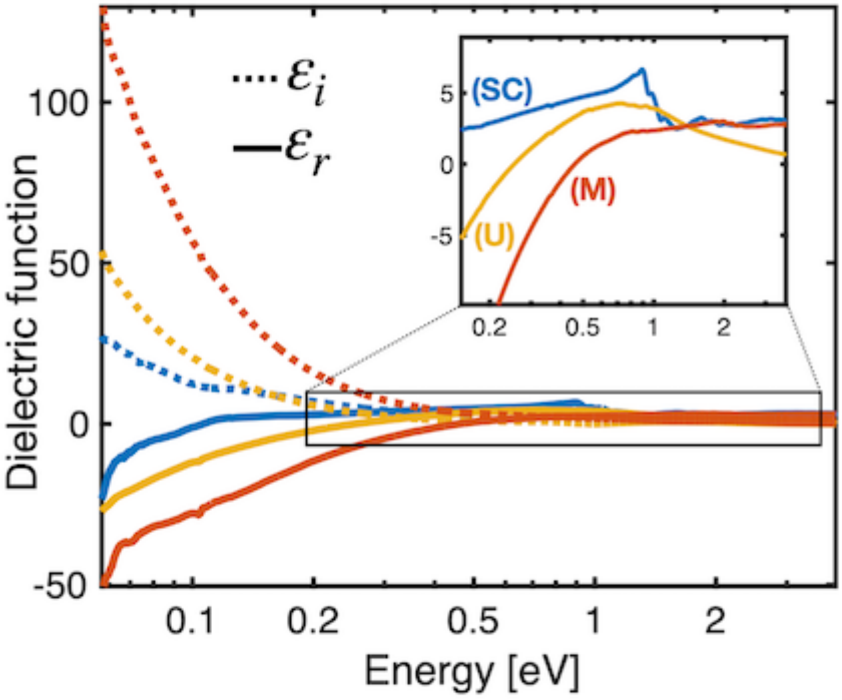
Carbon nanotubes are one-dimensional nano-objects that can have metallic or semiconducting behavior depending on their geometry. In order to study or predict the optical response of heterostructures made of carbon nanotubes, it is essential to know precisely their dielectric functions over a wide spectral range at optical frequencies. We propose to extract and compare the optical properties of sorted carbon nanotube films and investigate the effects of annealing. The complex dielectric functions of semiconducting and metallic carbon nanotube films are extracted from reflectance measurements carried out over a very wide spectral range from UV to FIR using electromagnetic modeling and Kramers-Kronig analysis. We demonstrate that the dielectric function of a metallic carbon nanotube film behaves like a metal perfectly described by a Drude term whose parameters (plasma frequency ω_p and damping γ) are extracted from experimental measurements[1]. We highlight the effect of annealing on the intra/interband transitions of metallic and semiconducting carbon nanotubes films and present their fundamental optical properties.



Dielectric function of metallic (M) (red), unsorted (U) (yellow) and semiconducting (SC) (blue) carbon nanotube films, real part in solid line and imaginary part in dotted line.

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OPTIMIZING THE THERMOELECTRIC PERFORMANCE OF CARBON NANOTUBE FILMS

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Carbon nanotubes (CNTs) are suitable materials for flexible thermoelectric (TE) devices due to their high flexibility and high electrical properties. Theoretical studies on the TE properties of CNTs have mainly focused on individual CNTs thus far, and their TE properties have been precisely analyzed [1]. Although as-grown CNTs are produced with a mixture of metallic and semiconducting CNTs in the ratio of 1:2 during the formation process, this ratio can be controlled and significantly influence the TE performance of CNT thin films [2]. Recently, two interesting experiments on the TE performance of CNT thin films were reported. There is a discrepancy in the mixture ratio dependence of the Seebeck coefficient of CNT thin films [3,4]. In another experiment, in an aligned CNT thin film, the Seebeck coefficient of the CNT thin film is isotropic, while the electrical conductivity of the thin film is significantly anisotropic [5]. Since it is difficult to understand the TE properties of such CNT thin films from individual CNTs, it is desirable to develop a new simulation method for CNT thin films consisting of large amounts of CNTs. In this study, we developed a new method to analyze the TE performance of CNT thin films by mapping CNTs on a random stick network model and performing electrical and thermal network analysis [6]. Using this method, we have successfully reproduced the gate voltage dependence of the electrical conductivity and Seebeck coefficient of CNT thin films with various types of mixture ratios reported by Ichinose et al. [2]. Furthermore, we succeeded in explaining the above-mentioned discrepancy in the two experiments regarding the difference in the chemical potential of CNT thin films. Finally, the same anisotropic electrical conductivity and isotropic Seebeck coefficient were reproduced for the aligned CNT thin film as in the experimental [5]. The cause of the anisotropy in the electrical conductivity was clarified from the difference in the effective number of contacts, and the cause of the isotropy in the Seebeck coefficient was clarified from the uniformity of the voltage and temperature gradients.

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P125

CONFINED SYNTHESIS OF ARMCHAIR GRAPHENE NANORIBBONS FROM VARIOUS PRECURSOR MOLECULES

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Contrast to gapless graphene, armchair graphene nanoribbons (AGNRs) possess remarkable energy gaps depending on their widths. Precision synthesis of AGNRs with desired width was only realized by on-surface polymerization of specific designed precursor hydrocarbon molecules [1]. Recently, we developed a method named confined synthesis [2] to synthesize AGNRs with controlled width inside single-wall carbon nanotubes [3]. Unlike the on-surface synthesis, the confined synthesis allows to synthesize specific AGNRs with various structures of precursor molecules [4,5], since the molecules are first decomposed and then reassembled into AGNRs, which is revealed through isotope experiments [6]. These results shed light on tailoring the structure of AGNRs by using the carbon nanotubes but not the precursor molecules.

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PERFORMANCE ENHANCEMENT OF CARBON NANOTUBE-BASED TRANSPARENT AND SOFT TRIBOELECTRIC NANOGENERATOR WITH FLUOROPOLYMER-PDMS MIXTURE DIELECTRIC LAYER

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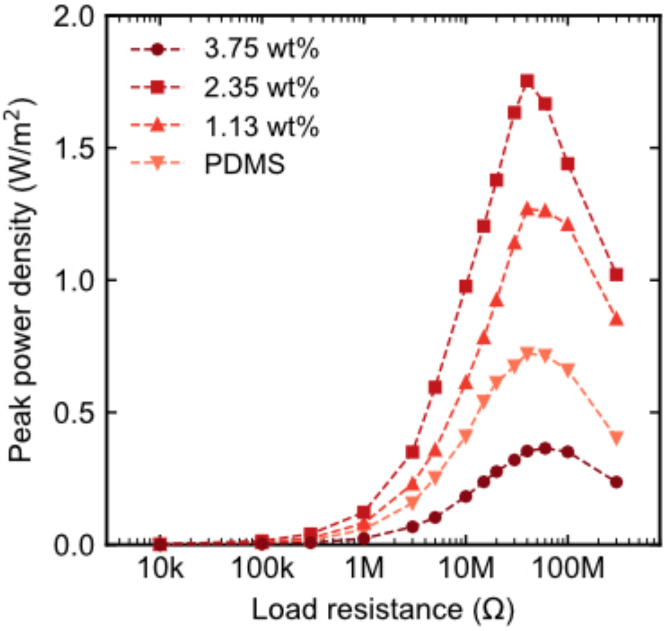
Triboelectric nanogenerator (TENG) is an energy harvesting technology that converts mechanical vibration into electrical energy by triboelectrification and electrostatic induction [1]. TENG is highly expected as a power source for self-powered wearable devices because of its remarkable features, such as high output, a simple structure, and low cost. Previously, we have reported a transparent stretchable TENG composed of carbon nanotubes and polydimethylsiloxane (PDMS) [2,3]. So far, we have improved the output performance by modifying the surface of the dielectric layer. However, problems such as the complicated process and the durability of the surface modification technique still need to be solved. In this study, we focused on the dielectric layer consisting of a mixture of fluoropolymer and PDMS to improve the durability and simplicity of the process. The TENG was composed of a carbon nanotube thin film as a transparent electrode and a mixture of PDMS and fluoropolymer as the dielectric layer. We fabricated several TENGs with a different fraction of the fluoropolymer. The output performance was evaluated by measuring the generated voltage through the external load resistance under a constant mechanical vibration (~2 Hz). The output power density of the fabricated TENG was enhanced with fraction of the fluoropolymer, and the maximum output power density of 1.75 W/m^2 was obtained at a fraction of 2.35 wt% as shown in Fig.1. Because the fluoropolymer has more negative triboelectric property than PDMS, the amount of the triboelectric charge was increased to enhance the output power of the TENG.



Peak power density versus load resistance as a function of fraction of fluoropolymer.

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PHOTOLUMINESCENCE FROM MAGNETIC IONIC LIQUID-GATED (6,5) SINGLE-WALLED CARBON NANOTUBE NETWORKS

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Excitons and charged excitons (trions) in Single-walled carbon nanotubes (SWCNTs) have been shown to be sensitive to their dielectric environment and charge carrier density.[1, 2] Despite extensive studies of the dielectric effects on excitonic states, the influence of a high spin environment on emission - especially from trions with non-zero spin - remains unexplored. Magnetic ionic liquids (MIL), which contain high-spin anions, are promising tools for creating such environments while also enabling controlled electrolyte-gating and hence charge accumulation. Here we employ a paramagnetic ionic liquid with the high-spin cobalt anion $[Co(NCS)_4]^{2-}$ as the electrolyte for (6,5) SWCNT network transistors. Tunable hole and electron accumulation are achieved and allows for the in-situ investigation of photoluminescence. Emission quenching and shifts of the exciton and trion energies are observed depending on the carrier polarity and hence the nature of the ions forming the electric double layer around the SWCNTs.

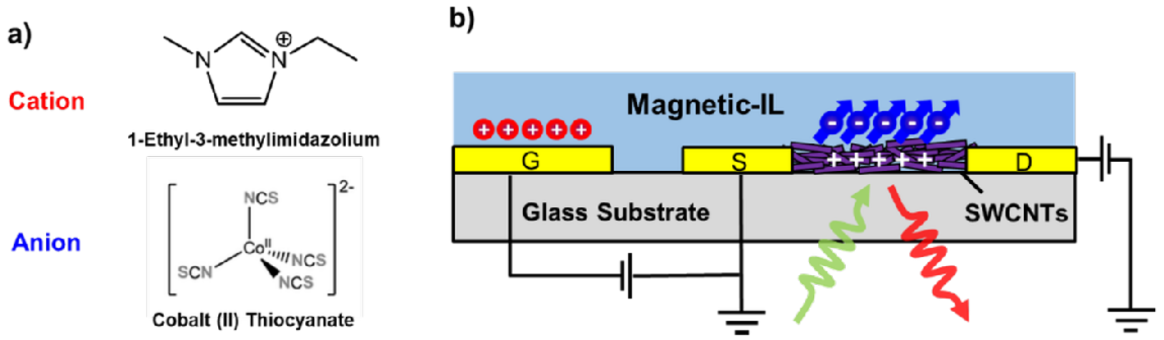

Figure Schematic. a) Molecular structure of magnetic ionic liquid and b) schematic of electrolyte-gated SWCNT networks transistor with side-gate.

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POLYIMIDE-CARBON NANOTUBE BASED CARBON AND GRAPHITE FIBER WITH HIGH STRENGTH AND MODULUS AND CONDUCTIVITY

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In this study, high performance polymer-CNT composite fibers with high tensile strength (4.8 ± 0.2 GPa) and modulus (390 ± 48 GPa) were fabricated through wet-spinning method without carbonization process [1]. Furthermore, composite polyimide (PI)-CNT composite fibers has improved interfacial shear strength (IFSS) with compared to pristine CNT fibers and thermally treated graphitic fibers [2]. With optimized content of PI (30%), carbonized and graphitized fibers represent exceptional mechanical and thermal properties through control of void size in fiber and increased crystal size. In this presentation, the processing condition including molecular weight of PI, CNT content, abd fiber alignment will be discussed.

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POLYMER-LIKE TOUGHNESS ENABLING RECYCLING OF CNT FABRICS FOR SUSTAINABLE COMPOSITES

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The carbon nanotube based continuous fibres (CNTF) synthesized by floating catalyst CVD process have already demonstrated high mechanical properties outperforming Kevlar, Vectran, and some conventional carbon (CF) and glass (GF) fibres [1]. The high degree of axial alignment and hierarchical structure of interconnected network of CNT bundles provide the basis for structural toughness and mechanical reinforcement of composite structures [2-4]. The next challenge in CNTF development, along with the scale-up process with reduced carbon footprint and CO_2 emissions, is demonstration of the ¨*recyclability-by-design*¨ principle. In this work we demonstrate, for the first time, the possibility of recycling the CNTF materials from their thermoset composite laminates retaining the structure and longitudinal properties of CNTF fabrics, which can be potentially re-processed for high value composite applications. The key feature of CNTF textile materials is their inherent ability to preserve the interconnected network of CNT bundles at the recycling step and intrinsic toughness, which enables their recycling with minimal deterioration to the format and electrical and mechanical properties at the macroscale. In contrast, monolithic fibres, such as CF and GF, are prone to introduction of defects during recycling due to their brittleness. Progressive degradation and sensitivity to defects such as surface flaws in absence of sizing during recycling, result in loss of continuity and alignment, reduction of length, and a rapid downgrade of mechanical performance, which restricts them from being suitable for the same applications. We discuss the structural features and their role in attaining the maximum retention of properties, such as full retention of modulus, and toughness of CNTF fabrics in general via Essential Work of Fracture concept. The work sets the path for using CNTF fabrics as a reinforcing material with superior material circularity and lifetime.

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PREFORMED NANO-POROUS CARBON NANOTUBE ARCHITECTURE FOR THE MECHANICAL REINFORCEMENT OF THE POLYMER MATRIX NANOCOMPOSITES

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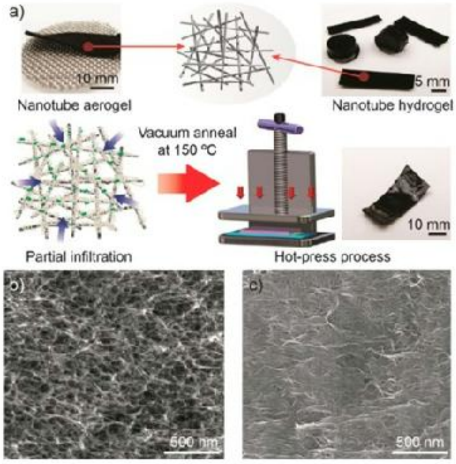
Foam structures made of low-dimensional nanomaterials are fascinating for various applications including electrodes for electrochemical energy storage, supports, templates, and membranes [1]. Especially, porous architectures made of carbon nanotubes, which exhibit exceptional high Young's modulus (~1 TPa) and tensile strength (~200 GPa), are attractive candidates for composite preforms. These porous nanotube monoliths are typically fabricated via chemical vapor deposition or chemical cross-linking methods, and they contain impurities from synthesis that cannot be removed without destroying the network. Furthermore, they offer limited control over porosity, pore size, surface area, form-factor, and properties of the constituent nanotubes. Here, we introduce a novel approach to creating a three-dimensional nanotube porous architecture with shape-controllability, using van der Waals interaction among isolated SWCNTs. The resulting isotropic SWCNT network acts as a composite preform that can be used to make thermoplastic polymer (Thermoplastic Polyurethane, TPU) nanocomposites achieved by resin impregnation process. The TPU/SWCNT composites we produced exhibit remarkable improvements in both tensile modulus and strength, showing enhancements of 40,000% and 9,700%, respectively, compared to both pristine SWCNT aerogel and bare TPU control sample [2]. The observed enhancements in tensile properties are consistent regardless of the tensile direction, indicating an isotropic behavior. Furthermore, we observed that the nanoporous nanotube networks have the ability to suppress the polymer glass transition and extend the mechanical integrity of the polymer well above its polymer melting temperature. This suggests that the TPU/SWCNT composites have potential for structural applications in high-temperature environments. Additionally, we found that both the nanotubes and polymer remain thermally stable above their decomposition temperatures, indicating good thermal stability.



Carbon nanotube preform based polymer composite. (a) A schematic of the fabrication steps. (b)Scanning electron microscopy imaging of a cross section of nanotube aerogels of 0.8 vol % showed three-dimensional network of isolated nanotubes. (c) Similar imaging of com posites with 25 vol % nanotubes showed that the nanotube networks were unaffected by polymer infiltration, and the composites did not have any voids.

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PREPARATION OF CARBON NANOTUBE COLD CATHODE MATERIALS WITH A WELL-ORIENTED MICROSTRUCTURE AS A FIELD ELECTRON EMITTING DEVICE

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Carbon nanotubes (CNTs) have gained attention as a field electron source for cold cathodes in X-ray tubes due to their low work function, good mechanical properties, and stability. [1] Various manufacturing methods such as chemical vapor deposition, tailored bucky paper, and annealed paste have been studied to produce CNT cold cathodes. [2-3] However, the relationship between the structure of CNT emitters and field emission properties has not been thoroughly explored. We prepared CNT fibers with different orientations using the direct spinning method and measured the field emission stability of the emitter through a duration test. This study found that as the orientation of the CNT fiber increased, the field emission stability of the emitter improved. These results suggest that the orientation of CNTs is a crucial factor that needs to be considered for developing efficient CNT cold cathodes. This work contributes to understanding the relationship between the structure of CNT emitters and their field emission properties and can serve as a reference for future studies in this field.

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PROBING INNER-TO-OUTER WALL ENERGY TRANSFER IN HIGHLY PURE DOUBLE-WALL CARBON NANOTUBES BY DETAILED OPTICAL SPECTROSCOPY

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Van der Waals interactions (VDW) in bulk materials are usually considered weak relative to the effects of strong chemical bonding. However, in low-dimensional systems, VDW coupling can significantly modulate physical properties, leading to photoluminescence quenching, appearance of new electronic transitions and significant shifts of existing optical resonance energies and phonon frequencies [1]. Here, we explore these effects in purified double-wall carbon nanotube[2] (DWCNT) samples by a combination of absorption, wavelength-dependent photoluminescence-excitation (PLE) and resonant Raman scattering (RRS) spectroscopy. The purified DWCNTs are obtained by careful solubilization that strictly avoids ultrasonication [3] or by electronic-type sorting [4], both followed by a density gradient ultracentrifugation to remove unwanted SWCNTs. Chirality-dependent shifts of the vibrational and electronic transitions of the inner and outer DWCNT walls, with respect to those of reference empty and water-filled SWCNTs, are determined by detailed two-dimensional fitting of RRS and PLE spectra and compared to theoretical predictions. This exhaustive data set verifies that fluorescence from the inner DWCNT walls is completely quenched through efficient inner-to-outer wall energy transfer.[5] By combining the PLE and RRS results, we provide evidence of the inner-to-outer wall energy transfer through observation of additional peaks in the PLE maps that can be related to particular inner and outer wall chiral combinations of the DWCNTs. Furthermore, the detailed fitting allows us to analyze the energy transfer as a function of the interlayer distance. The obtained results establish a novel structural characterization approach based on combined PLE and RRS spectroscopy for bulk DWCNT samples.[5]

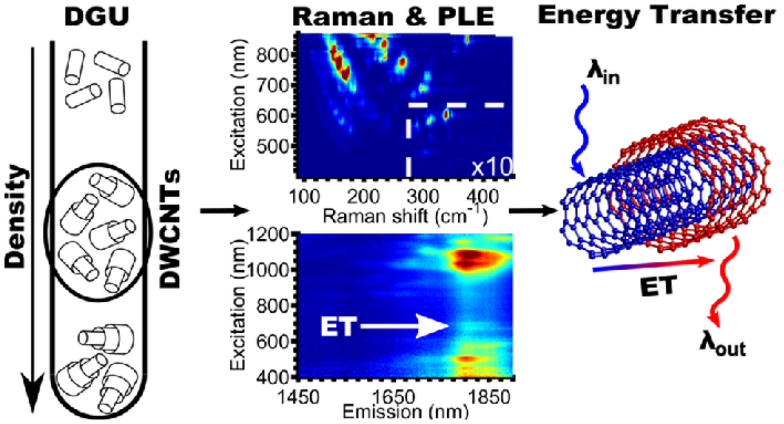

Figure 1. (left) separation of DWCNTs by DGU, (middle) wavelength-dependent Raman and PLE of purified DWCNTS and (right) energy transfer from inner to outer walls

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P133
PROMISING HEAVY-METAL FREE EMISSIVE MATERIALS

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In recent years, organic semiconductor materials have gained popularity due to their low-cost synthesis, chemical compatibility, ease of handling, and simplified manufacturing processes. Many emissive materials in semiconductive devices contain heavy and rare-earth metals and perform well. But heavy metals are toxic, and some are already restricted in the EU, so developing heavy metal-free emitters is an important task in organic electronics.

Fluorene derivatives have shown promise as emitters due to their high photoluminescence efficiency and good charge transport properties [1-2]. In this study, new family of fluorene-based emissive substances was synthesized using n-buthyllithium and n-hexylbromide treatment of fluorene in presence of bromine and FeCl3 and following Sonogashira coupling [3-4]. The film thickness was controlled using a Dektak® 150 surface profiler. UV-vis-NIR absorption and photoluminescence spectra were measured using an Ocean Optics HR4000 and fluorescence spectrometer FLS1000, respectively. All photoelectrical measurements were taken in a high vacuum cryostat.

The synthesized compounds were found to have absorption maxima at 320-420 nm, emission maxima at 390-430 nm, and a photoluminescence quantum yield of 53-59% for encapsulated samples. They also had an ionisation energy of -5.9-6.2 eV, adiabatic gap of -2.6-2.9 eV, and electron affinity of -2.9-3.3 eV. Based on these results, the synthesized substances show promise for use in organic electronic devices.

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P134
QUANTUM DEFECTS IN CARBON NANOTUBES FOR FUNCTIONALISATION AND SENSING

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Single wall carbon nanotubes (SWCNTs) are a 1D nanomaterial that shows fluorescence in the near infrared (NIR, >800nm). They have been assembled with biopolymers such as DNA to form highly sensitive molecular sensors. Such sensors change their fluorescence when they interact with analytes. Despite the progress in engineering of these sensors the underlying mechanisms are still not understood. In the past, covalent chemistry was less explored to functionalize SWCNTs as it impairs NIR emission. However, certain sp3 defects (quantum defects) in the carbon lattice have emerged that preserve NIR fluorescence and even introduce a new, redshifted emission peak capable of single-photon emission. Here, we report on quantum defects, introduced using lightdriven diazonium chemistry, that serve as anchor points for biomolecules. We show surface functionalization, measure experimentally the number of defects per SWCNT and their impact on photophysics. Additionally, we demonstrate how perturbation of a system with quantum defects reveals the photophysical mechanism of SWCNT-based sensors and provides opportunities for novel sensing concepts. Therefore, quantum defects are a versatile platform to tailor photophysical properties as well as surface chemistry of SWCNTs for sensing applications.

P135

RADIAL EFFECTS IN DOUBLE-WALLED TRANSITION METAL DICHALCOGENIDE NANOTUBES

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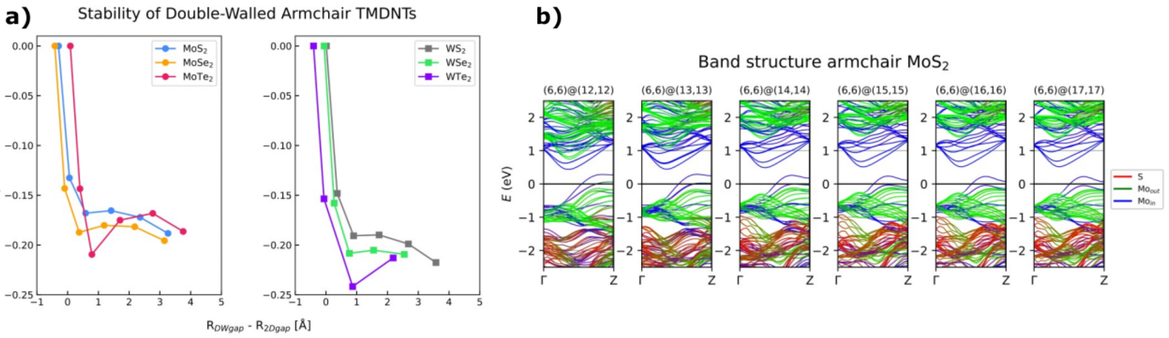
Transition metal dichalcogenide (TMD) nanotubes (NTs) have been the focus of much researched since the early 2000's. Computational studies have uncovered interesting properties of a wide variety of TMDNTs, especially Mo and W dichalcogenides [1]. Mo and W dichalcogenides have tunable band gaps dependent on structure and strain, hydrogen evolution reaction catalytic properties [2], high carrier mobility, high on/off current ratio, and good mechanical properties [3]. These properties make TMDNTs exciting for electronic, optoelectronic, electrochemical, and mechanical applications. However, the structure relationship between tubes in a multi-wall nanotube (MWNT) has not been comprehensively studied. Here, we report structure-property relationships for double-wall (DW) TMDNTs (MX2, M = Mo, W, X = S, Se, Te) as a function of the intertube distance. Interestingly, both armchair DW TMDNTs exhibit a metastable DW structure with relatively narrow diameter (<3 nm), coinciding with an intertube distance ~0.5-1 Å larger than the optimal 2D bilayer distance (Mo to Mo). The stability of this narrow diameter tube increases with chalcogenide size (i.e. Te>Se>S), see Figure 1(a). For zigzag DW TMDNTs, there are multiple metastable structures, and a range of outer tube diameters have energies in the metastable region. The electronic structure of these DW TMDNTs are structure-dependent; as the outer tube increases in diameter, the gaps between valence and conduction bands in both the outer and inner tubes increase.



Stability and band structure of DW TMD. Figure 1 - a) Stability of armchair double-wall (DW) Transition metal dichalcogenide nanotubes. The energy of the DW tubes show a clear metastable region, and b) the projected band structure of the MoS2 DW tubes, showing the band gap of the inner and outer tube increasing with outer tube diameter.

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P136

RAMAN FINGERPRINTS OF TWISTED BILAYER GRAPHENE WITH ISOTOPE LABELLING

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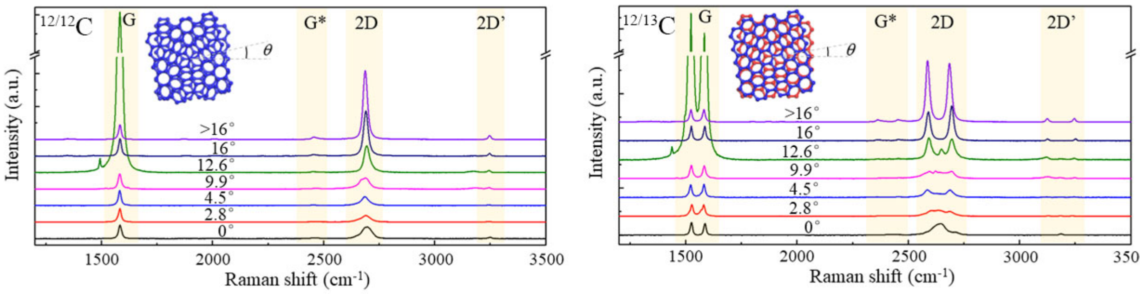
Raman spectroscopy has been widely used as a non-destructive technique to characterize graphene. Here we discuss the different interlayer and intralayer electron-phonon interactions underlying the different Raman peaks of bilayer graphene with different rotation angles using ^{13}C-substitution for one of the layers. Different from several previous reports[1,2], our results reveal that the G, R and R' peaks are from the intralayer electron-phonon interactions for all rotation angles, whereas the interlayer electron-phonon interactions make different contributions to the G*, 2D and 2D' peaks according to the rotation angles. Moreover, based on the same resonant rotation angle of the R' peak as that of the G peak, a possible scattering process of the R' peak in bilayer graphene is given.

Raman spectroscopy has been widely used as a non-destructive technique to characterize graphene. Here we discuss the different interlayer and intralayer electron-phonon interactions underlying the different Raman peaks of bilayer graphene with different rotation angles using ^{13}C-substitution for one of the layers. Different from several previous reports[1,2], our results reveal that the G, R and R' peaks are from the intralayer electron-phonon interactions for all rotation angles, whereas the interlayer electron-phonon interactions make different contributions to the G*, 2D and 2D' peaks according to the rotation angles. Moreover, based on the same resonant rotation angle of the R' peak as that of the G peak, a possible scattering process of the R' peak in bilayer graphene is given.



Raman spectra of bilayer graphene. Raman spectra of (a) 12/12C bilayer graphene and (b) 12/13C bilayer graphene with different twist angle.

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P137

RAMAN STRATEGY FOR DETERMINATION OF CHARGE TRANSFER IN INTERCALATED CARBON NANOTUBES

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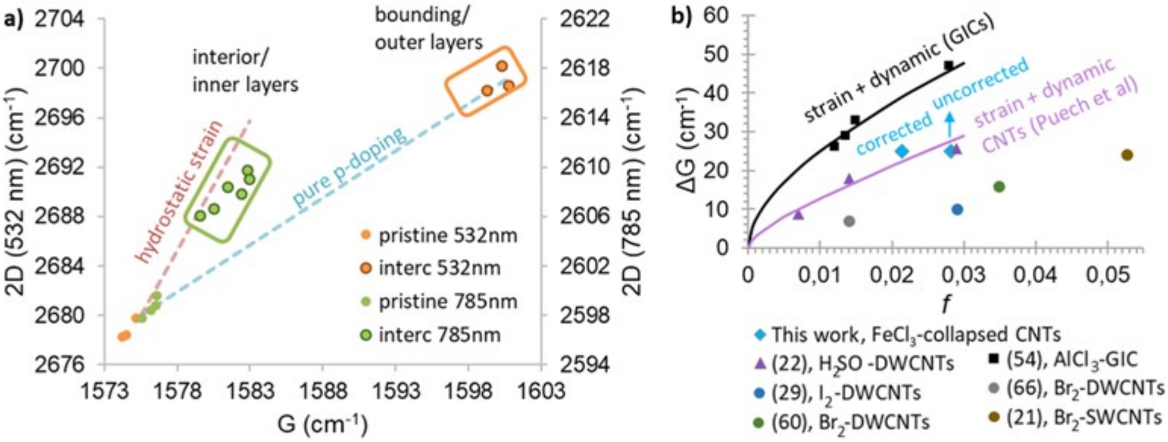
The difficulty in calculating charge transfer (*f*) through Raman spectroscopy in CNTs resides in that multiple contributions lead to shifts of the so-called G modes upon doping, among them a strain effect produced by the shortening/elongation of the carbon-carbon bond lengths upon doping with acceptors/donors [1]. A wise way of obtaining charge transfer in acceptor-intercalated DWCNTs was proposed by Puech et al. [2]. Briefly, strain caused in the hexagonal lattice of the outer wall upon acceptor doping causes hydrostatic compression of the inner wall, whose ratio of G-shifts is known by Raman experiments ($\Delta G_{\epsilon}^{out}=1.7\cdot\Delta G_{\epsilon}^{in}$). In their study, the total G shift of the inner wall is entirely attributed to the compression caused by the outer wall, because it is of general knowledge in this field that most of the charge transferred by the dopant is kept at the wall in contact. Then, charge transfer is obtained from the known factor of proportionality of the strain contribution to the G-shift ($\Delta G_{\epsilon}^{out}=350\cdot f$). The contribution of this work [3] in the analysis of charge transfer through Raman measurements is to separate (and thus accounting for) the charge transferred by the dopant to the inner wall, in order to obtain the overestimation of charge transfer to the outer wall (and thus Fermi level shift) at neglecting it. For that, we make use of the different ratios of Δ2D/ΔG observed upon hydrostatic compression alone and upon p-type doping (see Figure 1.a). The results indicate that charge transfer is being overestimated by ~30% (blue diamond labeled uncorrected in Figure 1.b). Interestingly, there is a correlation between our $FeCl_3$-intercalated collapsed DWCNTs and Puech's H_2SO_4-intercalated DWCNTs, as shown in Figure 1.b, giving hope for a master curve in which analysis of G-shifts alone directly give us charge transfer with any acceptor dopant.



a) Raman 2D-G representation for pristine and FeCl3-intercalated fibers of collapsed DWCNTs. b) Data plot of ΔG as a function of charge transfer for acceptor doping of different systems [3].

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P138

RAPIDLY MODULATED WIDE-SPECTRUM INFRARED SOURCE MADE OF SUPER ALIGNED CARBON NANOTUBE FILM FOR GREENHOUSE GAS MONITORING

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Non-dispersive infrared (NDIR) gas monitoring has advantages of environment stability, convenient operation and maintenance, wide detection range, and multi-gas-detection capability. However, the conventional IR sources for NDIR gas monitoring, such as miniature lamps, microelectromechanical system (MEMS) light sources, and light-emitting diodes (LEDs), can only work at narrow modulation frequency and spectral range, or require complicated design and fabrication, because of the constraint of materials and work principle. These issues cause low data acquisition rate, poor anti-interference ability and limited gas compatibility to NDIR. Here, the super-aligned carbon nanotube (SACNT) film is developed as an IR source in NDIR gas monitoring system. It has a wide spectral range (0.2–334 µm), a facile fabrication method, and can work up to a high frequency ≈150 kHz. A mechanicalchoper-free and wide-concentration-range monitoring equipment for CO2 and CH4 greenhouse gases is demonstrated with SACNT film IR source. The concentration ranges for CO2 and CH4 investigated in this paper are 0.0195–20.10% (v/v) and 0.10–17.11% (v/v), respectively. It can be easily applied to monitor other kinds of gases as well.

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P139

REAL-TIME MYCOTOXIN DETECTION USING GRAPHENE-BASED APTASENSORS

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Mycotoxins are secondary metabolites produced by microfungi such as Aspergillus and Penicillium genera and one of the most common and dangerous contaminants in food, feed, and agricultural products [1]. They can be found in a variety of foodstuffs, including cereals, dried fruit, and drinks [2]. A specific graphene field-effect transistor (GFET)-based aptasensor was developed for the detection of highly toxic Ochratoxin A (OTA), which relies on an array of GFETs integrated on a single silicon chip. We experimentally studied the aptamer reconfiguration process during binding a specific target molecule, i.e. OTA, the interaction of an aptamer with graphene, and how the variation of ionic strength of a solution influences the sensitivity of our biosensor [3]. We suggest that aptamer, when free-standing, is weakly adsorbed on graphene's surface via π-π stacking, which is experimentally confirmed by a left-shift of Dirac point in transfer characteristic of GFET (n-doping) compared to PBASE-modified graphene. On the other hand, when the aptamer binds the OTA molecule, it undergoes 3D reconfiguration into G-quadruplex and desorbs from the graphene surface, which initiates the right-shift of charge neutrality point (p-doping). We showed that, by decreasing ionic strength 10 times, the sensitivity can be improved due to increased electrostatic gating from aptamer G-quadruplex structure, which confirms the idea of aptamer desorption from the graphene surface upon OTA binding. The graphene-aptamer sensors reported here demonstrate fast assay with the lowest detection limit of 1.4 pM for OTA within a response time as low as 10 s [4], which is more than 30 times faster compared to any other reported aptamer-based methods for mycotoxin detection.

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P140

RELEASE OF SELECTED ANTICANCER DRUGS FROM THE INTERNAL SPACE OF CARBON NANOTUBES FUNCTIONALIZED BY DNA FRAGMENTS ANALYZED BY MEANS OF MOLECULAR DYNAMICS

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In this study we are going to show, on the molecular level, how carbon nanotubes, CNT, functionalized by cytosine-rich DNA fragments interact with doxorubicin (DOX) and that it is possible to engineer an interesting pH-controlled carrier of doxorubicin in that way. Our predictions are based on the application of molecular dynamics simulations with the adequately chosen force fields for each component of the system. We found that at neutral pH the cytosine-rich DNA fragments (i-motif precursors) and DOX molecules intercalate each other and the whole object can be attached to the carbon nanotube using covalent linkages. Reduction of pH leads to folding of these DNA fragments into noncanonical i-motif DNA structure which weakly interacts with DOX. Thus, we will show that cytosine-rich DNA fragments linked to the CNT tips form together a pH sensitive carrier of DOX. The carrier keeps DOX molecules locked within DNA chains and inside the CNT at neutral pH and unlocks them at slightly acidic pH. [1]We also found [2] that another anticancer drug, carmustine, can be stored in the carbon nanotube interior for a long time due to hydrophobic interactions. The access of water to carmustine phase in the CNT interior can be controlled by the state of cytosine rich DNA fragments covalently bound to the CNT tips and to the presence of doxorubicin molecules intercalated within bundles of DNA fragments. More effective control of water access and subsequent decomposition of carmustine due to the contact with water was observed when some small amount of doxorubicin molecules cork the CNT ends. Our analysis shows that carmustine decomposition products naturally separate when decomposition occurs within the CNT. The alkylating agent, chloroethyl carbonium cation, spontaneously escapes from the CNT but the carboamoylation agent, chloroethyl isocyanate, is still kept within the nanotube interior. The separation process and release of the alkylating agent needs uncorking the nanotube by doxorubicin molecules. The latter process is likely to occur spontaneously at acidic pH when intercalation of doxorubicin within the DNA fragments becomes ineffective. The features of the proposed molecular model, obtained form molecular dynamics simulations, can be beneficial in design of novel smart drugs carriers to a tumor microenvironment revealing the reduced extracellular pH.

Acknowledgment: This work was supported by Polish National Science Centre grant 2017/27/B/ST4/00108.

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P141
RESONANCE RAMAN SCATTERING OF (7,7) ARMCHAIR CARBON NANOTUBES

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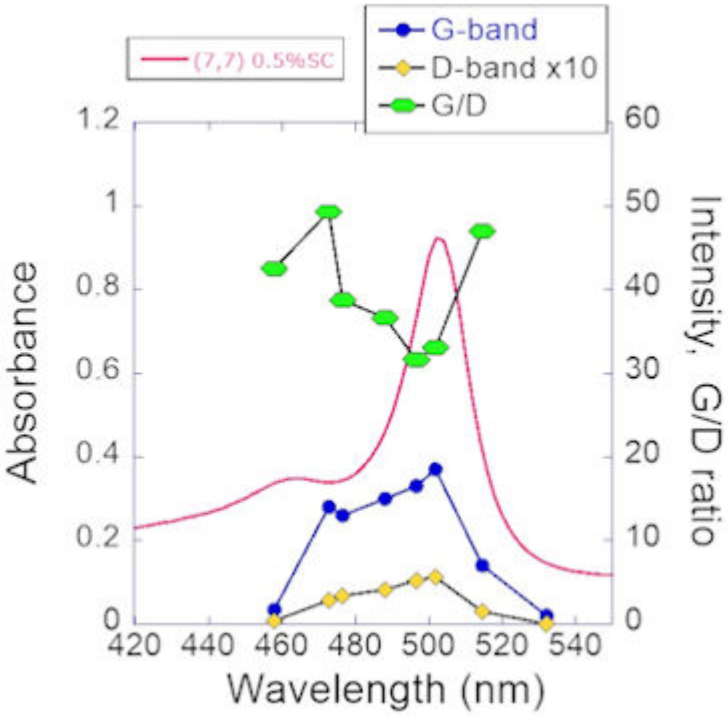
The analysis of Raman spectra of carbon nanotubes (CNTs) is almost well established. However, the defect-derived D-band has not yet been fully discussed. The D-band in graphene is explained by the double resonance effect, but it is not obvious whether a similar argument is possible for CNTs. Since a typical CNT sample is a mixture of various structures, it has been difficult to determine the resonance effects of individual CNTs. In this study, we measured resonance Raman scattering of (7,7)-armchair single-chirality CNTs and investigated the resonance effects of each vibrational mode. The figure shows the optical absorption of (7,7) and the intensity changes in G-band and D-band. Since the (7,7)-type is metallic, a double resonance effect similar to that of graphene is expected. However, we found that the D-band shows a typical resonance effect similar to the G-band, and the double resonance effect as seen in graphene is not so pronounced. This result suggests that the G/D ratio of CNTs is not enhanced by the G-band resonance effect. This result indicates that G/D can be a comparable metric for defect evaluation of CNTs to that of graphene, but the meaning of the value should be carefully discussed.



Results of Resonance Raman Scattering. Optical absorption spectrum and the intensities of G-band and D-band of (7,7) armchair CNTs dispersed in water.

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ROBUST METHOD FOR V2O5 COATING OF CARBON NANOTUBES FOR NEXT GENERATION TRANSPARENT ELECTRODES AND LI-ION BATTERIES

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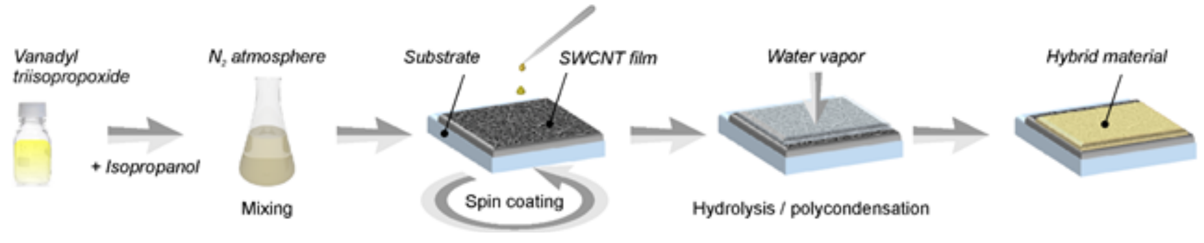
Composite materials comprising vanadium pentoxide (V_2O_5) coating on a surface of single-walled carbon nanotubes (SWCNTs) are a promising component for emerging applications in transparent conductors, solar cells, chemical and electrochemical sensors, etc. In this work, we propose a novel, simple, and facile approach for SWCNT coating with V_2O_5 by means of a simple spin coating under ambient conditions. With the mechanism, involving hydrolysis of V_2O_5 precursor (vanadyl triisopropoxide) followed by polycondensation directly on the surface of carbon nanotubes under ambient conditions, we observe the produced nm-thick layer oxide to be amorphous with a work function of 4.6 eV. The heating to 500-600ºC allows the material to recrystallize, achieving the work function of 5.8 eV. The method addresses the key advantages of the production of V_2O_5/SWCNTs composite material: the obtained coating is uniform with a tunable thickness and it does not require vacuum or heating during the processing. We prove the method applicability by achieving groundbreaking results for two V_2O_5/SWCNT applications: transparent electrodes and cathode for Li-ion batteries. As a transparent electrode, the composite shows stable sheet resistance of 160 Ω/sq at a 90% transmittance in the middle of the visible range – the best performance for SWCNTs doped by metal-oxides. As a cathode material, the obtained specific capacity (330 mAh/g) is the highest among all the other V_2O_5/SWCNT cathodes reported so far. These results open new horizons for the next generation of composite materials based on vanadium oxides for various applications, including optoelectronics and electrochemistry.

This work was supported by Russian Science Foundation grant number: 22-13-00436.



Scheme of SWCNT coating at ambient conditions by nanometer-thick V2O5 layer using vanadyl triisopropoxide (VTIP) dissolved in isopropanol.

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SCALE-UP PROCESS, MORPHOLOGY CONTROL AND MULTI-PROPERTIES OF AEROGELS FROM RECYCLE FIBERS OF VARIOUS WASTES

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At present, commercial aerogels on the market are costly, and largely used for heat and sound insulation. The manufacturing process also releases toxic levels of carbon emission. To solve these challenges, we have devised sustainable methods of upcycling different types of waste such as paper, textile, plastic, rubber, metal, fly ask, agriculture waste, food waste etc. into multi-functional large-scale aerogels. Compared to standard aerogel methods, our aerogel technologies are very cost-effective (due to 70% of energy saving), faster (18 times) and environmentally friendly (no toxic usage and much less CO2 emission with 0.1 kg CO_2 emission/aerogel m^2). The affordable aerogels products can be reused, recycled and disposed safely. The aerogel products can be used for engineering applications such as:

- Cheap fire-retardant coats/jackets and carbon dioxide absorption masks that help people escape a fire safely. When coated with flame retardants, our products can withstand temperatures of up to 1400^{o}C – 15 times more fireproof than the thermal lining in conventional fire-fighting suits, but at about 20% of the weight.
- Better heat and sound insulation in buildings to reduce energy use of air conditioners and heating systems and reduce 70% of the ambient (e.g., vehicle) noise. Our products reduce sound better than any conventional insulation foam, and it also insulates against heat many times better than fibreglass.
- Cleaning oil spills and organic solvents at factories. E.g., when our aerogel products are coated with certain water-repellent chemicals, they absorb up to seven times more oil than existing commercial sorbents can – and at a faster rate.
- Personal care products like diapers.
- Medical uses as human fat trappers. Based on our product test results, one capsule of pineapple leaf fibres can absorb almost all the saturated fats from eating one hamburger.
- Rapid haemorrhage control in trauma settings (e.g., conflict zones). Our compressed pellets expand and apply pressure on the wound to stop the blood flow. Each pellet can expand to 16 times its size in 4.5 seconds and absorb more blood three times faster than existing pellets.

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P144

SCANNING TRANSMISSION ELECTRON MICROSCOPY TO CHARACTERIZE THE STRUCTURE AND CHEMICAL STATE OF IODINE CHAINS IN CNT WIRES

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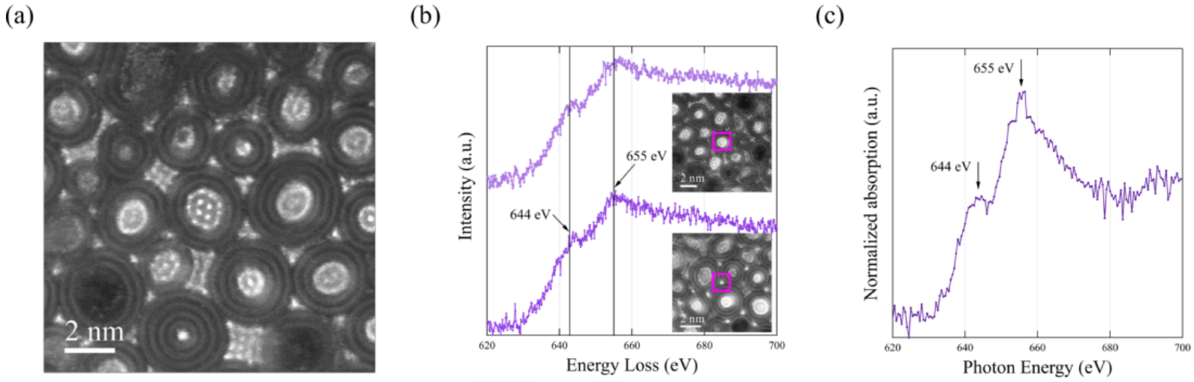
Carbon nanotubes (CNTs) are expected to be an electrical conductor for the next generation of electrical wires due to their low electrical resistance and lightweight [1]. CNT wires have a hierarchical structure in which multiple CNTs of a few nm in diameter are assembled into bundles, and these bundles are further agglomerated. The main difficulty in developing CNT wires is the increase in electrical resistivity as the hierarchical structure moves up. Iodine doping is a method to reduce the electrical resistivity of CNT wires, and it has been reported that the electrical resistivity is reduced by doping iodine into CNT wires [2]. However, there are few reports on the detailed structure, position and chemical state of iodine in CNT wires. Therefore, we doped CNT wire with iodine elements under high temperature and high pressure, and evaluated the structure, position and chemical state of doped iodine using scanning transmission electron microscopy (STEM) - electron energy loss spectroscopy (EELS) for iodine-doped CNT wire. X-ray absorption fine structure (XAFS) measurements were also performed to confirm the bulk chemical state of the doped iodine. Fig. 1 (a) shows the cross-sectional STEM image of the iodine-doped CNT wire. The bright areas are iodine and it can be seen that the iodine is encapsulated within the CNTs and between the CNT-CNTs. The EELS spectra of these iodine materials show no significant differences in their chemical states, with peaks at E = 644 & 655 eV (Fig. 1 (b)). Fig. 1 (c) shows the XAFS spectrum (M-edge) of the iodine-doped wire, which is in good agreement with the EELS spectrum. It has been confirmed that the electrical resistivity of CNT wires decreases by 15-20 % after iodine doping, and the origin of this phenomenon will be reported on the day as other structural analysis results.



STEM-EELS and XAFS. Fig. 1 (a) Cross-sectional STEM image of iodine-doped CNT wire. (b) EELS spectra of iodine in CNT wire. (c) XAFS spectrum of iodine-doped CNT wire.

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P145

SEALING OF SINGLE-WALLED CARBON NANOTUBES ENCAPSULATING WATER MOLECULES

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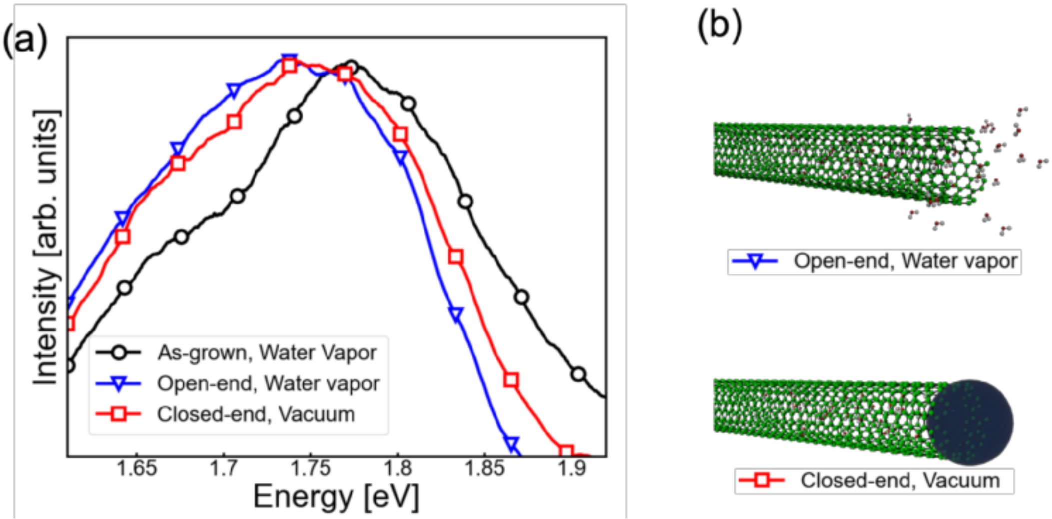
Single-walled carbon nanotube (SWCNT) is a nanomaterial with hollow structure. Water molecule encapsulation into SWCNT has been investigated by Raman scattering[1] and photoluminescence[2]. There is a limit to the chirality that can be measured with these methods, however, Rayleigh scattering spectroscopy can measure SWCNTs of all chirality. The previous research[3] revealed that SWCNTs encapsulate water molecules at high water vapor pressure and release them at low pressure or vacuum, but there are no reports about sealing water molecules in SWCNTs. In this study, we observed water encapsulation in SWCNTs by Rayleigh scattering spectroscopy and performed opening and closing SWCNTs by pulse laser irradiation. The suspended SWCNTs were synthesized on SiO2/Si slit substrates by fast-heating gas-flow CVD[4]. Rayleigh scattering spectroscopy was performed in an environmental chamber with controlling the water vapor pressure. The Rayleigh scattering spectra from as-grown(○) and opened(∇) SWCNT in water vapor are shown in Fig. 1(a). After opening, the peak energy red-shifted in water vapor and no red-shift was observed in vacuum. The red shift was caused by water molecule encapsulation and the water molecule went out when the SWCNTs were in vacuum (Fig. 1(b)). Pulse laser irradiation with higher power density in water vapor was performed to close the SWCNT, and its spectrum is shown in Fig. 1(a) as red curve with square markers(□). The red-shift was observed even in vacuum. This suggests that the SiO2 layer was melted by higher power laser irradiation and it sealed the once opened SWCNT (Fig. 1(b)). In conclusion, we successfully opened and closed the suspended SWCNT with pulse laser irradiation, and sealed water molecules in it.



(a)Rayleigh scattering spectra of as-grown(○), open-end(∇) and closed-end(□) SWCNTs, and the schematic images of water molecule encapsulation in (b)open-end and (c)closed-end SWCNT.

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P146

SEM IMAGING OF INSULATING SPECIMEN THROUGH A TRANSPARENT CONDUCTING VEIL OF CARBON NANOTUBE

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Observing the morphology of insulating specimen in scanning electron microscope (SEM) is of great significance for the nanoscale semiconductor devices and biological tissues. However, the charging effect will cause image distortion and abnormal contrast when observing insulating specimen in SEM. A typical solution to this problem is using metal coating or water-removable conductive coating. Unfortunately, in both cases the surface of the specimen is covered by a thin layer of conductive material which hides the real surface morphology and is very difficult to be completely removed after imaging. Here we show a convenient, residue-free, and versatile method to observe real surface morphology of insulating specimen without charging effect in SEM with the help of a nanometer-thick film of super-aligned carbon nanotube (SACNT). This thin layer of SACNT film, like metal, can conduct the surface charge on insulating specimen through the sample stage to the ground, thus eliminating the charging effect. SACNT film can also be used as the conductive tape to carry and immobilize insulating powder or particles during SEM imaging. Different from the metal coating, SACNT film is transparent, so that the real microstructure of the insulating specimen surface can be observed. In addition, SACNT film can be easily attached to and peeled off from the surface of specimen without any residue. This convenient, residue-free, and versatile method can open up new possibilities in non-destructive SEM imaging of a wide variety of insulating materials, semiconductor devices, and biological tissues.

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SIMULTANEOUS MEASUREMENT OF THE IN-PLANE AND INTERLAYER THERMAL CONDUCTIVITIES OF BILAYER GRAPHENE USING ISOTOPE-LABELLED RAMAN SPECTROSCOPY

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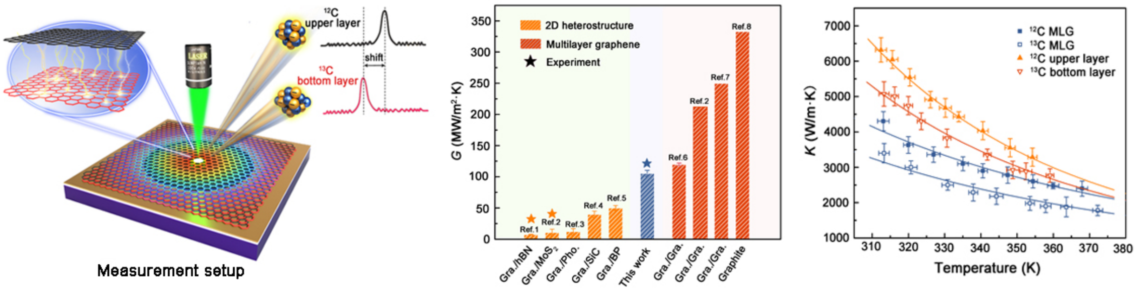
The thermal properties of bilayer graphene (BLG) play an important role in the development of its promising electronic devices, but the low temperature gradient and overlapped Raman signals have presented bottlenecks for the measurements using the widely used technique of time-domain thermoreflectance and Raman spectroscopy. Here we synthesize BLG with the bottom layer labelled by ^{13}C atoms by chemical vapor deposition, and simultaneously measure the interlayer thermal conductivity (G) and in–plane thermal conductivity (K) of each layer utilizing their different Raman feedbacks. Based on the experimental data, a modified heat diffusion equation suggests that the G has a considerable high value of 105±3 MW/m^2•K, and of each layer is significantly reduced compared with their monolayers. We believe the result can provide a support for more BLG thermal engineering research and the method can be extended to other 2D stacks as well.



Thermal measurement of bilayer graphene and experimental results using isotope-labeling Raman spectroscopy.

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P148

SINGLE-WALLED CARBON NANOTUBES SYNTHESIZED BY LASER ABLATION FROM COAL

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Developing methods to synthesize single-walled carbon nanotubes (SWCNTs) in a greener way is of long-term interests. Laser ablation, developed in 1995, is an important method to synthesize SWCNTs. [1] However, different from chemical vapor deposition and arc discharge, it uses solid carbon sources without preference in conductivity. This endows a great flexibility in carbon source selection for laser ablation. Using coal as the carbon source and Co/Ni as the catalyst, we synthesized high-quality SWCNTs (Fig. 1a, 1b). We studied the effects of temperature, pressure, Ar flow rate, and the ratio of Co/Ni on the yield and diameter distribution of SWCNTs. Separations based on diameter and conductivity were realized by aqueous two-phase extraction. Semiconducting SWCNTs (Fig. 1c) sorted by PCz ((poly[9-(1-octylonoyl)-9H-carbazole2,7-diyl]) were used to fabricate high-performance field effect transistors.

Acknowledgement: We thank Prof. Yohji Achiba and Prof. Shigeo Maruyama for the helpful discussion.

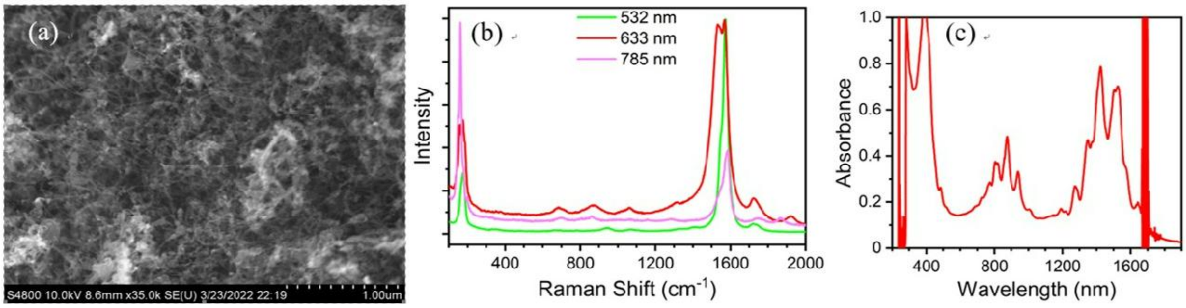

Fig.1. Characterizations and separation results of SWCNTs synthesized by LA. (a) SEM image. (b) Raman spectra with different excitation wavelengths. (c) Absorption spectrum of semiconducting SWCNTs sorted by PCz.

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P149

PIEZORESISTIVE AND THERMORESISTIVE RESPONSES OF CARBON NANOTUBE FIBERS: TOWARDS ENABLING INTEGRATED SENSING

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Carbon nanotube (CNT) yarns (CNTY) are fiber-like structures composed of thousands of carbon nanotubes in their cross-section. The hierarchical structure and microscale dimensions of CNTYs make them candidates for the development of sensors that could be integrated in materials [1]. The change in the electrical resistance of CNTYs when subjected to a mechanical strain, known as piezoresistivity, is the principal mechanism in strain sensing using CNTYs. The piezoresistive response in the direction of the yarn (axial direction) is relatively well-known experimentally [2], but the axial piezoresistive response under compression had not been studied due to the complexities associated with the nature of the experiments involving subjecting a slender fiber to compression loading in its axial direction. More recently, their piezoresistive response under axial compression has been determined using a single CNTY embedded into a polymeric resin (CNTY monofilament composite). The effect of the strain rate on the sign of piezoresistivity and the sensitivity are discussed in detail for both the freestanding CNTYs and the CNTY monofilament composites. Also, the piezoresistive responses under axial tension and axial compression are compared and discussed including insights into the various mechanical and physical mechanisms. Currently, the piezoresistive of the CNTYs in its lateral direction is being investigated experimentally and some preliminary results are presented along with the novel experimental setups. Piezoimpedance is the change of electrical impedance upon the application of a mechanical strain and recent results about the impedance and the piezoimpedance response of CNTYs are also discussed for frequencies up to the GHz-range. The electrical resistance of CNTYs can also vary due to a temperature change and the thermoresistive sensitivity is quantified by the normalized variation of electrical resistance change per unit of temperature given by the temperature coefficient of resistance (TCR) [4]. The cyclic thermoresistive response of CNTY monofilament composites under heating–cooling, incremental heating–cooling, and incremental dwell cycles is discussed considering the effect of the curing temperature of the polymeric matrix on the electrical response of the CNTY monofilament composites [3]. The intrinsic thermoresistivity of CNTYs and the resin infiltration of the CNTY are used to explain the analyzed thermoresistive response. The progress in developing sensor prototypes to measure strain, temperature or detect damage and others, relying on the above mechanisms, is described including the present challenges.

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SOLID-STATE DEFECT INTRODUCTION INTO NETWORKS OF (6,5) SINGLE-WALLED CARBON NANOTUBES

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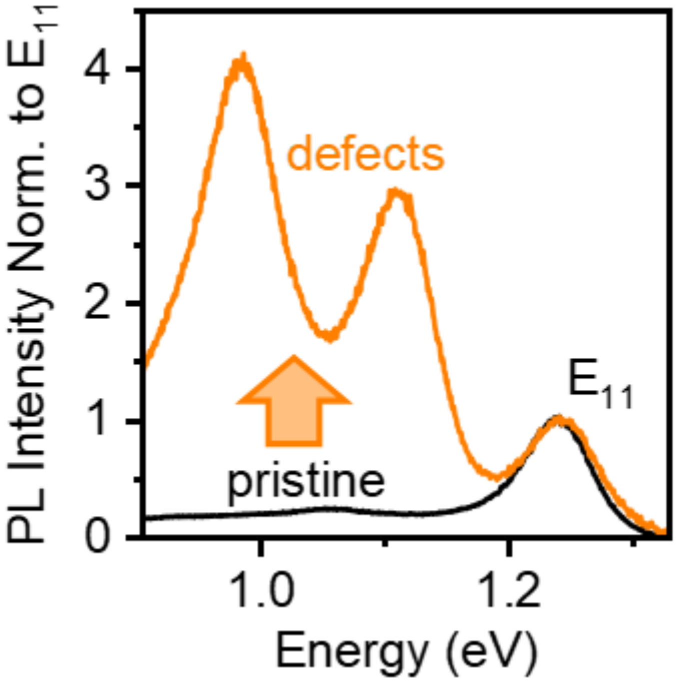
The optical properties of semiconducting single-walled carbon nanotubes (SWCNTs) are governed by excitons with narrow emission in the near-infrared. Covalent functionalization of SWCNTs can create luminescent defects with even further red-shifted emission and longer photoluminescence lifetimes. The defect emission energy is mainly determined by the binding configuration on the sp^2-hybridized SWCNT lattice, which can be controlled through the choice of synthetic conditions [1, 2]. To date, most functionalization routes rely on solution-based reactions. The resulting functionalized SWCNTs in dispersion can be deposited as random networks on substrates via spincoating but without spatial addressability. Here, we introduce luminescent defects into pre-deposited networks of (6,5) SWCNTs on reactive surfaces. We observe two types of luminescent defects with different optical trap depths that can be controlled through the reactivity of the surface and the reaction conditions. This solid-state functionalization method further allows us to introduce defects with high spatial resolution as corroborated by photoluminescence and Raman mapping.



PL of pristine vs functionalized SWCNT network. Normalized photoluminescence (PL) spectra from a network of (6,5) SWCNTs before and after solid-state functionalization.

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P151
SPATIALLY RESOLVED MOLECULAR ENGINEERING OF GRAPHENE

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Exploring the tailored physical/chemical properties is at the forefront of graphene research.[1] The emerging development of covalent molecular engineering represents a rather promising tactic for this purpose carrying several unique advantages. In this line, we have developed two scenarios, including reduction-mediated lithography and laser writing, for spatially resolved covalent 2D-patterning of graphene, affording a variety of well-structured graphene architectures.[2-3] Furthermore, based on the combination of 2D-patterning techniques and post-functionalization approaches, more promising hierarchically ordered multifunctional graphene architectures were facilely constructed. We further demonstrated that the chemical information of these built 2D systems can be finely manipulated by establishing complete write/read/erase circles.

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P152

STEPWISE ARTIFICIAL YARN MUSCLES WITH ENERGY-FREE CATCH STATES DRIVEN BY ION INSERTION

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Bivalve mollusks can keep their hard shells tightly closed while consuming very low energy. This muscle behavior is known as the catch state, which is enabled by Ca^{2+}-regulated trimeric compounds formed by actin filaments and myosin filaments in the anterior byssus retractor muscle. Endowing artificial muscles with a catch state is extremely important because it allows the retention of tensioned actuation states without continuous stimulations and energy consumption, and programmable stepwise actuation according to control profiles. Till now, various artificial muscles that can reversibly contract, bend, expand, or rotate when subjected to external stimuli have been developed. However, such a catch state featuring energy-free high actuation retention and stepwise actuation has rarely been achieved yet. Based on these considerations, a strong but dynamic "locker" that is energy-free should be built in an artificial muscle to retain the actuation state and allow programable actuation especially when the artificial muscle is actuating under a heavy load. Here, we proposed a new strategy that utilizes intercalation compounds that formed during an electrochemically reversible insertion reaction to well hold the CNT yarn muscles at any achieved stroke. $AlCl_4^-$ anions were faradaically and quantitively inserted in the collapsed CNT yarn muscles to form the intercalation compounds, resulting in a novel catch state during a long period as well as precious control of contraction at very small strain steps. This new actuation mechanism also allows the energy-free maintenance of high contractile forces generated by the muscles.

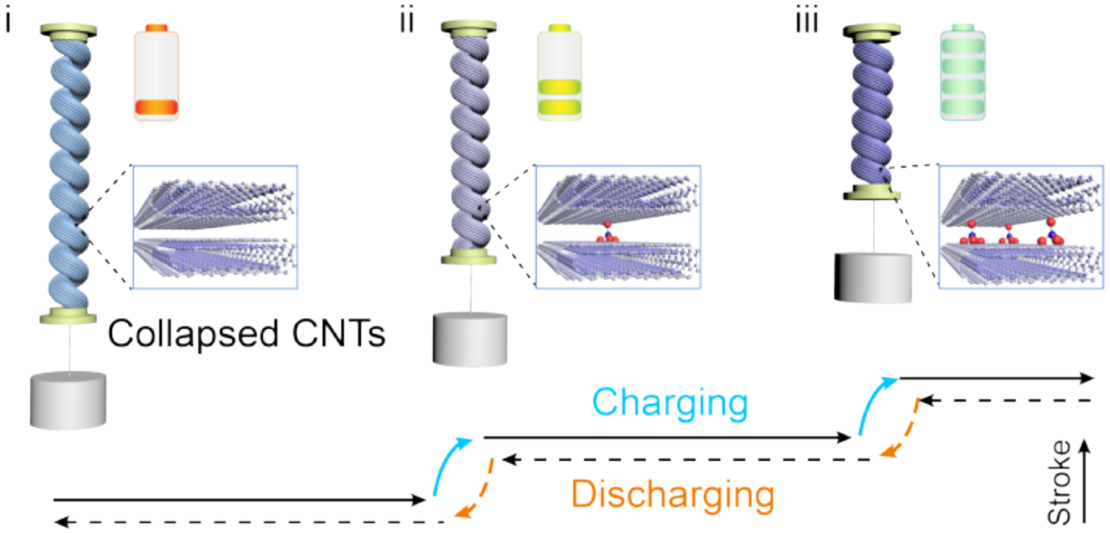

Figure 1. Actuation process showing stepwise actuation and catch state during a CNT coiled yarn charged at different capacity levels

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P153

STRUCTURAL SUPERCAPACITORS THROUGH VERTICALLY ALIGNED CARBON NANOTUBES FUNCTIONALIZED CARBON FIBER REINFORCED COMPOSITES

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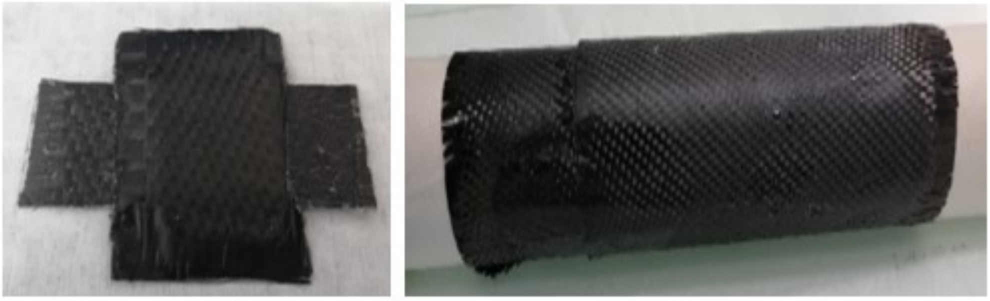
Structural energy storage can meet the target of saving weight in many applications where structural parts and energy source are required at the same location. This can be achieved by bringing multifunctionality in the design of carbon fibers reinforced composites (CFRC).

Here we report the modifications of a classical CFRC architecture so that it behaves like an Electrical Double Layer Capacitor (EDLC). These modifications include a specific formulation of the epoxy matrix leading to sufficient ionic conductivity and the use of carbon fibers on which Vertically Aligned Carbon Nanotubes have been grown.

Prototypes of structural supercapacitors of various shapes manufactured with this approach will be presented as well as their electrochemical properties.



Examples of flat (left) and cylindrical (right) structural supercapacitors

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STUDY OF THE BRAIN EXTRACELLULAR SPACE BY SINGLE CARBON NANOTUBE TRACKING AND SUPER-RESOLUTION IMAGING ANALYSIS IN HEALTH AND DISEASE

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Unraveling the extracellular space (ECS) structure and function represents a technological challenge due to its nanometric dimensions. Despite recent remarkable advances, its precise morphological and diffusional parameters are still mainly unknown in the healthy and pathological brain. The tracking of fluorescent Single-Wall Carbon Nanotubes (SWCNTs) in living tissue represents a powerful method to obtain information about this otherwise dark maze. Combining InfraRed single-particle tracking with super-resolution image analysis it is possible to rebuild the trajectory the probe has taken, and infer key properties such us instantaneous local diffusion or local channel width. Our recent work focused on the striatal extracellular space of the mouse. Understanding how ECS properties affect brain communication and change in disease is thus of fundamental importance. We studied key striatal ECS properties in a PFF model of synucleinopathy vs healthy controls. Results show an overall increase in diffusivity which cannot be explained by ECS volume augmentation. This highlights, first, the multiple factors affecting ECS diffusion. Second, that ECS may play a role in disease which has still to be elucidated.

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SUPER MACKAY ALLOY CLUSTER $FE_{42}CO_{13}$ FOR GROWTH OF SINGLE-WALLED CARBON NANOTUBES

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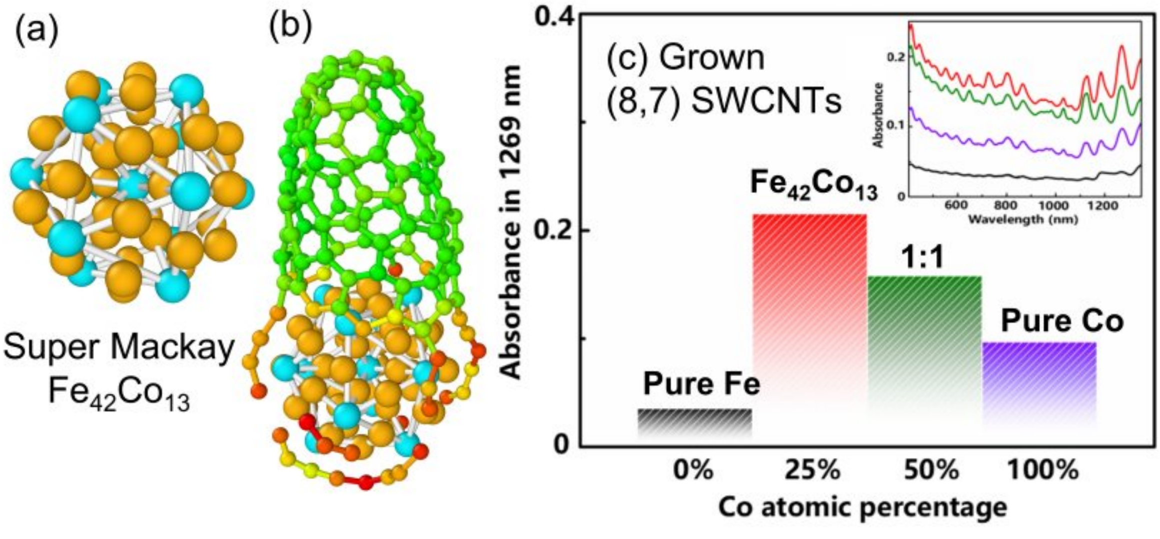
We propose a super Mackay cluster $Fe_{42}Co_{13}$ for the selective chirality growth of single-walled carbon nanotubes. The double icosahedral structure, the so-called Mackay structure, is well known by theoretical works[1,2]. However, the Mackay structure is meta-stable in our molecular dynamics simulation (MD). The most stable structure in MD simulation is shown in Fig. 1(a); internal core $Fe_{12}Co$ is rotated 15 degrees from the Mackay structure. If we let this cluster vibrate at high temperatures, we can observe the mode-crossing rotation of the inner core. From MD simulations, we found the extremely high melting point of $Fe_{42}Co_{13}$ cluster, 1800K. We believe the extremely high melting point originates from this unique mode-crossing vibration. By preliminary MD simulation of carbon nanotube growth, we found the solid behavior of this catalyst up to 1800K, as in Fig. 1(b). The chirality of SWCNT of the simulated nanotube will be discussed.

As we can guarantee the solid catalysts in the usual CVD condition, we try to grow chirality-specific SWCNTs based on this super Mackay cluster. Conventional ACCVD [3] used the 1:1 weight ratio of Fe and Co. Since the atomic ratio is not much different from the weight ratio, we compared the Fe: Co atomic ratio for 0:100, 42:13, 50:50, 100:0 at various temperatures 500-900 ºC, keeping the specific pressure of ethanol to 300 Pa. To our surprise, at 600 ºC, pure Co gives the best performance of growing (6,5) and (7,5). On the other hand, at 850 ºC, the alloy ratio corresponding to $Fe_{42}Co_{13}$ gives the highest efficiency as shown in Fig. 1(c). Exposure to higher temperatures could lead to more specific chirality distribution.



Super Mackay structure and growth of SWCNTs. (a) super Mackay structure of Fe42Co13. Co atoms are in cyan and Fe atoms are in orange. (b) Molecular dynamics simulation of growth. (c) CVD growth of SWCNTs by zeolite supported bimetallic alloy at 850 C. The absorption corresponding to (8,7) nanotubes.

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SUPER-RESOLUTION IMAGING OF DEFECT SITE FORMATION IN CARBON NANOTUBES

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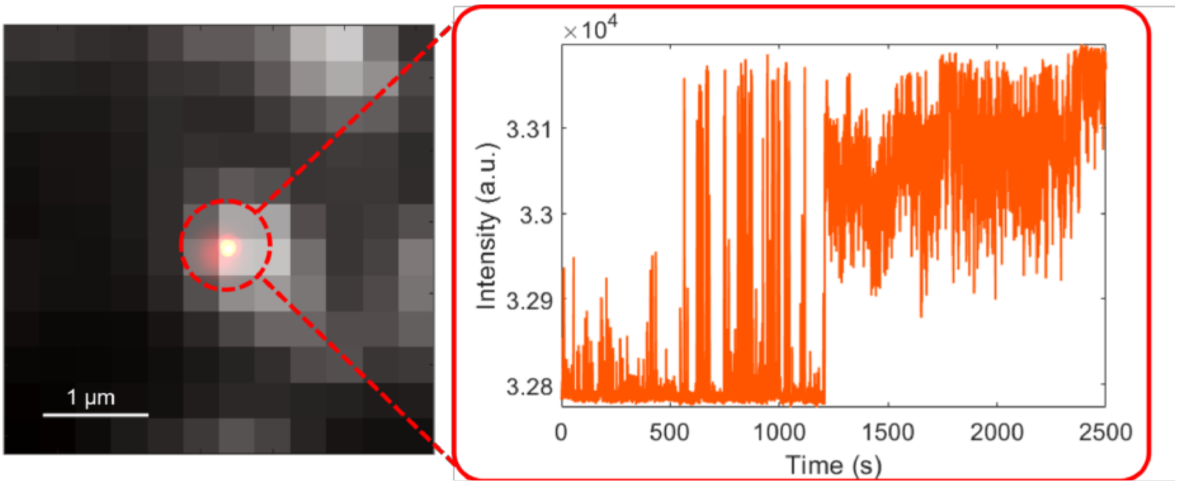
Semiconducting single-walled carbon nanotubes (SWCNTs) exhibit a photostable excitonic fluorescence in the short wave near-infrared (SWIR). Recently, the covalent functionalization of nanotubes opened new avenues to manipulate their excitonic fluorescence [1]. These "organic color centers (OCCs)", also known as "defects", act as localized potential wells on the nanotube surface, trapping locally otherwise diffusing excitons. This effectively results in an increase in the SWCNT emission, the trapped excitons avoiding possible quenching sites along the nanotube surface (structural defects, nanotube ends) [2]. This new radiative pathway results in a shifting of the SWCNT emission towards longer wavelengths and allows SWCNT excitation on their first-order excitonic transition (ca. SWIR) [3]. Altogether, these properties make OCC-functionalized SWCNTs particularly attractive for various applications ranging from biological imaging to quantum information. Yet, the functionalization reaction of SWCNTs with OCC is still poorly understood, stochastic and, as a result, poorly controlled. To gain knowledge and control over these reactions, we developed a two-color imaging platform to image simultaneously both the SWCNT and OCC emissions in situ during the functionalization reaction [4]. By performing super-localization on the OCC emission, we are able to determine the position of the OCCs in real time as they appear on the SWCNT at the nanometer scale. We will present how this platform allows to monitor the kinetics of the functionalization reaction and the possible coupling between different OCCs. We will further discuss our findings which provide insights on the interactions existing between OCCs and the SWCNT surface or between each other, and eventually help to have a more deterministic control of OCC implantation.



Super-resolution imaging of defect site formation. Left: super-resolved image of the defect localization (red circle) overlapped with the emission of a nanotube (grey). Right: intensity fluctuations of the defect emission as a function of time.

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P157

SURFACE DIFFUSION-LIMITED GROWTH OF MONOLAYER WS_2 USING SUBSTRATE-STACKED MICROREACTOR FOR OPTOELECTRONIC DEVICE APPLICATIONS

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Transition metal dichalcogenides (TMDCs), one of the two-dimensional semiconducting materials, have attracted attention for optoelectronic device applications due to their high flexibility, light absorption, and emission coefficient with direct band-gap. This research investigated the chemical vapor deposition (CVD) growth of monolayer WS_2 and their size control based on the vaper-liquid-solid (VLS) method with metal salt employing the microreactor constructed with two growth substrates [1].

Na_2WO_4 solution was spin-coated on a Si/SiO_2 substrate, and another Si/SiO_2 substrate was stacked on top to confine Na_2WO_4 in a microreactor consisting of two substrates. The microreactors were reacted with organosulfur ($(t\text{-}C_4H_9)_2S_2$) vapor in an infrared furnace to grow WS_2. We evaluated the photoluminescence (PL) of the grown crystals. The highest PL energy (~1.98 eV) and FWHM (~35 meV) were obtained at a growth temperature of 820°C, indicating its high crystallinity. Under this optimal growth temperature, we investigated the size and morphology of WS_2 crystals by adjusting the concentration of Na_2WO_4 solution and the sulfur supply rate. As a result, we succeeded in growing extremely large WS_2 crystals up to ~1100 µm (Figure 1). The systematic experiments to obtain the activation energy of growth and the calculations to estimate the surface diffusion energy of sulfur atoms on the growth substrate revealed that the growth mechanism is governed by the surface diffusion-limited process of sulfur atoms in the confined space. We found the fractally grown WS_2 crystals, which are also evidence for the surface diffusion-limited growth regime of WS_2. We fabricated the n-type field-effect transistors (FETs) with the full monolayer WS_2 grown under optimal conditions, exhibiting high on-off ratio ($\sim 5\times10^8$) and field-effect mobility ($\sim 7\ cm^2/Vs$). The wavelength-resolved response shows the specific three peaks corresponding to the photon absorption by the interband transition process. These results proved the intrinsic photoresponse realized by the clean interface of the WS_2-FET.

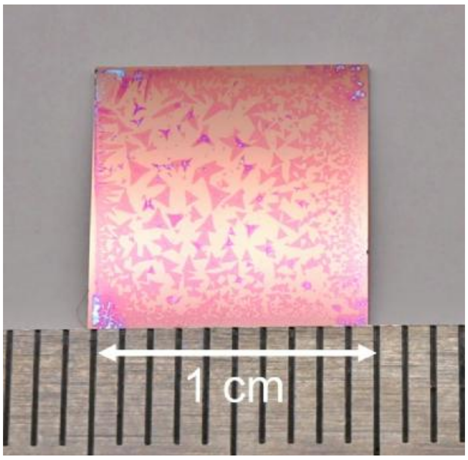

Figure 1: Photograph of the millimeter size WS2 crystals.

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P158

SURFACTANT DISPERSION OF BORON-NITRIDE NANOTUBES FOR BUILDING ONE-DIMENSIONAL VAN DER WAALS HETEROSTRUCTURES

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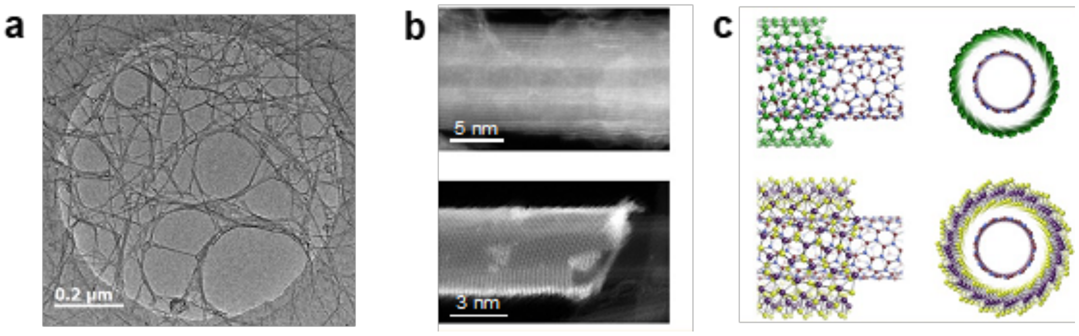
Transition metal dichalcogenide nanotubes (MX_2NTs) are one-dimensional (1D) materials that exhibit some intriguing phenomena such as exciton-polaritons and bulk photovoltaic effect[1]. Understanding the physical origin of these phenomena requires the isolation of well-defined single walls from typical multi-walled MX_2NTs. The recently developed coaxial growth of 1D van der Waals heterostructures yields single-walled (SW) MoS_2NTs around carbon nanotubes (CNTs)[2]. However, the intrinsic electronic properties of individual MoS_2NTs remain to be elucidated due to the significant interaction between carbon and MoS_2 walls[3]. In contrast to semiconducting or metallic CNTs, insulating boron-nitride nanotubes (BNNTs) can be recognized as an ideal template for the optical characterization of MX_2NTs, while their application as templates has been severely hampered by their poor dispersibility, which inevitably leads to the formation of thick bundles. Herein, we demonstrate the surfactant-assisted preparation of well-dispersed BNNT templates for the synthesis of 1D vdW heterostructures[4].The surfactant-assisted dispersion of BNNT bundles allows for the isolation of clean, crystalline BNNTs with diameters of 2~7nm. Transmission electron microscopy revealed that double-walled BNNTs are enriched by the chemical peeling of their sidewalls through the sonication process. We further demonstrate that the dispersed BNNTs can serve as templates for the construction of 1D vdW heterostructures. The BNNT-templated chemical vapor deposition can be applied for the enwrapping of carbon and MoS_2NTs. The isolation of single-walled MoS_2NTs allowed us to determine their chirality distributions[5]. The present methodology will accelerate the growing efforts to elucidate the electronic properties and potential applications of MX_2NTs.



(a)TEM image of BNNT network.(b)HAADF-STEM images and (c)atomic structures of CNTs and MoS2NTs coaxially grown on an individual BNNT.

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P159

MACHINE LEARNING METHODS FOR AEROSOL SYNTHESIS OF SINGLE-WALLED CARBON NANOTUBES

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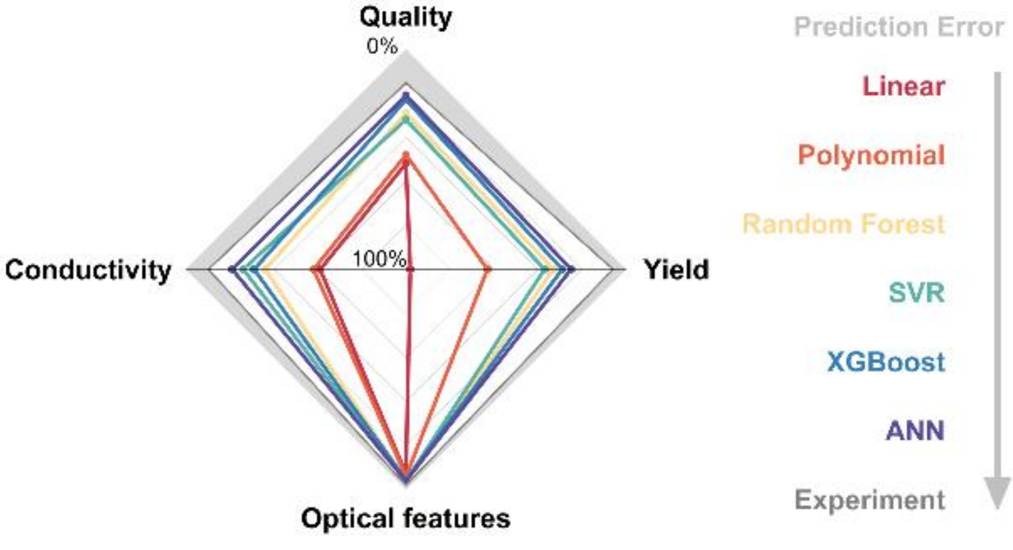
This work is devoted to the strategy towards the optimal development of multiparametric process of single-walled carbon nanotube (SWCNT) synthesis. Here we discuss the implementation of machine learning techniques, features of the optimal dataset size and density for aerosol chemical vapor deposition method with a complex carbon source [1]. We employ the dataset of 369 points, comprising synthesis parameters (catalyst amount, temperature, feed of carbon sources) and corresponding carbon nanotube characteristics (yield, quality, structure, optoelectrical figure of merit). Assessing the performance of six machine learning methods on the dataset, we demonstrate Artificial Neural Network to be the most suitable approach to predict the outcome of synthesis processes. We show that even a dataset of 250 points with the inhomogeneous distribution of input parameters is enough to reach an acceptable performance of the Artificial Neural Network, wherein the error is most likely to arise from experimental inaccuracy and hidden uncontrolled variables. We believe our work will contribute to the selection of an appropriate regression algorithm for the controlled carbon nanotube synthesis and further development of an autonomous synthesis system for an “on-demand” SWCNT production. This work was supported by RSF grant 20-73-10256.



Prediction error for all the methods used (as well as the experimental error) with respect to four output features of carbon.

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P160

SYNTHESIS AND CHARACTERIZATION OF GRAPHENE EPISULFIDES

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Li-S batteries face multiple obstacles, such as the weak chemical stability due to the polysulfide shuttle and subsequent irreversible loss of capacity and lifespan, which prevent them from being commercialized. Carbon nanostructures are investigated to solve these issues and stabilize the cathode via two methods chemical adsorption and physical confinement of sulfur with variable results of confinement and battery performance. The formation of covalent bonds between carbon and sulfur is a third approach and rarely applied to graphene [1].This work presents the synthesis and characterization of new compounds called graphene episulfides (GS). The GS compound is synthesized via gas phase reaction in moderate conditions of temperature by a catalyst and solvent free protocol. The reaction products are characterized using Raman and infrared spectroscopies, XPS, and DFT calculations. The results suggests that the vibrational signature of GS is consistent with the episulfide group at the surface of graphene.

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P161

SYNTHESIS OF JANUS TRANSITION METAL DICHALCOGENIDE NANOTUBES

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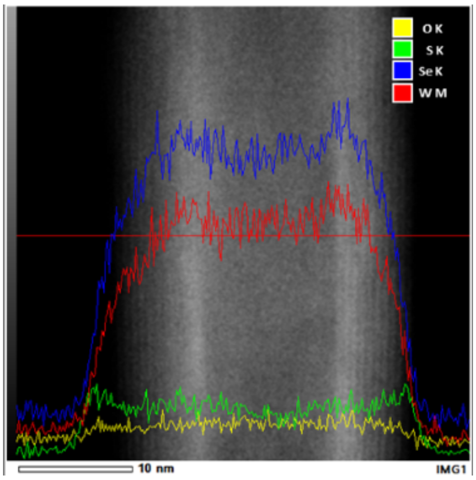
Transition metal dichalcogenide nanotubes (TMDC-NTs) are cylindrical nanotubes with rolled TMDC sheets. Because of their 1-dimensional and chiral structures, various unique properties such as bulk photo-voltaic effect and un-conventional super conductivity, have been observed. Violation of inversion symmetry is a key to generate these phenomena, and lowering the symmetry in the TMDC-NTs will enhance such unconventional properties. Here we report a method to produce Janus TMDC-NTs which have lower symmetry than conventional TMDC-NTs. Janus TMDC monolayer, which consist of different chalcogens on the front and back, was reported in 2017 and several interesting physical properties have been reported by the violation of the mirror symmetry[1]. From the discovery, lots of synthesis of Janus TMDCs were reported but none with the nanotube structures. Based on the reported approach, we made Janus TMDC-NTs. As the TMDC-NT templates, we used WSe2 nanotubes [2], assuming that replacing heavy atoms with light atoms would require less energy. Synthesis of WSe2 nanotubes were conducted by selenization of WOx nanowire precursors on quartz substrates and Mo TEM grids. For selenization, WOx NWs were placed in a quartz tube and reacted with Se vapor at 650-700°C for 1 h under Ar/H2 gas flow. We confirmed the success of synthesis of WSe2 NTs through TEM and Raman measurements. For Janus nanotube formation, the surface Se was first replaced by H through hydrogen plasma processes to perform sulfidation at low temperatures. Sulfurization was then performed under vacuum. The obtained Janus NTs were first evaluated using Raman spectra. The Raman spectra showed two peaks: a large WSe2 peak and a small peak of WSSe which is reported in the previous study[3]. This indicates that WSe2 layers were maintained and some of them changed to WSSe. The scanning TEM(STEM) and Energy Dispersive X-ray Spectroscopy (EDS) are shown in Fig. We observed the increase of the signals from S at the outermost layer of the NT indicating that multilayer Janus NTs have been successfully synthesized.



STEM image and EDS

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P162

THE ORIGIN OF AMPHIPATHIC NATURE OF SHORT AND THIN PRISTINE CARBON NANOTUBES

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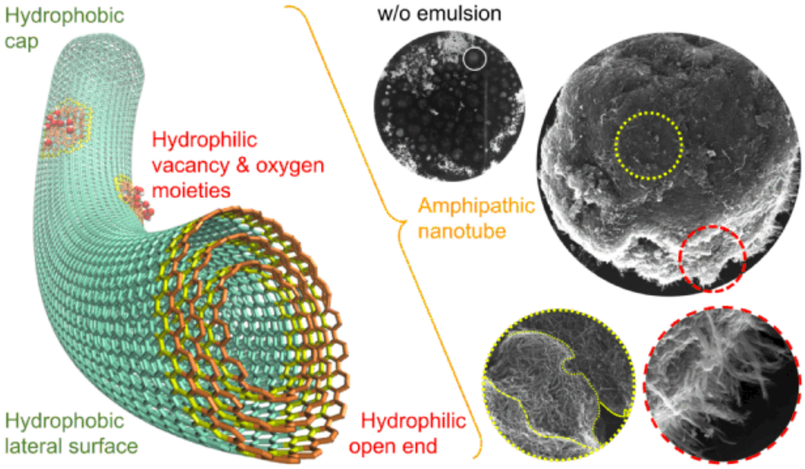
Short and thin pristine carbon nanotubes (CNTs) emerge as 1D emulsion stabilizers capable of replacing aquatoxic low-molecular surfactants [1]. However, inconsistencies in understanding of water–solid interfaces for realistic CNTs hamper their individualization-driven functionalities, processability in benign media, and compatibility with a broad scale of matrices. Pristine CNT processing based on water and inexpensive *n*-alkanes within a low-energy regime would constitute an important step toward greener technologies. Therefore, structural CNT components are quantitatively assessed, placing various CNTs on the scale from hydrophobicity to hydrophilicity. This structural interweave can lead to amphipathicity enabling the formation of water-in-oil emulsions. Combining experiments with theoretical studies, CNTs and CNT emulsions are comprehensively characterized establishing descriptors of the emulsifying behavior of pristine and purified CNTs. They emerge as having hydrophilic open-ends, a small number of oxygen–functionalized/vacancy surface areas, and hydrophobic sidewalls and full caps (**Fig. 1**). The interplay of these regions, like in 2D graphene [2], allows short and thin CNTs to be utilized as fully recyclable 1D surfactants stabilizing water/oil emulsions which, as demonstrated, can be applied as paints for flexible conductive coatings. It is also shown how the amphipathic strength depends on CNT size, the pristine-to-oxidized/vacancy domains, and the oil-to-water ratios.



Left: diagram explaining the amphipathic and hydrophobic natures of open-end and capped CNTs. Hydrophilic edges of CNT are marked in orange, while hydrophobic basal plane and caps in turquoise and dark green; Right: optical imaging and SEM micrographs of w/o emulsion droplets revealing: (1) a dense coverage of isotropically arranged, and (2) perpendicularly protruding, aligned nanotubes.

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THE SYNERGETIC RELATIONSHIP BETWEEN THE LENGTH AND ORIENTATION OF CARBON NANOTUBES IN DIRECT SPINNING OF HIGH-STRENGTH CARBON NANOTUBE FIBERS

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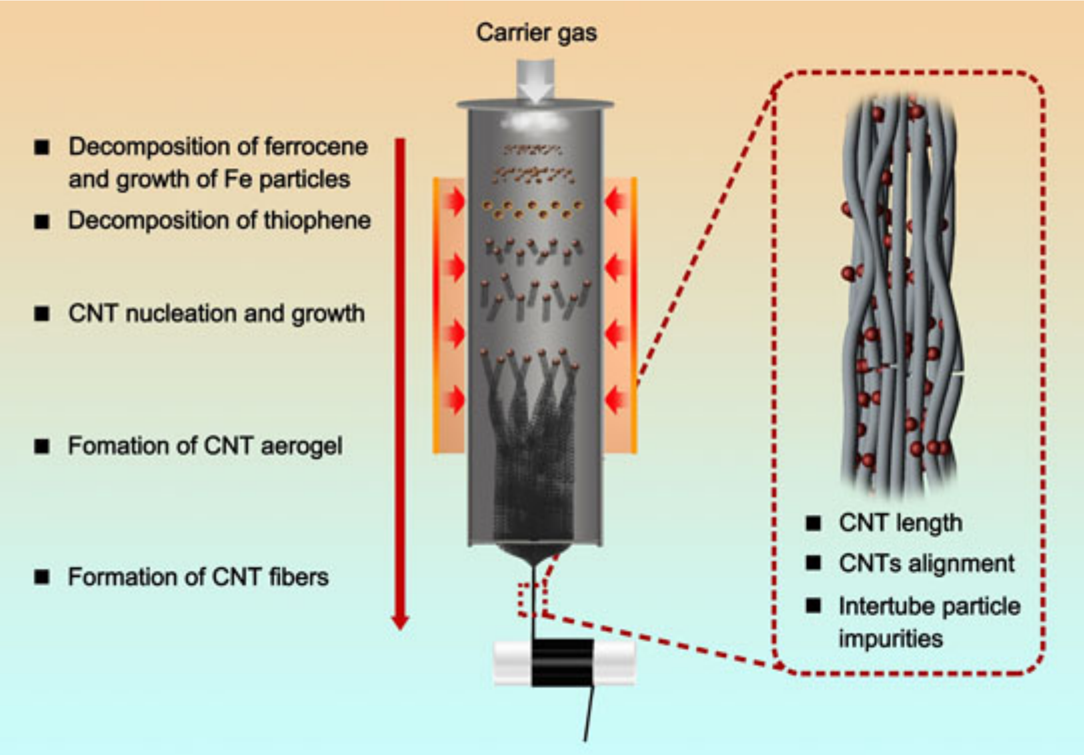
Carbon nanotube (CNT) fibers have already been considered as one of the most promising candidates for the next generation high-performance fiber materials. Floating catalytic chemical vapor deposition (FCCVD) is an attractive method for synthesizing high-strength CNT fibers. During the process of CNT fiber synthesis, the assembly structure, such as the CNT orientation, CNT length, and the inter-tube particle impurity inside the CNT fibers, are the key factors to determine the mechanical properties of CNT fibers. However, the regulation mechanism of the assembly structure during the process of CNT fiber synthesis is still unclear. In this study, in order to obtain high-strength CNT fibers, we demonstrated the synergistic relationship between the orientation and length of CNT inside the CNT fibers during the FCCVD growth process by adjusting the winding rate and the length of the high-temperature reaction zone. It also revealed that the particle impurities inside the fibers could greatly reduce mechanical strength of CNT fibers. By optimizing the assembly structure of CNT fibers, the stable and continuous synthesis was realized, with the specific tensile strength of 3.1 N/tex without any post-treatment process.



Schematic diagram of CNT fiber synthesis. Schematic diagram of continuous synthesis of CNT fibers by FCCVD. The synthesis process of CNT fibers includes the decomposition of ferrocene, the decomposition of thiophene, the nucleation and growth of CNTs, the formation of CNT aerogel and the formation of CNT fibers. The schematic diagram in the dashed frame shows the microscopic morphology of the formed CNT fibers, in which the red particles represent inter-tube particle impurities.

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THEORETICAL PREDICTION OF THERMOELECTRIC PERFORMANCE OF IMPURITY-DOPED CARBON NANOTUBES

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Carbon nanotubes (CNTs) are attractive materials because of their flexibility and high electrical conductivity. Recently, it has been reported that CNTs exhibit high thermoelectric power factor (*PF*), and the research on their application to thermoelectric devices has been active [1]. The development of CNT-based thermoelectric devices requires both p-type and n-type semiconducting CNTs. In this study, we focus on nitrogen-doped (N-doped) CNTs, which are typical n-type CNTs, and investigate their thermoelectric properties using the Kubo-Luttinger formula combined with thermal Green's function technique [2-5]. We show the dependence of electrical conductivity σ, Seebeck coefficient (S), and *PF* on N concentration. As the N concentration decreases, the system transitions from the ionization region to the intrinsic region through the exhaustion region. S increases from the ionization region to the exhaust region because the chemical potential is away from the band edge. In contrast, S decreases in the intrinsic region where hole excitation increases rapidly and, consequently, *PF* ($=\sigma S^2$) also decreases. From the above, it was found that there is an optimal N concentration that maximizes *PF* at each temperature. This optimization is strongly dependent on the band gap of the CNTs, and thus we scaled the thermoelectric parameters by the band gap, to predict the optimal thermoelectric properties for CNTs with various band gaps, i.e., various diameters. In addition, we reveal that the maximum *PF* increases exponentially as the CNT diameter decreases. This is because the thermal excitation from the valence band to the conduction band is suppressed for small-diameter CNTs.

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P165

THERMAL AND ELECTRICAL CONDUCTIVITY THROUGH ULTRA-THIN FILMS MADE FROM DRY-TRANSFERRED TRANSITION METAL DICHALCOGENIDE

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Energy harvesting techniques have recently attracted attention due to shortages and increased prices in the oil, gas, and electricity markets. Thermoelectric conversion under 100 °C is worthwhile because the heat waste is not recycled. Artificially stacked transition metal dichalcogenide (MX_2) films show ultra-low thermal conductance along out-of-plane directions originating from van der Waals interfaces and their mismatches,[1-3] which is promising for thermoelectric candidates. However, out-of-plane heat and electrical conductivity through MX_2 films in thermoelectric module configuration (*i.e.,* sandwiched by metal electrodes) are not well investigated. Our developed time-domain thermoreflectance method, in which Au is used as a thermal transducer (Au-TDTR), has the potential to measure both out-of-plane heat and electrical conductivity.[4] Au-TDTR is one of the pump-probe techniques. A pump laser pulse generates heat flux by irradiating Au, and then a probe laser pulse measures Au reflectance, which reflects thermal decay until the next pump irradiation. Additionally, Au is an appropriate electrode due to its stability. Here, we attempt to investigate heat and electrical conductivity through dry-transferred MX_2 films by Au-TDTR. Mo (an adhesion layer of few nm) and Au (100 nm) were deposited onto the quartz substrate by DC magnetron sputtering. Large MX_2 (MoS_2 and WS_2) monolayers on Si/SiO_2 were purchased by 2D semiconductor. Polymethyl methacrylate (PMMA) was spin-coated on top of the MX_2 monolayer, and the resulting film was peeled off the Si/SiO_2 substrate using thermal release tape (TRT). The MX_2/PMMA/TRT was mounted on Au, and then heating and acetone removed the TRT and PMMA films, respectively. Repeating these procedures three times resulted in homotrilayer (MoS_2 only) or heterotrilayer (MoS_2/WS_2/MoS_2) films. Finally, the top electrode (Au, ca. 100 nm) was deposited onto the trilayer film by thermal evaporation. Therefore, thermal and electrical conductivity were evaluated by the Au-TDTR and sourcemeter, respectively. The thermal conductance of the homotrilayer and heterotrilayer are found to be 36 $MWm^{-2}K^{-1}$ and 143 $MWm^{-2}K^{-1}$, respectively. The former value is plausible, but both thermal conductance values are relatively high compared with a previous study (ca. 17 $MWm^{-2}K^{-1}$).[1] Furthermore, both electrical resistance and Au-Au contact are almost the same. These phenomena suggest that the thermally evaporated Au penetrates the trilayer film through some cracks. As the experimental methodology was appropriate, we adapted the damage-free Au transfer process and will discuss the results in the presentation. This study is supported from KAKENHI (No. 22H05469) and the Precise Measurement Technology Promotion Foundation (PMTP-F).

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P166

THERMAL RADIATION FROM AN ELECTRICALLY MODULATED ALIGNED CARBON NANOTUBE FILM

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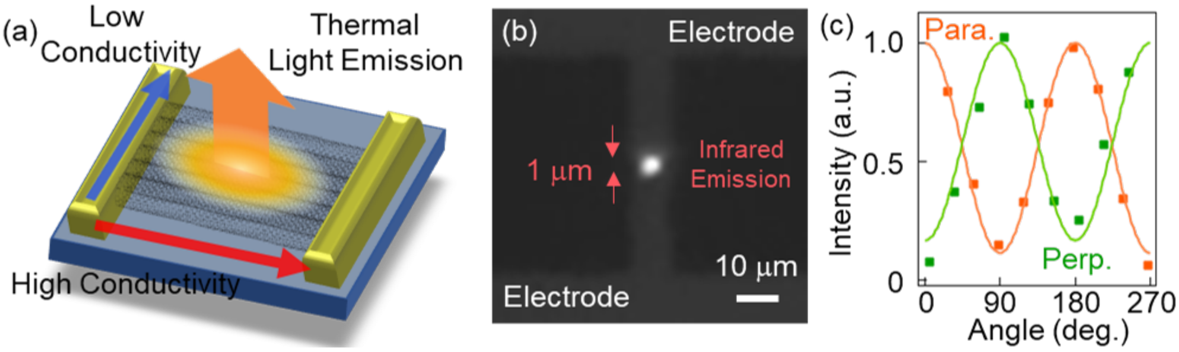
A compact on-chip source of broadband light is a promising tool for various optical applications. A thermal light source based on carbon nanomaterials such as carbon nanotubes (CNTs) and graphenes is a potential candidate for the compact light source because of its easy integration process on silicon chips [1, 2]. In particular, aligned CNT films can produce polarized and broadband light due to CNTs' one-dimensional structure [3]. However, anisotropic effect of transient thermal emission from an aligned CNT film has not been observed. Here, we report on our observation of anisotropic time-dependence of thermal radiation from an electrically modulated aligned CNT film (Fig. 1a). We fabricated a thermal light emitter with a lateral size of 1 μm^2 using an aligned CNT film (Fig. 1b), which was prepared with the controlled vacuum filtration method [4]. Thermal radiation emitted from the device was polarized along the CNT alignment direction regardless of the direction of the applied voltage (Fig. 1c). Through time-resolved measurements, we found that the response speed of thermal emission depends on the CNT alignment direction due to the film's anisotropic electrical and thermal conductivities. This work was supported by A-STEP from JST and KAKENHI from JSPS. This work was technically supported by KISTEC, Spintronics Research Network of Japan, the Core-to-Core program from JSPS, and NIMS Nanofabrication Platform. S.M. and Y.S. acknowledge support from JST SPRING. J.K. acknowledges support from the U.S. National Science Foundation (through Grant PIRE-2230727) and the Robert A. Welch Foundation (through Grant No. C-1509).



A thermal emitter based on an aligned CNT film. Fig. 1 (a) A schematic image of thermal radiation from an aligned CNT film and anisotropic characteristics of the film. (b) An infrared thermal radiation image of the device (driving voltage: 4.2 V). (c) Polarization dependence of emitted light, with a voltage applied parallel and perpendicular to the CNT alignment direction (0 degree: driven voltage direction).

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THERMOELECTRIC PROPERTIES OF A ALIGNED SINGLE-WALLED CARBON NANOTUBES THIN FILM

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Single-walled carbon nanotube (SWCNT) is a promising candidate for thermoelectric material because of its one-dimensional properties, chemical stability, and flexibility.[1] Previously, we have investigated the thermoelectric properties of SWCNTs with different electronic structures and morphology.[2] The alignment of SWCNTs can enhance the electrical conductivity (σ) without decreasing the Seebeck coefficient (S), that is, thermoelectric figure-of-merit (ZT) improves. ZT is given as $\sigma S^2 T/\kappa$, where T and κ are the absolute temperature and thermal conductivity, respectively. ZT needs to be about 0.5 at room temperature for practical use. However, for thin-film systems, the understanding of the relationships between σ, S, and κ has still been limited. In this study, we employed the aligned SWCNT film to simultaneously evaluate σ, S (perpendicular to the tube direction), and κ (thickness direction) in the same device. Noted that perpendicular to the tube direction is almost same as the thickness direction in the aligned SWCNT film thus we can evaluate the ZT. Semiconducting SWCNTs were separated by density gradient ultracentrifugation and then the aqueous dispersion was filtered with a grooved membrane at reduced pressure.[3] Subsequently, an adhesion tape peeled off the random layer and then only the alignment layer was transferred to a quartz substrate with designed gold electrodes. σ and S perpendicular to the tube direction with different Fermi levels were evaluated by a thermocouple and an electrolyte transistor.[2] Furthermore, out-of-plane κ with different Fermi levels was evaluated by our developed time-domain thermoreflectance where Au is a thermal transducer.[4] When the Fermi level of the aligned SWCNT thin film is modulated by electrolyte gating, we observed peaks in σS^2 (power factor) as a function of gate voltage, reflecting van Hove singularities. As out-of-plane κ is independent of the gate voltage, the behavior of ZT corresponds to that of σS^2. The maximum ZT at 300K is found to be about 0.044. κ of the quartz substrate is higher than that of the film perpendicular to the tube direction, suggesting the overestimated temperature difference in Seebeck measurement. Therefore, improvement in ZT could be expected. We improve the experimental condition and will discuss the detail in the presentation.

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P168

TIME-RESOLVED SPECTROSCOPY OF DOPED SINGLE-WALL CARBON NANOTUBES

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The electronic and optical properties of semiconductors are strongly influenced by doping [1,2]. Therefore, understanding the dynamics of excitons and charged excitons (trions) is crucial for improving our knowledge of the doping process. Prior optical studies of semiconducting single-wall carbon nanotubes (s-SWNTs) have shown that the character of exciton transport and non-radiative decay at room temperature is diffusive [3,4]. In contrast, non-radiative decay of the trion photobleach is indicative of unimolecular, i.e. non diffusive trion dynamics, providing evidence of localized and immobile charged excitons [4,5,6]. The coupling between excitons and trions can be further investigated by studying their temperature dependence but no such data have been reported to date. The initial data reported here are aimed at clarifying photoinduced dynamics and the dependence of experimentally measured exciton sizes on the doping level in thin films of polymer-wrapped (6,5) s-SWNTs.

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TOWARDS UNDERSTANDING THE OPTICAL PROPERTIES OF ZIG-ZAG CHIRALITY SORTED SINGLE-WALLED CARBON NANOTUBES

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Understanding the optical properties of single-walled carbon nanotubes (SWCNTs) is of major interest to bring their applicability in optoelectronics, photonic and bioimaging to reality. From the theoretical point of view, several predictions have shown that the physical properties of SWCNTs depend on the geometrical configuration of the carbon atoms that construct their walls. This implies a definition for the chiral vector, chiral angle and consequently the chiral indexes (n,m). However, from the experimental point of view, observing those predicted properties imposes challenges that still embrace the production of the nanotube-material. For each specific chirality, defined and unique optical transitions are expected. These can be nicely identified with methods like optical absorption and Raman spectroscopy, and this has been done even in chiratily mixed samples given that a reasonable debundling is achieved. Nevertheless, every foreign chirality in a batch represents an impurity. For that reason, it is extremely important to produce chirality sorted samples. Since many years now, various methods have been developed. Among these, gel chromatography has been very successful to produce high yield and high purity samples at large scale quantities. This method is based on the selective adsorption of surfactants with different hydrophobicity on the nanotube´s surface at given adsorption sites, while leaving others free to stick in the gel for further gradient elution. Therefore, a careful load of surfactants and a controlled flow of the nanotubes through the gel are key parameters to explore how to increase the purity on single chirality sorting experiments. chirality species are otherwise obtained after second purification processes in which most of them use surfactants to separate nanotubes by electronic character, diameter or chirality. In this work, we show a full optical characterization of single-chirality sorted SWCNTs processed by a modified gel chromatography process where the temperature dependence plays a crucial role. The preferential adsorption mechanism of the surfactants with different hydrophobicities onto the nanotubes' surface is shown. We focus on how their diameter and chiralitycan be correlated with a controlled-flow that involves a careful monitoring of the temperature.. The (10,0) zig-zag chiralitiy will be used as an example of how a sigle chirality sample can be obtained in a 2 step process. Additionally, first results of high purity (11,0) chirality sorting is shown.

P170

CELL UPTAKE STUDIES OF GRAPHENE QUANTUM DOTS

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Graphene quantum dots (GQDs) have emerged as a forerunner of carbon nanotechnology due to their multifunctional delivery and imaging platform as they present fluorescence in the visible and near-infrared, high biocompatibility, and water solubility. These abilities put GQDs forward as a compelling cancer therapeutics drug delivery platform. Understanding the cell internalization routes of GQDs is crucial while delivering drugs in different types of cell lines. Herein, we performed cell uptake studies on various types of top-down and bottom-up synthesized GQDs by the comparative study of their preferred endocytosis paths on healthy cell line HEK-293 and cancer cell line HeLa. The concentration and cell viability of GQDs were determined by MTT assays. Endocytosis paths were investigated through confocal fluorescence microscopy on cells co-incubated for 1 to 24 hours. The potential for GQD interactions with the cell membrane is further examined via zeta (ζ) potential measurements. Our findings provide insights into the internalization mechanisms of the GQDs into cell membranes of healthy and cancer cells. The optimization of these mechanisms can serve for the enhancement of a variety of novel GQD applications in biomedicine including therapeutic delivery disease detection through sensing as well as diagnostic imaging.

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TRANSPARENT TERAHERTZ–INFRARED SENSORS BASED ON ULTRA-THIN METAL-SEMICONDUCTOR CARBON NANOTUBE HYBRID FILMS

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Photo-thermoelectric image sensors with carbon nanotube (CNT) films have attracted much attention. Specifically, it is capable of broadband sensing of visible and infrared light, and even terahertz waves, and has realized non-destructive inspection of multilayered composite structures. Furthermore, due to the mechanical softness of CNT film, it is specialized for omni-directional imaging without any blind spots. Following the use of CNT film as non-destructive imaging techniques, it is expected that CNT film will be developed into smart inspection devices cooperating with human senses. Toward image sensor application, it is essential to have transparent structures that does not interfere with human vision. However, not enough research has been conducted to realize highly transparent CNT film-based photo-thermoelectric image sensors. Here, we developed highly transparent terahertz–infrared sensors using ultra-thin metallic and semiconducting hybrid CNT films. In contrast to the conventional device structure [1], the metallic film absorbs light and generates heat, and the semiconducting film performs the subsequent thermoelectric conversion.

Fig. 1a shows the device structure. A polyurethane film with a 25-µm-thickness is used as the transparent stretchable substrate. PEDOT:PSS is used as the transparent stretchable electrode. The transparent THz–IR absorbent film is made of metallic-CNT. Semiconducting-CNT is used for the transparent thermoelectric conversion film.

Fig. 1b shows the optical properties of the transparent absorbent film and the transparent thermoelectric film. Both are highly transparent in the visible light band. Wheras, in the IR–THz bands, changes in the optical properties of both are observed. Transparent thermoelectric conversion films (semiconducting-CNTs) still show high transmittance. Transparent light-absorbing films (metallic-CNTs) show an absorption of more than 80 % in the terahertz band and 50-60 % in the infrared band. Therefore, the device structure allows the heat generated by THz-IR absorption to be concentrated locally in the metal-CNT. This light-absorbing film is located at the edge of the thermoelectric film with the Seebeck coefficient of more than 200 µV/K. This allows generating the photo-thermoelectric effect. Other basic performance and sensing and imaging applications will be presented at the conference.

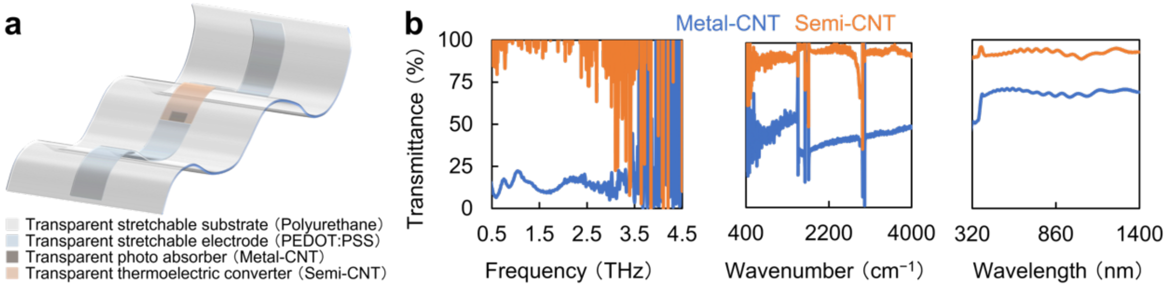

Figure 1. a, Conceptual schematic of the presenting device. b, Comparisons in broad transmittance of the device materials.

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ULTRA-HIGH CHARGE CARRIER DENSITY IN MONOLAYER GRAPHENE BY INTEGRATED FLIP-CHIP ALKALI DOPING

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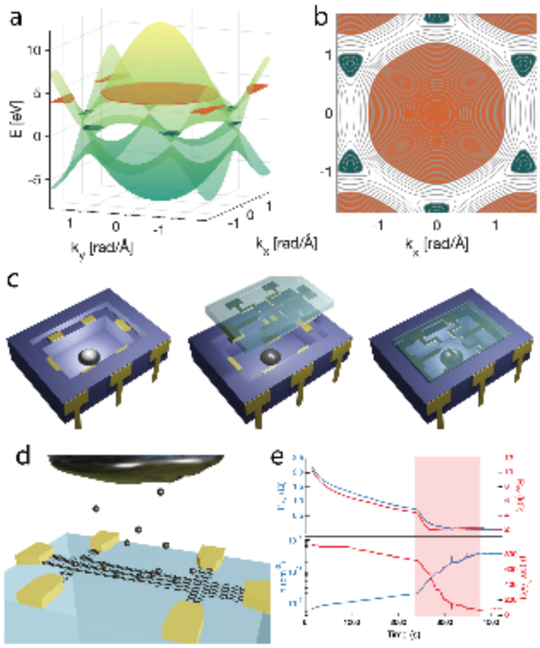
Adsorbates enable the modification of the electronic properties of graphene, with alkali metal adatoms being notable as efficient dopants due to their high electronegativity. Studies of the lithium/graphene system have revealed evidence of superconductivity[1,2], while lithium diffusion is found to be strongly enhanced by intercalation in a bilayer[3]. Lithium, calcium, potassium and cesium adatoms have been used to investigate the van Hove singularity of graphene, including many-body interactions, the Lifshitz transition, and flat band formation[4-7], as observed by Raman spectroscopy and photoemission. The Lifshitz transition in graphene, wherein the Fermi surface abruptly changes from electron-like to hole-like, has yet to be studied by charge transport. Ionic gating, typically used for high-density transport measurements, limits carrier density to $<1\times10^{14}\mathrm{cm}^{-2}$ in monolayer graphene[8]. We present a flip-chip method for alkali doping, enabling charge transport measurements of cesium/graphene at carrier densities as high as $4\times10^{14}\mathrm{cm}^{-2}$, corresponding to ~85% of the electron density required to reach the Lifshitz transition. A monolayer graphene Hall-bar on a quartz substrate is bonded to a ceramic chip carrier in a nitrogen environment(Fig.a). A droplet of cesium elevates the cesium vapour pressure inside the hermetically-sealed cavity(Fig.b). Real-time ac Hall measurements enable simultaneous measurement of longitudinal and transverse resistivity, and thus charge carrier density and mobility, during doping(Fig.c) The Fermi surfaces corresponding to the observed doping(Fig.d) are estimated by a third-nearest-neighbour tight-binding model[9], illustrating proximity to the Lifshitz transition. Magnetoresistance and weak-localization(Fig.e) of high-density samples were studied at high magnetic field(7T) and low temperature(1.3K), with electron densities up to $4\times10^{14}\mathrm{cm}^{-2}$ confirmed by high-field Hall resistance. Raman spectroscopy provides independent confirmation of high doping. This method may be refined to enable the study of the transport coefficients of graphene at the Lifshitz transition, other 2D materials and van der Waals heterostructures at high carrier density.



a)Flip-chip assembly. b)Cesium adsorption onto graphene. c)Real-time ac Hall results during doping. d)The Fermi surfaces corresponding to the observed doping levels. e)Magnetoresistance and weak-localization of high-density samples.

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VERTICALLY ALIGNED CARBON NANOTUBES GROWN ON FIBROUS CARBONS - TOWARDS NOVEL APPLICATIONS

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Different scientific groups have evidenced the need to pre-deposit nanometric diffusion barrier layers (DBL), as the most promising and commercially sustainable way, to successful grow VACNTs (vertically aligned carbon nanotubes) on carbonaceous materials. Aside of well-studied insulating DBL [1], anticipated conductive DBL show higher activity with the catalyst layer (required for the growth of VACNTs), such as interdiffusion and alloy formation, which further affects the microstructure of the DBL and dewetting of the catalyst layer into dense network of nanoparticles [2]. Thus, the growth of VACNTs have been reported on different conductive DBL materials, such as aluminium [3], molybdenum aluminide [4], tantalum nitride [5], titanium aluminide [6] or titanium nitride [7]. Imperatively, the introduction of a conductive DBL is shown to support the growth of VACNTs and boost the conductive/mechanical properties of the overall composite. Nowadays, different techniques are studied for the deposition of DBL, such as, chemical vapour deposition (CVD), physical vapour deposition (PVD), or atomic layer deposition (ALD) [8].

The upper-cited DBL have already been used on various flat or 3-D substrates, and potentially can be re-/-investigated for the growth of VACNTs on carbon fibres (CF) [9]. Within the scope of development and application of high-performance all-carbon materials, one issue is to distinguish suitable solutions to achieve advanced 3-D carbon composites with enhanced conductive and mechanical properties for energy storage application.

For the purpose, we have examined the competence of CVD/PVD ways to deposit conductive DBL for the growth of tuneable VACNTs on CF or flat carbone substrates via aerosol-assisted CVD (AACVD) [1], at low temperatures (600 °C). As one of the used solutions, PVD was carried out for the deposition of bi-metal conductive DBL on CF, followed by AACVD for the growth of VACNTs. The resultant composite morphologies (VACNT length, alignment) have been examined by scanning or transmission electron microscopy (SEM/TEM) with the aim of understanding the effect of the performed modification on the final hybrid material. Finally, we highlight the importance of the initial materials/precursors, DBL deposition technique and VACNTs' CVD growth technique, all playing extremely important role for producing VACNTs-CF composite.

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VERTICALLY ALIGNED CARBON NANOTUBES ON ALUMINUM FOILS: ONE-STEP SYNTHESIS FROM BIO-SOURCED PRECURSORS AND ELECTROCHEMICAL CHARACTERIZATION

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In order to meet the growing demand for devices able to store efficiently electrical energy, supercapacitors are emerging as good candidates due to their attractive balance between their energy density and their power density. However, their performance remains to be improved, which is highly dependent on the material of the electrodes.Vertically aligned carbon nanotubes (VACNT) have been used instead of activated carbon as electrode for supercapacitors applications. Indeed, owing to their anisotropy, VACNT offer easy ionic diffusion pathway and great specific power[1]. The Aerosol Assisted Catalytic Chemical Vapor Deposition method allows the controlled one-step growth of Vertically Aligned Carbon Nanotubes (VACNT) carpets on conductive substrates[2,3]. This process has been optimized for the growth of dense VACNT on aluminium foils at low temperature (580 to 615°C) with acetylene as carbon precursor, leading to a single-step process that meets industrial requirements for the development of low cost, highly conducting and light supercapacitors electrodes[4]. In order to meet the challenges of energy transition, the industrial sector urgently needs to develop more acceptable processes from the point of view of environmental preservation and decarbonization. The aim of this work is to replace the current carbon precursor (acetylene) by bio-based carbon sources compatible with an industrial process. Our approach was to first identify the most relevant carbon sources and to develop the synthesis conditions adjusted to these carbon sources in order to achieve VACNT growth at a temperature as low as the one required on thin Al collectors. The challenge is a better control of the growth process under these conditions where the physical and chemical phenomena occuring can be modified or slowed down. Different bio-based precursors (liquid or gaseous) were selected and used alone or associated for a parametric study in order to assess the interest in term of VACNT growth. First results show that we were able to grow VACNT on thin Al collector with each carbon precursor selected. VACNT from alcohol precursors have larger diameter and less volumetric mass than acetylene VACNT but their density is similar (1011 CNT.cm-2). Moreover, VACNT height of 100µm can be reached in 80 minutes by using a combination of ethylene and butanol as carbon sources at the temperature of 640°C. Electrochemical capacitances measured for alcohol-based VACNT are in most cases lower than the ones of VANCT synthesized with acetylene. However volumetric capacitance from some samples can compete with acetylene VACNT and will be presented. With the goal of mass production of VACNTs on Al electrodes for supercapacitors, these encouraging results lead us to scale-up the process on larger Al surfaces from lab-scale up to an industrial production line.

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VIOLET PHOSPHORUS TRANSMISSION AND PHOTOCONDUCTANCE SPECTROSCOPY

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Phosphorus and its extensive catalog of allotropes have been a fascinating source of various material properties for hundreds of years [1]. Black phosphorus (bP), a narrow bandgap semiconductor known for its buckled honeycomb layers with interlayer van der Waals bonding, has been the subject of intense study in the last decade. Meanwhile, violet phosphorus (vP) has only seen recent interest following advances in crystalline vP synthesis and exfoliation [2,3]. The crystal structure of vP is now well known, consisting of orthogonally oriented layers of phosphorus chains with P2[P8]P2[P9] repeating units [4], while its electronic and optoelectronic properties are far less understood than for bP [3, 5, 6]. We report a complementary study of exfoliated vP, including optical transmission measurements and photoconductance measurements of mechanically exfoliated vP in the bulk thin-film limit. The spectral dependence of optical transmission and photoconductivity of vP leads us to identify optical transitions at van Hove singularities corresponding to energies E1 = 1.80 +/- 0.05 eV and E2 = 1.95 +/- 0.05 eV. Through a comparison with density functional theory and a transition dipole analysis, transitions at Z and A0 of the Brillouin zone are assigned to the observed photoconductivity spectral features. Exfoliated vP samples are obtained following mechanical exfoliation of chemical vapor transport synthesized crystals. The thickness is >100 nm, insufficiently thin for quantum confinement to affect the bandgap, as was shown to be the case for bP [7]. Charge carriers may however accumulate at the surface of exfoliated flakes due to band bending effects [8, 9]. This naturally leads to sensitivity of the surface conditions, and considering the tendency of bP and vP to oxidize in ambient conditions [7, 10], an inert gas environment was used to suppress oxidation and study vP's intrinsic properties. We experimentally observed that exposure of vP to an ambient environment for several minutes suppresses photoconductivity, confirming the importance of maintaining an inert environment for the study of vP's intrinsic optoelectronic properties. Exposure of vP to ambient conditions for several hours leads to the formation of blisters on the vP surface. Further investigation using energy dispersive X-ray spectroscopy (EDS) reveals this blistering to be due to oxidation.

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FISHING CARBON NANOTUBES WITH SURFACTANT MIXTURES AS NANO-BAIT

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Single-walled carbon nanotubes (SWCNTs) are among the most extensively researched materials of our times. Unfortunately, they are always obtained as polydisperse mixtures, which must be sorted to unlock their implementation potential. One of the most convenient methods of doing so is through aqueous two-phase extraction, which does not require sophisticated equipment or niche chemical compounds [1]. This contribution will display our recent breakthroughs in the differentiation of SWCNTs using this technique. Through a thorough examination of the separation process, we managed to enhance the resolution of the system considerably. Consequently, we isolated (7,5) [2] and (6,4) [3] SWCNTs in a single step. Furthermore, the application of previously unrecognized non-ionic surfactants and modeling enabled us to gain more insight into the mechanism of the ATPE [3,4].

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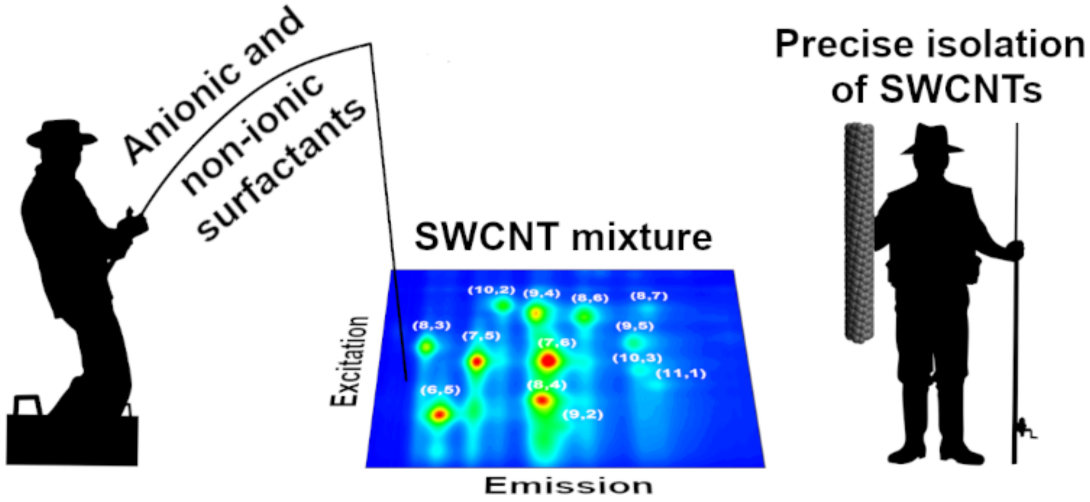

Extraction of specific SWCNTs using mixtures of anionic and non-ionic surfactants

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STRAIN-RELAXATION PROCESS FOR STRENGTH REINFORCEMENT OF CARBON NANOTUBE FIBERS

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Carbon nanotube (CNT) fibers provide a rich potential for the next-generation light-weight structural materials. Despite extensive research on the fiberization techniques of CNTs, CNT fibers exhibit far below the tensile strength of commercially- available chemical fibers (e.g., 2.3 (N/tex) for Kevlar), mainly due to the inter-tube defects originating from insufficient load transfer and stress concentration caused by local misorientation and low packing density. Here we show a way to improve the tensile strength of CNT fibers through the iteration of strain and releasing processes. In this study, aligned CNT bundles were fabricated using a laboratory-designed reactor based on floating-catalyst chemical vapor deposition [1]. Ferrocene and thiophene were used as a catalyst source and a promotor, respectively. Toluene and ethylene were used as carbon sources. The feedstock was injected to the reactor simultaneously through a spray nozzle with pure hydrogen. The resulting CNT bundles were collected as a macroscopic fiber (as-made CNT fiber). To remove remaining inter-bundle voids, as-made CNT fiber was immersed in chlorosulfonic acid (CSA) and stretched to ~270% compared to the initial length. The wet-stretched fiber was rinsed with chloroform and dried under vacuum (denoted as CSA-CNT fiber). As-made CNT fiber and CSA-CNT fiber were pulled until elongation reached to ~1% and subsequently released the strain. The strain-relaxation process was performed for 100 times. After the strain-relaxation process, the specific strength of as-made CNT fiber increases from 0.62 (N/tex) to 1.5 (N/tex) with decreasing the breaking strain. This trend is also observed for CSA-CNT fiber, reaching to a specific strength of 2.8 (N/tex) after the strain-relaxation process. This result indicates that repeating the strain-relaxation process in a quasi-elastic elongation (~1%) could gradually reduce the entanglement of CNTs and/or the inter-bundle voids, leading to the reconstruction of CNT bundles and the strength reinforcement of CNT fibers (Fig. 1).

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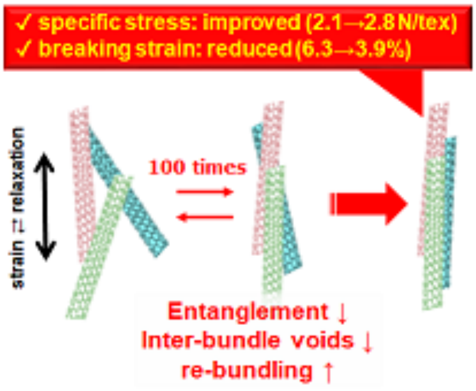

Fig. 1. The strain-relaxation process for improving the strength of CNT fibers.

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TARGETED EXTRACTION OF SPECIFIC SINGLE-WALLED CARBON NANOTUBES WITH CONJUGATED POLYMERS IN ORGANIC SOLVENTS

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Semiconducting single-walled carbon nanotubes (SWCNTs) are highly valuable in a broad spectrum of exploitation fields such as photonics, microelectronics, etc. Currently, one of the main obstacles limiting their implementation is the scarcity of chirality-defined fractions with a particular set of desired properties. To tackle this problem, the community has developed various sorting methods to provide such materials [1]. Conjugated Polymer Extraction is particularly useful, as it offers high selectivity, and the isolated SWCNTs are already suspended in volatile organic solvents, which are highly convenient for making devices. Unfortunately, the mechanism of the process is not fully understood, so, so far, only (6,5) and (7,5) SWCNTs can be isolated with truly monochiral purity. This contribution will disclose how we extract specific SWCNTs from their complex mixtures using self-made conjugated polymers and organic solvents. Thoughtful selection of separation medium and tailoring of the polymer characteristics enable the generation of suspensions highly enriched with (7,3) or (6,4) SWCNTs [2-3]. The conducted experiments highlight the importance of a number of factors, which are crucial for reaching satisfactory yield and selectivity.

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ADVANCED FABRICATION AND MULTI-PROPERTIES OF CARBON NANOTUBE- GRAPHENE OXIDE HYBRID AEROGELS

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Electromagnetic interference is considered a serious form of environmental pollution, ranging from minor disturbances to possible fatal accidents due to the malfunction of critical control system. One crucial way to prevent the electromagnetic interference is to provide shielding against the interference. Shielding devices not only reduces the electromagnetic emissions but also improves the devices' performance. But common electromagnetic shielding materials are mostly made from heavy metals due to their high electrical conductivity. To overcome the current shielding material problems, we develop successfully the alternative lightweight carbon nanotube (CNT) and graphene oxide (rGO) hybrid aerogels with excellent electromagnetic performance in various GHz bands, mechanical properties, and thermal properties. The rGO sheets have the thickness range of 10 - 15 nm. The CNTs have an outer diameter range of 8 -15 nm and the average length of 50μm.

Ultralightweight CNT-rGO aerogels are fabricated via solution mixing and freeze-drying processes. After the freeze-drying process, the uniform hybrid aerogels have the densities of 0.11 - 0.15 g/cm3 and the very high porosities of 80-90%. The aerogel with 3.1mm thickness exhibits the excellent reflection loss of below -10dB throughout the entire X-band (8-12 GHz) and reaches the maximum reflection loss of -68 dB at 9.40 GHz. The hybrid aerogels also have the low thermal conductivities of 0.041 – 0.063 W/m.K and the high thermal stability of 220°C. The aerogels also have the excellent compressive strength with their young's modulus of 1.25 – 1.46 MPa. The developed aerogels can be used for shielding coating to protect critical electronic equipment and for military stealth technologies.

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ARE OUR DFT MODELS OF ONE-DIMENSIONAL VAN DER WAALS HETEROSTRUCTURES RELIABLE? A JANUS NANOTUBE CASE STUDY

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The recent translation of van der Waals heterostructures from 2-dimensions to 1-dimensions has established a new class of materials with exciting optoelectronic properties.[1] Synthesis of complex CNT@BNNT@MoS2 multiwall heteronanotube architectures have displayed interesting properties such as ultrafast optoelectronic processes[2] and inner core nanotube dependent photoluminescence quenching.[3] In order to understand, model and predict the structure and behaviour of these new architectures, the field invariably turns to plane wave density functional theory (DFT). And while in reality 1D vdW heterostructures do not induce lattice deformation of their component tube layers, the use of periodic boundary conditions in plane wave DFT calculations can induce significant artificial strain in the material. This occurs since a single axial lattice dimension must be applied, despite individual layers having incommensurate axial lattice vectors. The fact that low-dimensional TMD materials have well-established strain-induced properties[4,5] then begs the question – are our DFT predictions of 1D vdW heterostructures reliable? In this work we consider the effects of artificial axial strain, radial strain, exchange correlation functional and dispersion approximation on the stability and properties of 1D vdW nanotubes using plane wave DFT, focusing on Janus SWCNT@MoSX (X = Se, Te) heterostructures as a case study.[6]

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BROADLY TUNABLE UNIDIRECTIONAL HYPERBOLIC METASURFACES OF ULTRATHIN PERIODICALLY ALIGNED CARBON NANOTUBES

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Self-assembled quasiperiodic finite-thickness single-wall carbon nanotube (SWCN) arrays and films have been recently shown experimentally to exhibit extraordinary optoplasmonic properties [1-3], which is why they are getting more and more attention of nanomaterials communities. Here, using the low-energy plasmon response calculation technique [4] and the many-particle Green's function formalism in the Matsubara formulation [5], we study the in-plane dynamical electromagnetic (EM) response for ultrathin (<~ a few tens of nm) plane-parallel periodic SWCN arrays and weakly inhomogeneous SWCN films in the broad spectral domain of IR to visible [6,7]. Our theory demonstrates strong EM response anisotropy, whereby the system becomes metallic in the SWCN alignment direction (even for semiconductor SWCN arrays) and dielectric in the perpendicular in-plane direction [6]. This can be controlled by the volume fraction of constituent SWCNs, the active component of the film, which can be done not only by varying the parameters of the SWCN content (CN diameter and/or intertube distance) but also by varying the thickness of the CN embedding dielectric layer. For homogeneous single-type periodic SWCN arrays and weakly inhomogeneous quasi-periodic multi-type SWCN films, the real part of the EM response function in the CN alignment direction is negative in a wide domain around quantum interband (exciton) transitions of constituent SWCNs, to form relatively broad negative refraction (NR) bands, whereby the system behaves as a unidirectional hyperbolic metasurface (MS) at higher frequencies than those (typically in the IR) the classical intraband plasma oscillations have to offer. We show that by decreasing the CN diameter it is possible to push such a unidirectional NR band to the visible range and using weakly inhomogeneous multi-type SWCN films makes it broader compared to that of a single-type SWCN array. We also show that by varying the relative weights of the constituent SWCN array components in a properly fabricated two-component SWCN film, it is possible to tune its optical absorption profile to make the film transmit or absorb light on-demand. Other, more fundamental applications we study include: (a) highly efficient unidirectional SERS (Surface Enhanced Raman Scattering) substrates for single atom/ion/molecule detection, trapping, and manipulation; (b) precision directional control of polarized spontaneous emission, absorption and scattering by atomic type emitters trapped near ultrathin finite-thickness SWCN metasurfaces; (c) near-field control of Casimir-Polder forces in close proximity to ultrathin finite-thickness SWCN films. This research is supported by the U.S. National Science Foundation under Condensed Matter Theory Program Award No. DMR-1830874 (I.V.B.).

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ENHANCED PHOTOCATALYTIC OXIDATION OF NOX OVER TIO2-CARBON NANOTUBE HYBRID COATINGS

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Nitrogen oxides (NOx), originating from combustion reactions, can have detrimental health and environmental effects resulting from high amounts of nitrogen oxide (NO) and nitrogen dioxide (NO2), the most common forms of NOx. To reduce concentrations of NOx in the atmosphere, heterogeneous photocatalysis using semiconductors has been studied as an effective method for NOx abatement. Complete oxidation of NOx results in the generation of harmless concentrations of nitrates (NO3-), whereas partial oxidation generates NO2, the most hazardous form of atmospheric NOx. Real-world humidity levels in major cities across the globe have been assessed, and our experiments have been conducted under representative conditions. The De-NOx index—a measure of photonic efficiency during NOx oxidation—has been used to quantify catalyst efficiency in completely oxidizing NOx to nitrates. Our results show substantial photocatalytic enhancement of TiO2 during NOx oxidation by coupling with multi-walled carbon nanotubes (MWCNTs). We have investigated the effects of initial concentration, humidity, and reactor headspace on De-NOx for commercial TiO2 (P25) and TiO2-MWCNT under practical conditions. To obtain further insight into the reaction mechanisms and specific role of the nanotubes in enhanced NOx abatement, a variety of characterization techniques have been used to probe the photocatalysts.

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HYDROGEL MATRICES FOR NEAR-INFRARED MONITORING OF ASCORBIC ACID RELEASE

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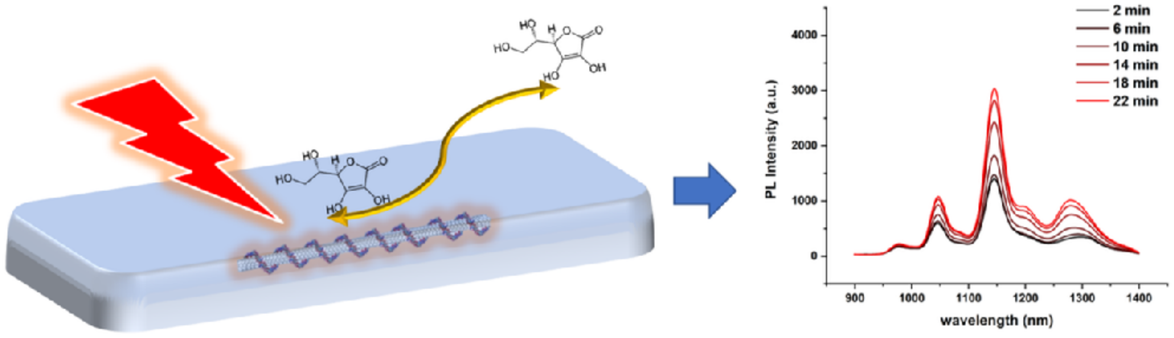
Single-walled carbon nanotubes (SWCNTs) have excellent optical properties for sensing applications. On excitation, semiconducting SWCNTs emit fluorescence that varies with the chirality and the environment of the nanotube. Because the near-infrared fluorescence emissions are minimally absorbed by biological tissue and biofluids, SWCNTs can be used for deep-tissue imaging and sensing. These applications, however, require SWCNT immobilization and encapsulation strategies that are stable and biocompatible.

Herein, we develop a hydrogel-encapsulated SWCNT sensor to study the release of ascorbic acid, a model agent for delivery applications. We examine the response of SWCNTs wrapped in (GT)$_{10}$, (GT)$_{20}$, (GT)$_{40}$, (CCG)$_{4}$, (CCG)$_{8}$ and (AT)$_{15}$ DNA sequences to ascorbic acid. The strongest response is observed for the (GT)$_{10}$ sequence. The (GT)$_{10}$-wrapped SWCNT sensors also show the greatest sensitivity to ascorbic acid concentrations over the range of 10 - 100 µM. We further compared the performance of the (GT)$_{10}$-wrapped SWCNT sensor in different hydrogels, including alginate, hyaluronic acid, and agarose matrices loaded with ascorbic acid. The agarose gels show the most promising performance, undergoing the largest intensity change on release of 100 µM ascorbic acid. Scanning electron microscopy (SEM) images of the agarose hydrogel loaded with and without the SWCNTs confirm no significant perturbation of this matrix on SWCNT encapsulation under the tested conditions. Finally, the encapsulated sensor was applied to monitor cyclic ascorbic acid loading and release. These results highlight the promising application of SWCNT hydrogels for the reversible optical monitoring of bioactive agents.



Hydrogel-encapsulated SWCNT sensors

Near-infrared fluorescence response to ascorbic acid

Construction of SWCNT-hydrogel structure

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MACHINE LEARNING MOLECULAR DYNAMICS SIMULATION OF SINGLE-WALLED CARBON NANOTUBE GROWTH

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In the past few decades, many classical molecular dynamics (MD) simulations were carried out to reveal the growth mechanism of single-walled carbon nanotubes (SWCNTs), demonstrating a series of growth processes from the nucleation to the sidewall elongation [1]. Although these studies provided insights into the primary growth mechanism of SWCNTs, the discussion of the chirality was difficult because the simulated SWCNTs had a number of defects. This difficulty in simulating defect-free growth can be attributed to the limited accuracy of the interatomic potentials.

Recently, the application of artificial neural networks to interatomic potentials has been actively studied to overcome the limitations of conventional interatomic potentials, and such interatomic potentials are called neural network potentials (NNPs).

We developed an NNP to describe the defect formation energetics of graphitic structure for more realistic MD simulations of SWCNT growth. As shown in Fig. 1, the SWCNTs grew through carbon saturation, cap formation, and side wall elongation, which are typical growth stages. During the growth, defects were frequently formed on the open edge and healed into hexagons by metal-mediated C-C bond recombination, resulting in defect-free SWCNTs with exactly six pentagons in their cap. The simulated SWCNTs' side walls had few defects, which allowed us to investigate the detailed processes of hexagon formation at zigzag and armchair sites on the open tube edge. Our realization of the defect-free growth MD simulation will give insights into the mechanism of SWCNT growth.

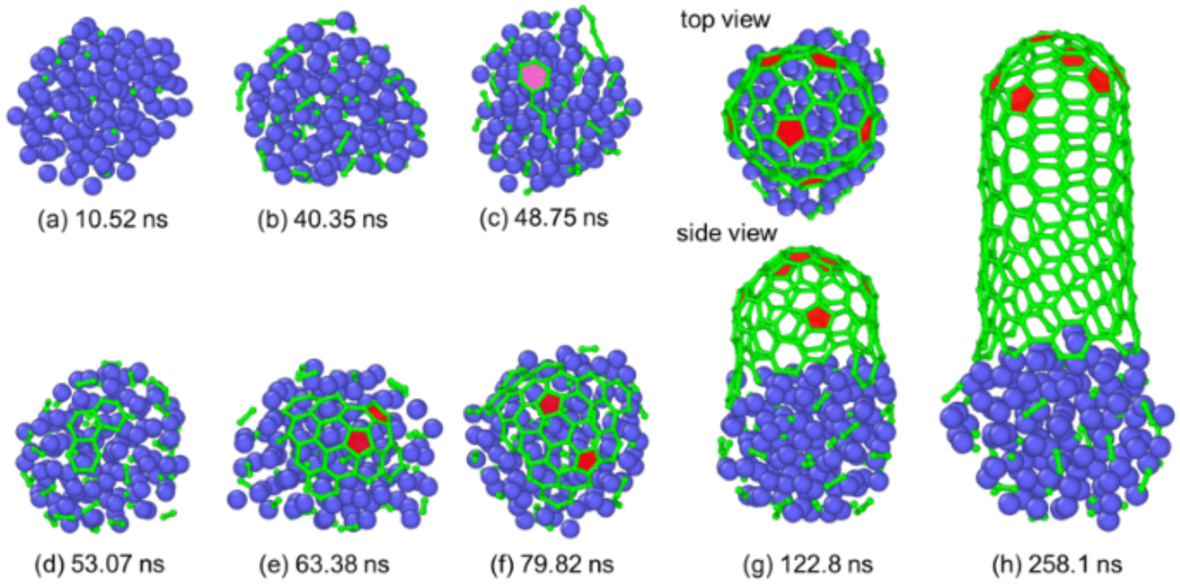

Fig. 1. (8,7) SWCNT growth on Fe120 at 1500 K. The blue and green atoms denote Fe and C, respectively. The red polygons are pentagons. The pink polygon is the first hexagon.

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NANOFUNCTIONALIZATION TOWARDS SCREENING NANOCATALYSTS FOR AGROCHEMICAL NEUTRALIZATION: EFFECTS OF COVERAGE, SUPPORT, GROUP AND NEIGHBORING

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Agrochemicals and chemical warfare have a lot in common, since they constitute the class of organophosphates, known to be highly toxic. Abusive use, intoxication, terrorist attacks, civil war, unsafe food are some of the issues that concern regarding these compounds. Hence, it has been of great interest to develop efficient methods for alerting attacks, monitoring crops/food and overall neutralizing undesired stocks and warheads. Catalysts-by-design is a promising approach, since the reactions of organophosphates are extremely slow. Our group has been focused in combating organophosphates, mainly seeking: (i) milder conditions for the neutralization/synthetic processes; (ii) nanocatalysts derived from graphene oxide and carbon nanotubes. We pursued site-selective mono and bifunctionalization with thiol, imidazole and hydroxamate groups (covalently linked) and applied as neutralizing agents. The catalysts were obtained as powder (for carbon nanotube with magnetic properties) and thin film, which facilitates separation and reuse. For the bifunctionalization, two different groups were anchored on specific sites of the material: (i) carboxylic acid for the cellulosic residues; and (ii) both carboxylic acid and epoxy sites for the graphene oxide. The catalysts are able to act as neutralizing agents for organophosphates, accelerating the process to less than 1 day, that otherwise could take millions of years. The process guarantees less toxic products and is selective and recyclable. The bifunctionalized catalysts showed an interesting relationship between coverage degree, group identity and neighboring effects. The materials with the highest degree of functionalization were not the best catalysts. This was attributed to cooperative effects between neighbouring groups that promote multiple catalyses (acid, basic and nucleophilic). In addition, a higher coverage by functional groups can disturb or even inhibit possible catalytic mechanisms, either by steric effect or non-ideal positioning of the groups. This finding was extremely important since it shows that the functionalization process pursued should be driven by the application wanted since not always what we expect as a better functionalization methodology will lead to the best response for a specific application. In summary, indeed the strategic design of various materials seeking optimal catalysts opens a myriad of possibilities for achieving prominent catalysis, especially for promoting worldwide chemical security by fighting agrochemicals and chemical warfare.

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ONE-DIMENSIONAL VAN DER WAALS HETEROSTRUCTURES AS THE ACTIVE LAYER MATERIAL OF SOLAR CELLS

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Carbon nanotubes have demonstrated great potential in photovoltaic applications credited to their strong chemical stability, high electrical conductivity, and tunable energy levels, which enable them to function as electrodes or the active layer components of solar cells. In 2020, our group successfully synthesized one-dimensional van der Waals heterostructures [1], composed of a coaxial stacking of boron nitride (BN) on carbon nanotubes (CNTs), followed by transition metal dichalcogenide (TMDC) coating on BN layer, which finally forms 1D triple structure CNTs-BN-MoS2 nanotubes. Preceding research results by examining the ultrafast response of 1D heterostructures to infrared light pulses demonstrated a strong intertube excitonic coupling [2], indicating a potential of 1D heterostructures as the active layer material for solar cells.

The chemical vapor deposition (CVD) method was adopted for 1D heterostructure synthesis [3]. Carbon nanotube films on graphite substrate went through two stages of CVD growth for BN and MoS2 coverage successively. For solar cell fabrication, a laminated structure was adopted where the ITO electrode, electron transport layer, 1D heterostructure active layer, hole transport layer, and gold electrode were deposited on the glass substrate successively. The fabricated device was finally set under the solar light simulator to test the I-V curve and power conversion efficiency.

Compared with conventional silicon solar cells whose active layer component is fixed, the novel 1D heterostructure solar cells possess a larger diversity facilitated by free combinations of carbon nanotubes with different chirality and TMDC with different band structures and energy levels [4]. The inner carbon nanotubes act as the foundation of the entire structure, not only mechanically supporting outer layers, but also determining the electrical properties of devices. We fabricated the devices using the metallic and semi-conducting mixture CNTs [5] and achieved a power conversion efficiency (PCE) of around 0.05% for the best device. We believe that PCE can be further enhanced by removing the metallic component in the CNTs film to suppress the electrical leakages. We also are working on film fabrication from high-purity semi-conducting CNT dispersion [6]. Through the filtration and annealing process [7], we acquired semi-conducting CNT films and removed the most of surfactant on CNTs, ready for the 1D heterostructure growth in the next step.

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THE EFFECT OF SINGLE-WALLED CARBON NANOTUBE FILM ELECTROCHEMICAL TREATMENT ON THE PROPERTIES AND FILLING CAPABILITY

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Metal encapsulated Single-Walled Carbon Nanotubes (SWCNTs) are in the focus of the extensive research over the last years because their possible application in various fields from electrocatalysis and energy storage to nanoelectronics and magnetic materials [1-3]. Most metal encapsulated SWCNT applications require control over SWCNTs structure, while demand them to be opened for filling. Structure control is crucial not only because SWCNT shell protects filler material from the interaction with surrounding medium, but also because several applications rely on the electronic properties when nanotube band structure is altered by the filler material [4]. The commonly used technique for SWCNT opening is treatment with inorganic acids, but heat treatment in oxidizing atmosphere is also utilized [5,6]. Although these procedures allow to efficiently oxidize SWCNT caps and purify nanotubes, they also generate structural defects on the side walls. To allow precise control over the SWCNT cap removal the alternative electrochemical treatment can be utilized [7]. It enables accurate dozing “opening power” (potential) and duration that finally can lead to the better filling capacity. In this work, we have examined the effect of electrochemical treatment on the SWCNT film’s properties and filling capability. The investigated material was SWCNT film of ~90% transmittance in the middle of the visible region (550 nm) supported on the polymer substrate with the opening. The film was comprising chaotically oriented SWCNTs synthesized using aerosol chemical vapor deposition method [8]. The electrochemical treatment consisted of the potential cycling of SWCNT film immersed into the 0.5 mol l^{-1} sulfuric acid electrolyte for 100 cycles at 20 mV s^{-1} sweep rate between the bottom limit potential 0.2 V vs. RHE and top limit potential 0.7-1.5 V vs. RHE. In the result we revealed optical and electrical properties behavior as well as functional and structural changes, which were attributed to the I-V curves. We established that SWCNT internal voids opening could be easily tracked by electrochemical means or with UV-vis-NIR spectroscopy. We show that SWCNT internal channels filling ability reaches maximum of ~2000 m cm^{-2} of nanowire length per film unit area. This highest filling capacity is achieved with electrochemical treatment at 1.1 V vs. RHE, and decays at severer treatment.

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TRACKING ELECTRICAL PROPERTIES OF INTERMEDIATE STATE BETWEEN MOSE2 AND JANUS MOSES DURING PLASMA TREATMENT

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Transition metal dichalcogenides (TMDCs), typified by MoS2 and MoSe2, are promising materials for next-generation semiconductor device applications, including optoelectronic devices, chemical-biological sensors, and energy conversion devices. The structural freedom of TMDCs through atomic substitution is key to controlling the electrical properties of TMDCs. The Janus TMDCs, which have different chalcogen atoms on each side of the TMDCs, have attracted much attention due to the out-of-plane intrinsic polarization in the monolayer TMDCs. The plasma process for the synthesis of Janus TMDCs by the atomic substitution of surface chalcogen atoms of non-Janus TMDCs at room temperature has been proposed [1,2]. However, the electrical properties in the intermediate state between non-Janus and Janus TMDCs have not been investigated. In this study, we investigated the electrical properties of the intermediate state between MoSe2 and Janus MoSeS during the atomic substitution process. Monolayer MoSe2 was synthesized by vapor-liquid-solid growth-based chemical vapor deposition. To measure the electrical properties, a field effect transistor (FET) with the channel of monolayer MoSe2, was fabricated by the lithography techniques. The changes in electrical properties during the synthesis of Janus MoSeS from MoSe2 were tracked by alternating plasma treatments and FET characterizations. We observed a significant increase in the current after plasma treatment in the initial treatment stage; however, we also observed a decrease in the current in the near state of Janus MoSeS. The change of Raman spectra in the repeated plasma treatments was also traced. We observed unknown Raman peaks during the repeated treatments, which may originate from the intermediate state between MoSe2 and Janus MoSeS. These results suggest that the intermediate state may contribute to the increase in the current. The possible origin of this behavior is the formation of Mo-H bonds during the substitution process, leading to the semiconducting to metallic phase transition [3].

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ADVANCED FABRICATION AND PROPERTIES OF POLYETHYLENE TEREPHTHELATE (PET) AEROGEL COMPOSITES FROM PLASTIC WASTE

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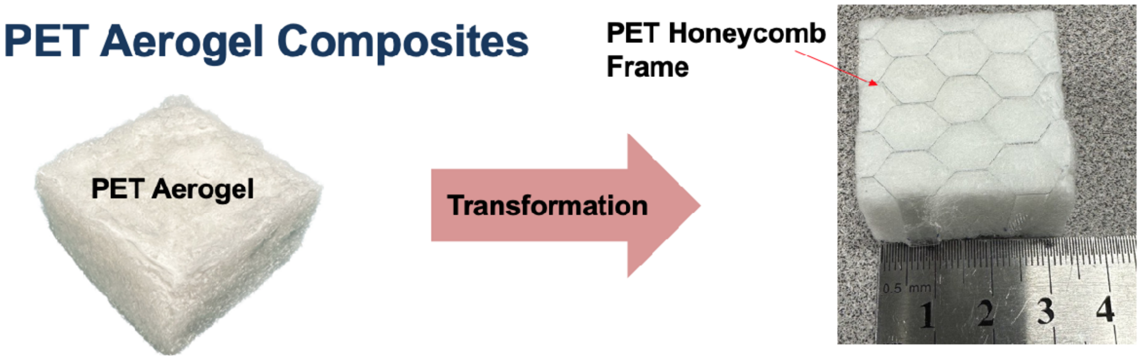
In order to solve environmental problems of plastic waste, the polyethylene terephthalate (PET) aerogel composites from PET bottle waste are developed successfully in this work. The PET honeycomb structures with various cell width are made by layering PET sheets and formed by ethyl cyanoacrylate. The honeycomb cells are filled up with the recycled PET fibers and a cross-linker solution and then freeze-fried at – 70 oC, 0.1 mbar for 48 hours to obtain the PET aerogel composites (PACs). Effects of the various honeycomb cell width (5 - 10 mm), the recycled PET fiber amount (5 - 20 g) and the cross linker amount on thermal conductivities and mechanical properties of the PACs are investigated comprehensively. Due to the PET aerogel contribution, the PACs have the low densities of 0.042 – 0. 072 g/cm^3 and the low thermal conductivities of 33 – 37 mW/m.K. The compressive strength of the PACs in the out-of-plane direction is up to 320 times larger than those in the other in-plane directions. Due to the smallest cell width of the honeycomb structure, the PAC with the 5-mm cell width exhibits the highest compressive strength of 11.56 MPa in its out-of-plane direction and 0.06 - 0.12 MPa in the other in-plane directions. The PAC properties are better than those of aramid honeycomb reinforced silica aerogel composites. The PACs can be the better alternatives for insulative panels in building, cryogenic, and cold chain applications.



POLYETHYLENE TEREPHTHELATE (PET) AEROGEL COMPOSITE

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EXTRAORDINARY IMPACT RESISTANCE OF CARBON NANOTUBE FILM WITH CROSSLINKS UNDER MICRO-BALLISTIC IMPACT

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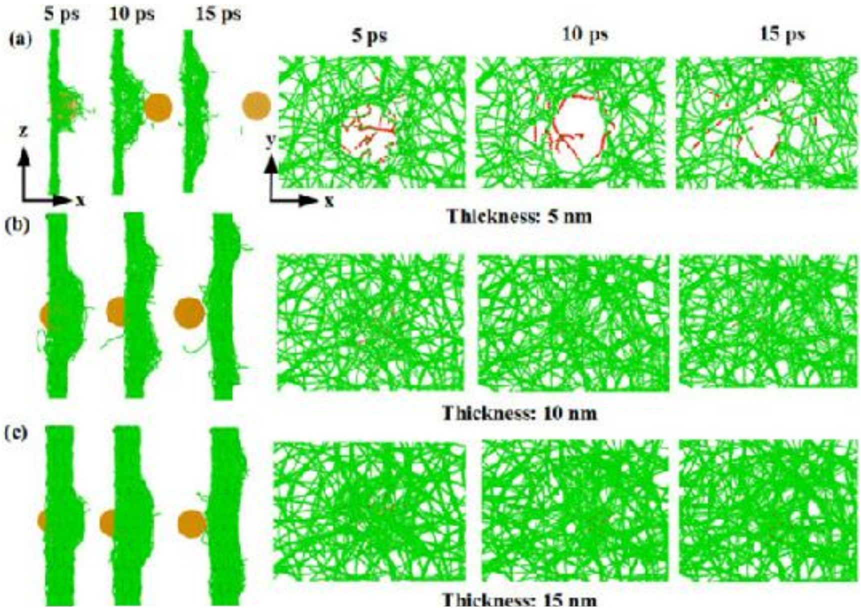
The crosslinks of carbon nanotubes (CNT) film has been demonstrated to owing the ability to reinforce the quasi-static mechanical properties. But it is unclear whether crosslinks improve the ballistic impact resistance of CNT film. Here, we investigated the impact resistance of CNT film with crosslinks by combining micro-ballistic impact experiments with coarse-grained molecular dynamics (CGMD) simulations. The impact resistance is quantitatively characterized in terms of the specific penetration energy. Meanwhile, the effective enhancement of impact resistance contributed to the crosslinks is directly observed in the experiment. CGMD simulations are employed to unveil the corresponding mechanisms in terms of deformation behavior, energy dissipation mode, and failure behavior. Our results indicate that with the increase of crosslink density, the energy dissipation mode of the CNT film transforms from bending-dominated to stretching-bending-dominated due to enhanced interaction between the adjacent CNTs. This leads to a transformation of perforated morphology from cascaded interfaces sliding to crosslink-restricted deformation with crosslinks. Our simulations also indicate that the length, bending stiffness of CNTs, and film's thickness play essential roles in the impact resistance of CNT film at various crosslink densities. These results provide a feasible strategy to improve the protective performance of CNT film.



Simulated morphologies of the CNT films with thicknesses of (a) 5 nm, (b) 10 nm, and (c) 15 nm for ρ = 10 during impact. (A colour version of this figure can be viewed online.)

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IMPROVING THE PERFORMANCE OF ALIGNED CARBON NANOTUBE-BASED TRANSISTORS BY REFRESHING THE SUBSTRATE SURFACE

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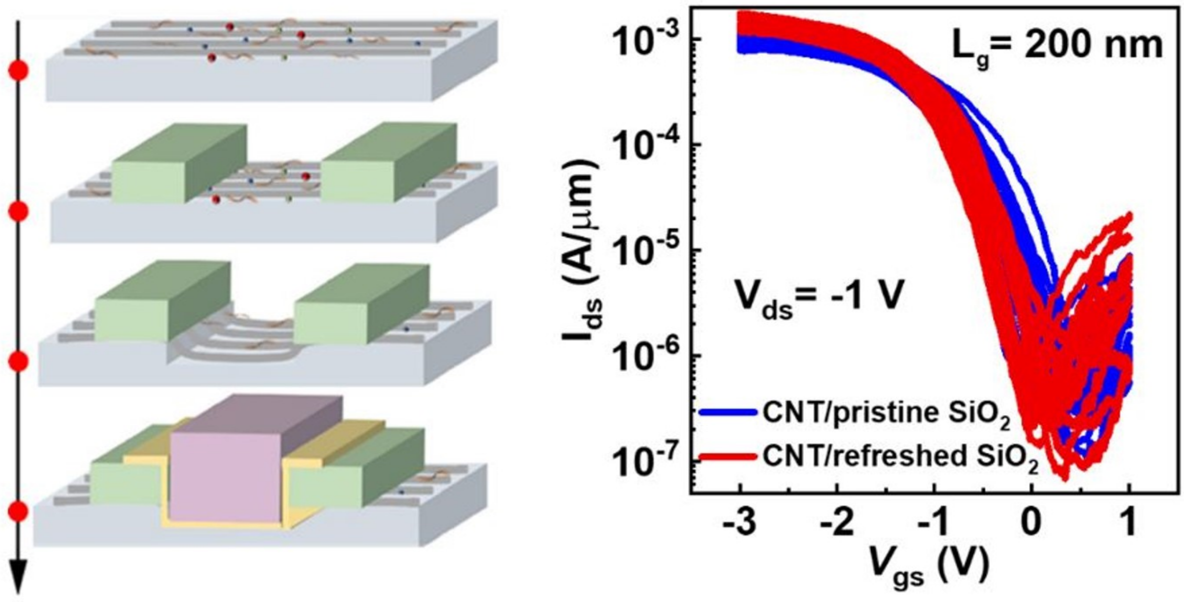
Aligned semiconducting carbon nanotube (A-CNT) array has been considered as an excellent channel material to construct high-performance field-effect transistors (FETs) and integrated circuits (ICs). The purification and assembly processes to prepare semiconducting A-CNT array require conjugated polymers, introducing stubborn residual polymers and stress at the interface between A-CNTs and substrate which inevitably affects the fabrication and performance of the FETs. In this work, we develop a process to refresh the Si/SiO_2 substrate surface underneath the A-CNT film by wet etching to clean the residual polymers and release the stress. Top-gated A-CNT FETs fabricated with this process show significant performance improvement especially in terms of saturation on-current, peak transconductance, hysteresis, and subthreshold swing. These improvements are attributed to the increase in carrier mobility from 1025 to 1374 cm^2/Vs by 34% after the substrate surface refreshing process. Representative 200 nm-gate length A-CNT FETs exhibit an on-current of 1.42 mA/μm and a peak transconductance of 1.06 mS/μm at a drain-to-source bias of 1 V, subthreshold swing (SS) of 105 mV/dec, and negligible hysteresis and drain induced barrier lowering (DIBL) of 5 mV/V.



Schematic showing the substrate surface refreshing process and the transfer characteristics of top-gated A-CNT FETs with and without this process

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MULTI-FUNCTIONAL CARBON NANOTUBE COMPOSITE FIBERS WITH ULTRAFAST AND LOW-VOLTAGE ELECTROTHERMAL RESPONSE FOR WEARABLE FABRICS

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CNTs have been considered to be the final building blocks of a new generation of high-performance multifunctional fibers owing to their high strength, high thermal conductivity and high electrical conductivity [1]. The van der Waals forces between CNTs were overcome by the interaction of superacid protons, and the liquid crystal dopes with the formation of anisotropy and dynamic alignment was facilitated by fluid shear. This liquid crystal CNT dopes could be assembled into carbon nanotube fibers by wet spinning method, which shows excellent performance of high strength, electronic conductivity and thermal conductivity [2-5]. The application of lightweight and high-performance fibers for reinforcement of composite materials in frontier fields and functional and intelligent fibers in wearable electronics has a greater prospect in the future. In our work, we enhance the electrothermal performance of carbon nanotube fibers by increasing the inter-tube interaction to enhance the phonon and electron transfer rate. In addition, the polymer molecules produce directional drainage, enhancing the viscoelastic and liquid crystal phase of the CNT dispersion, ensuring better spinnability and fiber microstructure integrity during the assembly process. The tensile fracture strength, electrical conductivity and thermal conductivity of the carbon nanotube composite fibers prepared in this study were 3.67±0.4 GPa, 3.25±0.1 MS·m-1 and 376±50 W·m-1·K-1, respectively. We investigated the electrothermal properties of carbon nanotube fiber, and found that it can achieve a stable temperature in 0.13 s to 260 °C under the condition of low voltage of 4V, and achieve an ultrahigh electrothermal response speed of 2000 °C·s-1, which is far beyond the response speed of all electric heating materials on the market today.

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A HIGH-RATE SUPERCAPACITOR WITH A 90% CAPACITANCE RETENTION AT -100 °C ENABLED BY A HYBRID-ALIGNED STRUCTURAL DESIGN

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In the development of low-temperature storage devices, ultralow-temperature tolerance, rate performance, and the trade-off between performance and working temperature represent critical obstacles, which stem from the problem of inhibited ion mobility.[1-3] Here, we report a unique hybrid aligned CNT structure where adjacent aligned bundles with large space connected with traversing CNTs were synthesized in a single assembly. This architecture affords the formation of highly orientated ion-transport channels due to its large and low tortuous ion-transport channels. Neutron scattering in conjunction with other techniques revealed that the presence of orientated macropore channels created by the specially designed hybrid aligned CNT architecture was the key for the enhanced electrolyte permeability, even allowing electrolyte to be infiltrated into the deepest inner volume of the electrode, thereby mitigating the degradation of ion kinetics at low temperatures. At -100 °C, a capacitance retention of 90% was achieved at a scan rate of 20 mV s^{-1}, breaking the commonly observed trade-off between the electrochemical performance and working temperature. Finally, a highest-reported power density of 40 kW kg^{-1} and an energy density of 75.3 Wh kg^{-1} were presented at -100 °C, far surpassing the previously reported low-temperature supercapacitors.

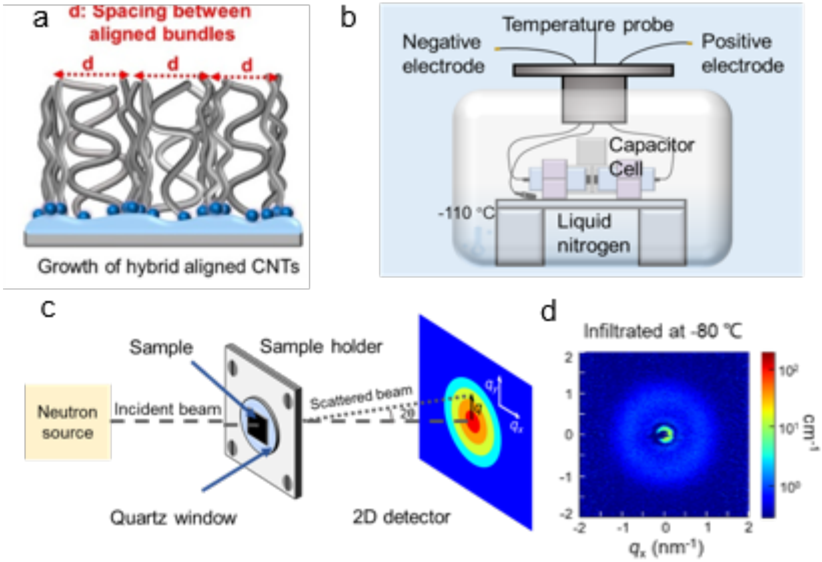

Figure 1. Structure design of a) hybrid aligned CNTs, b) Device assembly, c) Schematic of experimental setup for SANS measurements of electrolyte-infiltrated CNT electrodes, d) 2D SANS images for the hybrid aligned CNTs after electrolyte infiltration at -80 °C.

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