Graphene Flagship EU-China Workshop on *Graphene and related 2D materials*

Dresden, Germany
07 – 08 December 2018

Workshop report

Workshop chairs: Jari Kinaret (Sweden) and Hongjun Gao (China)

Programme chairs: Xinliang Feng (Germany), Francesco Bonaccorso (Italy) and Shixuan Du (China)

Contents

Overview

The 2nd Graphene Flagship EU-China Workshop on Graphene and related 2D materials was held on 07-08 December 2018 at Hotel Pullman Dresden Newa, Dresden, Germany.

The workshop aimed at being a forum for the exchange of experiences, practices and ideas related to the current and emerging topics associated with the fundamental materials synthesis, physics and devices for graphene and related 2D materials. In addition, the objective was to explore further possibilities for collaborative research opportunities between researchers in Europe and China.

This was a follow up of the China-EU Workshop held in Beijing, China, on June 29 –July 2, 2017.

The workshop gathered 34 participants (16 from China and 18 from Europe), coming mainly from academic institutions. Speakers gave 29 talks that have shown the breadth of activities and topics covered by their respective research groups. The selection of the scientific speakers and participants was done by the two groups of organizers. All presentations stimulated questions and discussions. Several Graphene Flagship work-packages (Enabling Research, Spintronics, Photonics and Optoelectronics, Energy Generation, Functional Foams & Coatings, Innovation, Management) and leading Chinese institutions active in GRM research were represented at the meeting which offered a unique opportunity for direct exchanges and development of new collaborations.

The workshop was opened by Prof. Feng and Prof. Gao who set the scene and introduced the overall goals for the meeting. Prof. Kinaret presented the status of the Graphene Flagship and the plans for the Core3 project. Prof. Gao, the workshop chair from China, highlighted the major opportunities for research support available in China. The Chinese Academy of Sciences has set-up a new programme to support the research on 2D materials, with a total budget of 2bilion CNY (approximately 250M Euro) over 5 years. This available funding will continue support the research in the field of 2D materials but will also allow to set-up new collaborations and opportunities.

Common challenges and opportunities for collaborations

In the final discussion session, participants identified areas of common interest that include mainly fundament science of graphene and related materials (GRM) growth, heterostructures, devices and physics. While the results presented by the Chinese speakers were mostly on fundamental science, the Europeans have presented more results on applied science and graphene-related devices. As such, there was no significant overlap between the presentations of the two sides.

At the end of the meeting, there was clear interest to continue the series of workshops by organising the next workshop again in Shanghai, China, possibly in October 2019. The dates of the event need to be decided. Another option will be to organise the workshop in connection with another event, like GRAPCHINA conference, that will take place in September 2019 (the dates are not fixed yet), and have the workshop held before the conference. In this way, the EU partners can have opportunity to present in the session in GRAPCHINA conference.

It has also been agreed that for the next workshop, the topics should be selected as to increase the overlap and have complementary talks. The Chinese side has raised their strength in the materials synthesis side. Also, it was agreed that, in the next workshop, there should be more balance between the basic and applied/industry topics.

Some emerging or on-going collaborations exist already between European and Chinese participants, and this could be the driving force for the definition of topics for the 2019 workshop.

Some of the topics suggested by the participants were:

- Materials synthesis and characterisation;
- Nanoscale materials characterisation;
- Nanoribbons;
- Boron nitride (BN);
- Heterojunctions;

The instrument to further foster collaboration (grants for student exchanges) has been reminded. Such support could be very useful. This is already available within the Flagship, i.e., the mobility grants, which allow young researchers from Europe to perform research stays in laboratories in overseas countries.

Programme

December 7, 2018		
08:30	**Registration and welcome**	
08:45	*Xinliang Feng*	Welcome Words and opening workshop
08:55	*Jari Kinaret*	Graphene Flagship
09:05	*Hongjun Gao*	Graphene and 2D Materials activities in China
Session 1: Materials Growth and Heterostructures *Chair: Xinliang Feng*		
09:15	*Xiaoming Xie*	Synthesis and characterizations of graphene and graphene/superconductor hetero-structures
09:40	*Renhao Dong*	Interfacial Synthesis of 2D Conjugated Polymers: The Rise of Organic 2D Materials
10:05	*Xiao Lin*	Construction of Palladium Selenide Island on Graphene
10:30 – 11:00	**Coffee Break**	
Session 2: Materials Growth and Heterostructures *Chair: Shixuan Du*		
11:00	*Vladimir Falko*	Infrared and THz inter-subband optics of few-layer 2D materials
11:25	*Ping-Heng Tan*	Interfacial Interactions in van der Waals Heterostructures of MoS_2 and Graphene flakes
11:50	*Thomas Heine*	New 2D kids on the block: Noble metal chalcogenides and conjugated 2D polymers
12:15	*Andrea Ferrari*	Light scattering with Graphene and Related materials
12:40 – 13:45	**Lunch**	

Session 3: Materials Growth and Heterostructures *Chair: Francesco Bonaccorso*		
13:45	*Shixuan Du*	Novel Two-dimensional Materials beyond Graphene: DFT calculations and Scanning Tunnelling Microscope investigations
14:10	*Roman Fasel*	Topological quantum phases in graphene nanoribbons
14:35	*Yeliang Wang*	Epitaxial Growth and Properties of 2D Monolayer Antimonene
15:00	*Stephan Roche*	Charge, Thermal and Spin Transport in Graphene Composites & Polycrystalline Heterostructures
15:25	*Paolo Samori*	Leveraging the properties of 2D materials: chemical tailoring of multifunctional foams and coatings
15:50 – 16:15	**Coffee Break**	
Session 4: GRM based devices *Chair: Paolo Samori*		
16:15	*Xiaodong Zhuang*	Rational Design 2D Porous Organic Materials for Energy Storage and Conversion
16:40	*Emmanuel Kymakis*	Graphene and related 2D materials for perovskite solar cell applications
17:05	*Francesco Bonaccorso*	2D-materials for energy applications
17:30	Wrap-up of the first day	
17:45	***Visiting Dresden Christmas Market***	
19:30 – 22:30	**Dinner at Restaurant Genuss-Atelier** (departure from hotel at 19:15)	

December 8, 2018		
Session 5: GRM based devices *Chair: Stefan Roche*		
09:00	*Kaihui Liu*	Growth and Application of Meter-sized Single-crystal Graphene
09:25	*Vincenzo Palermo*	Selective gas permeation in graphene oxide-polymer self-assembled multilayers
09:50	*Guangyu Zhang*	Scalable monolayer MoS2 for electronic devices
10:15	*Aldo Di Carlo*	The role of graphene and other 2D materials in Perovskite photovoltaics
10:40 – 11:00	**Coffee Break**	
Session 6: GRM based devices *Chair: Guangyu Zhang*		
11:00	*Georg Duesberg*	Hybrid electronic devices with 2D Materials

11:25	*Lihong Bao*	Graphene and Beyond: Electronic Devices and Transport Properties
11:50	*Gianluca Fiori*	Promises and perspectives of two-dimensional materials for electronic applications
12:15	*Wenguang Zhu*	Theoretical Design of 2D Ferroelectric and Multiferroic Materials
12:40 – 13:30	**Lunch**	
	Session 7: Physics *Chair: Xiaoming Xie*	
13:30	*Qing Dai*	The properties and applications of graphene plasmons
13:55	*Kehui Wu*	Polymorphism of Elemental 2D Materials
14:20	*Wei Ji*	Interlayer engineering in tuning physical properties of two-dimensional materials
14:45	*Annick Loiseau*	Understanding optical absorption and luminescence in hBN: a tool for a characterisation metrics from bulk to the monolayer
15:10 – 15:30	**Coffee Break**	
	Session 8: Physics *Chair: Yeliang Wang*	
15:30	*Wu Zhou*	Exploring strain effect at 2D material interfaces at the atomic scale
15:55	*Chendong Zhang*	Atomic and electronic structures of transition metal dichalcogenides heterostructures
16:20 – 17:15	**Discussions on future collaborations** *Chair: Francesco Bonaccorso*	
17:15	*Xinliang Feng*	**End of the workshop**

List of participants

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Book of abstracts

Graphene and Beyond: Electronic Devices and Transport Properties

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Short biography:
I received the Ph.D for condensed matter physics in Institute of Physics, CAS in 2008. After the postdoctoral research at University of South Carolina and Iowa State University, USA, I joined in Institute of Physics, CAS as an associate Professor in 2013. Currently, my research is mainly focused on construction, electronic devices, and electrical transport properties of low-dimensional systems. The other important aspects of my research are in-situ measurement of electrical transport properties of low-dimensional materials and characterization of their structure-property relationship by UHV four probe-STM. In past years, I have published more than 40 papers in high-profile journals, including Nano Letters, Advanced Materials, Applied Physics Letters etc., and have been cited by others for more than 2000 times.

Abstract:

Grain boundaries (GBs) in polycrystalline graphene scatter charge carriers, which reduces carrier mobility and limits graphene applications in high-speed electronics. In this talk, I will demonstrate the extraction of the resistivity of GBs and the effect of GBs on carrier mobility by direct four-probe measurements on millimetersized graphene bicrystals grown by chemical vapor deposition (CVD). Measurements on seven representative GBs find that the maximum resistivities are in the range of several kΩ μm to more than one hundred kΩ μm. Furthermore, the mobility in these defective regions is reduced to 0.4 - 5.9 ‰ of the mobility of single-crystal, pristine graphene.
Black phosphorus (BP) has attracted great attention due to its high hole mobility, and a sizable and tunable bandgap, meeting the basic requirements for logic circuits application. To realize a complementary logic operation, it needs to control the conduction type in BP FETs, i.e., the dominant carrier types, holes (P-type) or electrons (N-type). In this talk, I will also demonstrate that capping the thin BP film with a cross-linked poly-methyl-methacrylate (PMMA) layer can modify the conductivity type of BP by a surface charge transfer process, converting the BP layer from p-type to n-type. Combining BP films capped by cross-linked PMMA to a standard BP, a family of planar devices can be created, including BP gated diodes (rectification ratio >102), BP barristors (on/off ratio >105), and BP logic inverter (gain ~ 0.75), which are capable of performing current rectification, switching, and signal inversion operations.
Inspired by the discovery of black phosphorus as channel material in FETs, the orthorhombic ones, such as GeS, GeSe, SnS, and SnSe, have attracted growing interest. I'll also demonstrate ultrathin SnSe single crystals have been epitaxially grown on molten polydimethylsiloxane (PDMS) by the chemical vapor deposition (CVD) method. Thickness-dependent Ramans spectroscopy measurements result in a red shift of the Ag3 mode and blue shift of the B3g and Ag2 modes, even when the thickness is over 10 nm, which is never observed in hexagonal Van der Waals structures. The octagonal SnSe nanosheets show an electrical anisotropic characteristic. Finally, the thermopower of SnSe nanosheets can be electrostatically tuned, and, when sweeping the gate voltage from -40 V to 40 V at 120 K, the thermopower can be tuned from 54 to 866 mVK-1, indicating the unique advantage of gate modulation compared to chemical doping in thermoelectric applications.

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2D-materials for energy applications

Francesco Bonaccorso
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Abstract:

In this talk, I will illustrate first the most promising areas of development of 2D materials.[1-5] In the context of the project it is of foremost importance the development of industrial-scale, reliable, inexpensive production processes for the implementation of 2D materials in flexible (opto)electronics and energy applications.
I will show how the production of 2D materials by solution processing[2,6] represents a simple and cost-effective pathway towards the development of 2D materials-based (opto)electronic and energy devices, presenting huge integration flexibility compared to other production methods. Here, I will first present our strategy to produce 2D materials on large scale by wet-jet milling[7] of their bulk counterpart and then an overview of their applications for flexible and printed (opto)electronic and energy devices. 3,8,9,10,11,12,13,14

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The properties and applications of graphene plasmons

Quin Dai
National Center for Nanoscience and Technology, CAS, China

Short biography:

Qing Dai received PhD degree in Nanophotonics at the Department of Engineering from University of Cambridge, after obtained MEng degree on Electronic & Electrical Engineering from Imperial College, London. Following postdoctoral appointments at Centre for Advanced Photonics and Electronics (CAPE) at University of Cambridge, he joined the faculty of National Center for Nanoscience and Technology (NCNST, located in Beijing) in 2012. Now he is a professor at NCNST and serving as the director of Division of Nanophotonics.

His research interests include low dimensional nanomaterials, plasmonics, nearfield optical characterization and ultrafast electron emissions. He has published over 70 peer-reviewed papers in reputed international journals, including Nature Communications, Nanoscale and Advanced Materials. He serves as the associate editor of Nanoscale since 2018 and is a regular reviewer of various high-impact journals such as Nature, Nature Materials, Advanced Materials.

He has been awarded various prizes, including Junior Research Fellowship at Wolfson College, University of Cambridge (2012), "Thousand Talent Program for Young Scientists" award (2012), LU JIAXI Award for Young Scientists (2014) and Chinese Academy of Sciences Professorship (2017).

Abstract:

Graphene plasmonics is of great interest for compact optical devices working in broad frequency due to its ultrahigh field confinement, electrical tunable resonance frequency and very low intrinsic damping. However, graphene plasmons can be easily affected by the dielectric environment, such as scattering from electrical impurities and strong plasmon-phonon coupling. We studied graphene plasmons on different substrates including SiO_2/Si, CaF_2/Si, BN/CaF_2, BN/SiO_2 and mica, which result in different interaction with graphene plasmon. Due to the strong coupling between graphene plasmon and BN phonon, we discover a new hybridized polariton mode in graphene/h-BN van der Waals heterostructures, which enables ultralong hybrid plasmon lifetime up to 1.6 picosecond. Such hybrid modes combine the high field enhancement feature of graphene plasmon and the long lifetime property of h-BN transverse optical phonon. By designing graphene plasmon on CaF_2/Si, we avoid the plasmon-phonon hybridization and obtain electrically-tunable graphene plasmon that can cover the entire molecular fingerprint region, based on which molecular fingerprinting at the nanoscale level are demonstrated.

On flexible mica, we experimentally demonstrated bendable graphene plasmonic devices exhibit no visible change at bending radius down to 1 mm and after 1000 bending cycles at a radius of 3 mm. These findings may help to understand the properties of graphene plasmon and pave the way for applications such as deep-subwavelength low-loss waveguides and enhanced mid-infrared spectroscopy.

The role of graphene and other 2D materials in Perovskite photovoltaics

Aldo Di Carlo
CHOSE – Centre for Hybrid and Organic Solar Energy, University of Rome Tor Vergata, Italy

Short biography:
Aldo Di Carlo is full professor of Optoelectronics and Nanoelectronics at the University of Rome "Tor Vergata" (Italy). Since 2006 he is director of the Centre for Hybrid and Organic Solar Energy (CHOSE) which involves more than 30 researchers for the development and industrialization of the organic and hybrid organic/inorganic photovoltaic technologies. Di Carlo is author/co-author of more than 400 scientific publications on international journals, 13 patents and several book chapters.

Abstract:

Hybrid Metal-Organic Halide Perovskite such as CH3NH3PbI3 (MAPI) have opened up new directions to fabricate cost effective and high efficient photovoltaic (PV) devices. Many factors can influence the efficiency and stability characteristics of Perovskite Solar Cells (PSCs). In particular, interfaces can influence layers deposition, charge recombinations and compound intermixing/diffusion, representing a critical aspect for scaling up activities aiming to exploit at industrial level perovskite photovoltaics. In this perspective, bidimensional (2D) nanomaterials, such as graphene and related materials can play a primary role owing to their 2D nature and the large variety of 2D crystals, whose complementary opto/electronic properties, can be on-demand tuned by chemical functionalization and edge modification. The so-called Graphene Interface Engineering (GIE) has shown to be extremely effective in PSC technology both at lab cells (small area) level and at large area (module) level. We demonstrate the use of graphene and 2D materials as an effective way to control the morphology [1] and to improve stability and efficiency [2,3]. By dispersing graphene flakes into the mesoporous TiO2 layer and by inserting graphene oxide (GO) as interlayer between perovskite and Spiro-OMeTAD layers, we demonstrate a PCE exceeding 18% with a two-step MAPI deposition, carried out in air [2] Further optimization of the 2D interface layers could promote the efficiency above 20% with a strong improvement of the stability. The proposed approach has been exploited for the fabrication of state-of-the-art large area perovskite modules with a PCE of 13.7% (active area exceeding 100 cm2) paving the way to an industrialization phase compatible with standard fabrication processes [4]. In this respect, the Spear Head project "Solar Farm" of the Graphene Flagship will make use of the GIE for a pilot-line fabrication of Graphene-Perovskite modules to demonstrate the feasibility of the approach in the realization of PV panels.

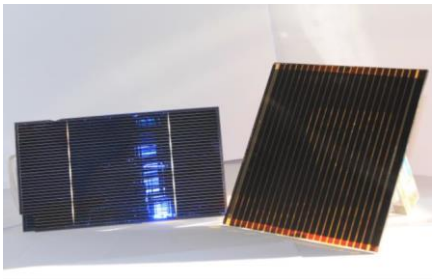

Figure 1: comparison between silicon solar cell (left) and graphene-perovskite solar module (right)

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Interfacial Synthesis of 2D Conjugated Polymers: The Rise of Organic 2D Materials

Renhao Dong
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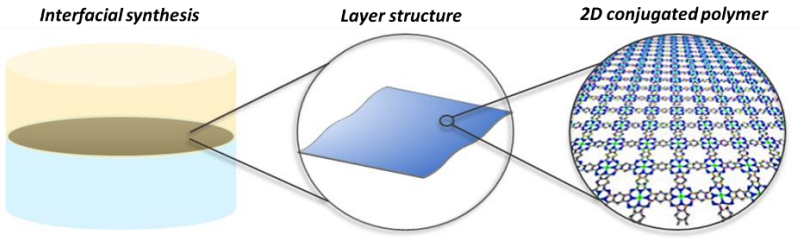
Short biography:
Renhao Dong obtained his B.S. degree in chemistry from Shandong University in 2008 and completed his Ph.D. study with a focus on colloid and interface chemistry under the supervision of Prof. Jingcheng Hao at Shandong University (China) in 2013. Then he joined Prof. Klaus Müllen's group as a Postdoctoral Fellow at Max Planck Institute for Polymer Research (Mainz, Germany) in August 2013. In 2015, he joined Prof. Xinliang Feng's group as an Alexander von Humboldt Foundation Fellow at Technical University of Dresden (Dresden, Germany). Since 2017, he has been a young research group leader in the Chair of Molecular Functional Materials at Technical University of Dresden. His current research interest focuses on design and synthesis (in solution/at
interfaces) of organic 2D materials such as 2D polymers, 2D covalent organic frameworks, and 2D metal-organic frameworks as well as their applications in opto-electronics, magnetics and energy storage/conversion.

Abstract:
The discovery of graphene one decade ago has triggered enormous interest in developing two-dimensional materials (2DMs). At present, various synthesis strategies have been exploited to produce 2DMs, such as top-down exfoliation and bottom-up chemical vapor deposition and solution synthesis methods.[1] In our work, we have employed the interfacial chemistry toward the controlled synthesis of organic 2D materials with varied structural features and diverse functions. For instance, we demonstrated the synthesis of 2D conjugated metal-organic framework (2D MOF) —crystalline porous coordination polymer—at the air-water or liquid-liquid interfaces via metal-bis(dithiolene)/-bis(diimino)/-catecholate complexes. Such 2D MOFs feature with large-area single layer or van der Waals stacked multi-layers and possess unique electronic properties, such as full delocalization of π-electrons, narrowed band gaps, largely improved conductivity and high charge mobility, which render 2D conjugated MOFs as advanced electronic materials. One representative triphenylene-fused iron-bis(dithiolene) 2D MOF exhibited a *p*-type semiconducting behavior with a band-like transport and high charge mobility of ~220 cm^2/Vs.[2] Owing to their electrical conductivity and tunable band gaps, the resultant 2D conjugated MOFs have been applied in transistors, sensing, magnetics, and energy storage and conversion.[3] Apart from the coordination polymer, we have synthesized 2D conjugated polymers by covalent linkages, such as imines, imides and pyrazines, at the air-water or liquid-liquid interfaces. For instance, we synthesized a single-layer polycrystalline 2D polyimine at the air-water interface in a Langmuir-Blodget trough. The resultant 2D polyimine displayed an outstanding Young's modulus (267±30 GPa) comparable to that of graphene and multi-functions such as an organic semiconducting layer for thin film field effect transistor (FET) and electrocatalyst for hydrogen generation from water.[4] Very recently, by employing surfactant monolayer as a soft-template at the air-water interface, we were able to synthesize highly crystalline imide-based 2D polymers with highly ordered square units along 2D directions up to remarkable ~4 μm^2 for a single crystalline domain. This preliminary result clearly highlights the feasibility to synthesize crystalline 2D polymers via soft-template-assisted interfacial synthesis strategy. In short, we expect to develop interfacial chemistry toward the controlled synthesis of organic 2DMs and achieve delineation of reliable structure-property relationships and superior physical and chemical performances of organic 2DMs.



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Novel Two-dimensional Materials beyond Graphene: DFT calculations and Scanning Tunneling Microscope investigations

Shixuan Du
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Short biography:
Shixuan Du studied at Peking University (B.S.), and received her Ph.D. in physical chemistry from Beijing Normal University in 2002. She was appointed as an Associate Professor in 2002 and became a Professor in Institute of Physics, Chinese Academy of Sciences in 2009. Her research interests focus on the nature of molecular assembly, graphene, silicene and other new two dimensional atomic/molecular crystals, and the growth mechanism of low-dimensional materials. She is the winner of the National Science Fund for Distinguished Young Scholars and the editorial board member of "Journal of Physics, Condensed Matter". She got the Award of the Chinese Young Women in Science Fellowship. As a Major Contributor, she won the 2013's Outstanding Science and Technology Achievement Prize of the Chinese Academy of Sciences. She has published more than 140 journal articles including Science and Nature series.

Abstract:
The discovery of graphene opened a door for manufacturing and investigating two-dimensional (2D) materials. After more than ten years of development, 2D materials have become one of the most important topics in materials research, with dozens of new materials having been synthesized experimentally and even more predicted theoretically. In this talk, I will talk about the fabrication of 2D materials based on epitaxial growth in an ultra-high vacuum (UHV) experimental environment and the investigation of their physical and chemical properties using scanning tunneling microscope combined with density functional theory (DFT) based first principle calculations. In particular, I focus on the novel materials constructed by direct selenization of metal substrates, for example, CuSe. At a high dosage of Se, a single atomic layer transition metal monochalcogenide (CuSe) with an intrinsic pattern of nanoscale triangular holes was fabricated on Cu(111). DFT calculations show that free-standing monolayer CuSe with holes is not stable, while hole-free CuSe is endowed with the Dirac nodal line fermion (DNLF). This very rare DNLF state is evidenced by topologically nontrivial edge states situated inside the spin-orbit coupling gaps. Motivated by the promising properties of hole-free honeycomb CuSe, we fabricated monolayer CuSe on a Cu(111) surface by molecular beam epitaxy and confirmed success with high resolution scanning tunneling microscopy. The good agreement of angle resolved photoemission spectra with the calculated band structures of CuSe/Cu(111) demonstrates that our sample is monolayer CuSe with a honeycomb lattice.

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Hybrid electronic devices with 2D Materials

Georg Duesberg
Bundeswehr University Munich, Germany

Short biography:
Georg S. Duesberg graduated in Physical Chemistry from the University of Kassel, Germany in 1996.
PHD Max-Planck-Institute for Solid State Research, Stuttgart from 1997 – 2001.
From 2001 – 2005 he worked at the Infineon AG, in the Corporate Research Department in Munich.
From 2005 – 2007 Prof. Duesberg was in the Thin Films Department at Qimonda AG, Dresden.
In 2007 Prof. Duesberg became Assoc. Prof. and then later Prof. in the School of Chemistry of Trinity College Dublin, Ireland and a Principal Investigator in at the National Research Institute CRANN.
In 2017 Prof. Duesberg took on the Chair for Sensortechnologies at the Universität der Bundeswehr in Munich.
He co-authored more than 230 publications with more than 18000 citations (H-index 55) and has filed more than 25 patents.
Prof. Duesberg´s research focuses on making novel devices to exploit the unique properties of low-dimensional structures.

Abstract:

Two-dimensional (2D) materials like graphene and transition metal dichalcogenides (TMDs) are intensively investigated because of their unique properties, such as tunable band gaps, which make them highly interesting for fundamental studies and emerging applications. While exfoliation techniques have paved the way too many exciting prospects, reliable and controllable deposition techniques are a prerequisite for real life applications. While chemical vapor deposition (CVD), atomic layer deposition and molecular beam epitaxy are investigated, the synthesis by thermally assisted conversion (TAC) of predeposited metal films yields homogenous films of a number of TMDs. The scalable process leads to polycrystalline films of controlled thickness which align well with the substrate when thin. The composition and morphology are investigated in detail by Raman spectroscopy [2], X-ray photoelectron spectroscopy, TOF-SIMS and transmission electron microscopy. The TAC films allow the investigation and device fabrication with these materials.

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Infrared and THz inter-subband optics of few-layer 2D materials

Vladimir Falko
The university of Manchester, National Graphene Institute, United Kingdom

Short biography:
Vladimir Falko is condensed matter theorist responsible for many advances in the theory of electronic and optical properties of atomically thin two-dimensional crystals and their heterostructures (graphene, transition metal dichalcogenides, post-transition metal chalcogenides), and he worked on various aspects of theory of quantum transport and fundamentals of nanoelectronics. His career has been marked by Humboldt Fellowship, EPSRC Advanced Fellowship, ERC Advanced Investigator Grant, Synergy Grant, and Royal Society Wolfson Foundation Research Merit Award. Falko is the initiator 'Graphene Week' conference series, founding Editor-in-Chief of the IoP Journal '2D Materials', and one of the initiators and leaders of the European Graphene Flagship Project. Currently, he serves as Director of National Graphene Institute and Professor of Condensed Matter Theory at the University of Manchester.

Abstract:
The science and applications of electronics and optoelectronics have been driven for decades by progress in the growth of semiconducting heterostructures. Many applications in the infrared and terahertz frequency range exploit transitions between quantized states in semiconductor quantum wells (intersubband transitions). However, current quantum well devices are limited in functionality and versatility by diffusive interfaces and the requirement of lattice-matched growth conditions. Here, we introduce the concept of intersubband transitions in van der Waals quantum wells, such as atomically thin films of MoS2, MoSe2, WS2 and WSe2 and post-transition metal chalcogenides (PTMC), InSe and GaSe. These are materials where a strong covalent bonding of atoms inside individual layers coexists with a weak van der Waals coupling of the consecutive layer of the bulk crystal. Van der Waals quantum wells are naturally formed by two-dimensional materials and hold unexplored potential to overcome the aforementioned limitations — they form atomically sharp interfaces and can easily be combined into heterostructures, without lattice-matching restrictions.

At the same time, van der Waals nature of these crystals coexists with strong hybridizations of – separately – conduction and valence band orbitals in the consecutive monolayers in the film, making the band structure of few-layer atomically thin TMDs and PTMCs sensitive to the number of layers in them [1,2]. In particular, few-layer films acquire multiple subbands in their electronic spectra, with a strong coupling of inter-subband transitions of carriers (electrons in n-doped and holes in p-doped materials) with out-of-plane polarised photons. Here, we show that, when n- or p-doped, few-layer films of TMDs and PTMCs become absorbers and emitters of infrared (IR) and THz light [1,2]. Our density functional theory modelling and a specially designed hybrid k'p theory for the monolayers of these materials, combined with the tight-binding model description of the interlayer hopping, predicts that optical activity of few-layer films of these two classes of compounds densely covers the range from IR (1.5 micron) for bilayer films to THz for the films with 3-10 layers.

The predicted spectral characteristics are confirmed [3] by SNOM studies of atomically thin films of WSe2. In a way, these thin films are analogous to quantum wells in conventional semiconductors, and, by choosing the number of layers, and/or n- or p-doping in one of TMD and PTMC compounds, one can tune such intersubband transition energy to the desirable application range, offering a new way how 2D materials can be harnessed for developing new technologies. This work enables the exploitation of intersubband transitions with unmatched design freedom and individual electronic and optical control suitable for photodetectors, light-emitting diodes and lasers.

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Topological quantum phases in graphene nanoribbons

Roman Fasel
EMPA, Swiss Federal Laboratories for Materials Science and Technology Switzerland

Short biography:

Roman Fasel received his Ph.D. in Physics in 1996 from the University of Fribourg (Switzerland) and joined Empa, the Swiss Federal Laboratories for Materials Science and Technology, after post-doctoral research fellowships at La Trobe University (Melbourne) and the Fritz-Haber-Institute (Berlin). He is currently the head of the nanotech@surfaces Laboratory of Empa, and since 2008 Tit. Professor at the Department of Chemistry and Biochemistry of the University of Bern. Roman Fasel has a strong background in experimental surface physics and chemistry, and follows an experimental approach building on state-of-the-art scanning probe methods (UHV temperature-controlled STM/STS) combined with structural and spectroscopic methods based on photoelectron emission (XPS, UPS, XPD). His group's research covers a wide range of topics at the interface of materials science, surface physics and chemistry, with a strong current focus on the on-surface fabrication and in-depth characterization of carbon-based nanomaterials. He has given numerous invited talks at international conferences and at research institutions and universities world-wide and has published more than 150 peer-reviewed papers totalling over 7800 citations.
Roman Fasel and his team are among the pioneers of the novel and rapidly evolving field of on-surface synthesis. Most importantly, he has pioneered the bottom-up approach to the synthesis of graphene nanoribbons (GNRs), which is based on a two-step process combining the surface-assisted activation and colligation of specifically designed precursor monomers and the subsequent surface-assisted intramolecular cyclodehydrogenation under ultrahigh vacuum conditions. It yields atomically precise GNR structures that are fully dictated by the design of the precursor monomers. Roman Fasel is the co-inventor of different aspects of GNR fabrication and application that have been covered by 6 patents filed in collaboration with the chemical company BASF.

Abstract:

Topological materials have attracted great interest in solid state physics due to their ability to support robust, yet exotic quantum states at their boundaries (or interfaces) such as spin-momentum locked transport channels or Majorana fermions. Very recently, it has been found theoretically that localized zero energy modes can be obtained at the junctions of topologically dissimilar graphene nanoribbons (GNR) [1]. We have experimentally realized GNRs exhibiting well defined periodic sequences of these topological electronic modes [2]. This leads to one-dimensional electronic bands which are described by the Su-Schrieffer-Heeger (SSH) Hamiltonian representing the dimerized atomic chain. By manipulating the intra- and inter-cell coupling strength we could create SSH analogs with different Chern number and therefore topological class. Experimentally, the topological class is determined by the presence or absence of zero energy end states at the termini of the corresponding GNR or its junctions to structurally dissimilar GNRs.
The realization of 1D topological quantum phases in GNRs enables a novel route to bandgap (and effective mass) control in GNR structures, which can be readily integrated in CMOS type electronic devices [3]. Furthermore, the topological GNR structures might be extended to a size where magnetic ordering occurs and 1D spin chains can be realized. In the longer term the topological end states might be used to host qubits for quantum information applications.

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Light scattering with Graphene and Related materials

Andrea Ferrari
Cambridge Graphene Centre, United Kingdom

Short biography:
Andrea Ferrari is Professor of nanotechnology at the University of Cambridge and a Fellow of Pembroke College. He founded and directs the Cambridge Graphene Centre and the Engineering and Physical Sciences Research Council Doctoral Training Centre in Graphene Technology. He chairs the management panel and is the Science and Technology Officer of the European Graphene Flagship. He is a Fellow of the American Physical Society, Fellow of the Materials Research Society, Fellow of the Institute of Physics, Fellow of the Optical Society and he has been recipient of numerous awards, such as the Royal Society Brian Mercer Award for Innovation, the Royal Society Wolfson Research Merit Award, the Marie Curie Excellence Award, the Philip Leverhulme Prize, The EU-40 Materials Prize.

Promises and perspectives of two-dimensional materials for electronic applications

Gianluca Fiori
University of Pisa, Italy

Short biography:
Gianluca Fiori received the M.S. degree in electrical engineering and the Ph.D. degree from the Università di Pisa, Pisa, Italy, in 2001 and 2005, respectively. In autumn 2002, he visited Silvaco International, developing quantum models, which are currently implemented in the commercial simulator Atlas by Silvaco. In summers 2004, 2005, and 2008, he visited Purdue University, West Lafayette, IN, USA, where he worked on models for the simulation of transport in nanoscaled devices. His main field of activity includes the development of models and codes for the simulations of ultrascaled semiconductor devices, with particular focus on two-dimensional materials-based transistors. G.F. is the leading developer of the open-source code NanoTCAD ViDES (http://vides.nanotcad.com). More information available at http://gianlucafiori.org.

Abstract:
Intensive research in the two-dimensional material field has led to huge progresses in terms of technology enhancement in material fabrication and exploitation of 2DMs in a wide range of applications.
In this talk, I will try to provide a personal opinion on the applications which I believe 2DMs could represent an enabling technology, focusing both on high-performance computing, as well as printable electronics.

Graphene and 2D Materials activities in China

Hong-Jun Gao
Institute of Physics, CAS, China

Short biography:

Hong-Jun Gao received his Ph.D. in physics from Peking University in 1994. He became a Professor in Institute of Physics, Chinese Academy of Sciences in 1995. He is an Academician of the Chinese Academy of Sciences and an Academician of the Developing-Country Academy of Sciences (TWAS). His research interest is on the construction and physical property of quantum nanostructures including two dimensional atomic/molecular crystals and scanning tunneling microscopy/spectroscopy. He has 6 international books/chapters and about 200 journal publications including Science, Nature series journals, Phys. Rev. Lett., J. Am. Chem. Soc., and Adv. Mater., etc. He was awarded the "OCPA AAA (Robert) Prize 2008" (OCPA: the Overseas Chinese Physics Association; AAA: Achievement in Asia Award), the "TWAS Prize in Physics 2009" (TWAS: Third World Academy of Sciences), and "Humboldt Research Award 2010"; 2012 Science and Technology Awards of the Ho Leung Ho Lee Foundation.

New 2D kids on the block: Noble metal chalcogenides and conjugated 2D polymers

Thomas Heine
Dresden University of Technology, Germany

Abstract:

First, I will report our latest results on noble metal chalcogenides and their properties that benefit from catalytic activity and strong quantum confinement [1-3].
In the second part, I will discuss 2D polymers that can be produced in virtually any crystal topology [4] and that act as semiconductors when conjugation is achieved during polymerization process [5]. Consequently, I will introduce a 2D material with kagome lattice which shows extraordinary electronic properties, namely multiple Dirac signatures and flat bands [6].

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Interlayer engineering in tuning physical properties of two-dimensional materials

Wei Ji
Department of Physics, Renmin University of China, China

Short biography:
Dr. Ji, Wei is a computational physicist, working in the field of surface and interface modeling of low-dimensional materials. His research interests include surface and interface modeling of emerging electronic materials and devices. Recently, he focuses on theoretical modeling of electronic, optical, and vibrational properties of two-dimensional materials. He has been also developing theoretical methods for describing beam effects in scanning transmission microscopy and understanding ultrahigh resolution in noncontact atomic force microscopy. He received his Ph.D in condensed matter physics from the Institute of Physics, Chinese Academy of Science in 2008. Prior to joining Renmin University of China, he spent four years in McGill University as a visiting scholar and then a postdoctoral fellow. He was originally appointed as an Associated Professor by Renmin University in 2010 and was early promoted to Full Professor in 2014. He was supported by the National Young Top-Notch Talent Program in 2014 and the National Science Fund for Excellent Young Scholars in 2016 and awarded Chang-Jiang Young Scholars in 2015. He also serves as trustees in the youth committee and computational materials science division of the Chinese Materials Research Society.

Abstract:
Van der Waals forces were believed dominant for interlayer interactions in layered two-dimensional (2D) materials. We recently found an emergent type of interlayer interactions, namely covalent-like quasi-bonding (CLQB) [1,2], in various 2D materials like black phosphorus [1,2], PtS2 [3], PtSe2 [4] and Te [5] few-layers. The existence of CLQB in Te allows to tune various Te phases from its bulk form (the alpha-phase) upon charge doping or external strain [6]. In addition to the known beta and gamma phases, At least three new phases, namely, delta, epsilon and zeta phases was found during charge doping and sliding of layers [7]. Among these phase, the alpha to gamma phases are semiconducting and the rest are metallic. In light of this, it might be a promising strategy to build all-Te electrical devices, since Te has both semiconducting and metallic phases, which show considerable stability and rather high carrier conductance. In addition, we discussed the interlayer magnetic couplings (IMC) of CrS2 and CrI3 bilayers. It is interesting that these two materials are at two extremes of IMC. The interlayer FM coupling in CrS2 is very robust and is nearly unable to be tuned under usual external fields, but the intra-layer magnetism does be varied under layer stacking [8]. An opposite case was found in CrI3 bilayers [9] where the intra-layer FM coupling is, however, very strong but the interlayer magnetism was found governed by a subtle change of interlayer stacking; this shows a decoupled magnetic interaction between intra- and inter-layer directions.

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Graphene Flagship

Jari Kinaret
Chalmers University, Sweden

Short biography:
Jari Kinaret is the leader of the Condensed Matter Theory (CMT) group at the Department of Physics at Chalmers University of Technology (Sweden) and the Director of the Graphene Flagship. He has a background in theoretical physics and electrical engineering and received his PhD in Physics from the Massachusetts Institute of Technology in 1992. He has been at Chalmers since 1995 and his research focuses on electrical and mechanical phenomena on the nanoscale. Jari Kinaret is a member of The Royal Swedish Academy of Engineering Sciences (IVA).

Graphene and related 2D materials for perovskite solar cell applications

Emmanuel Kymakis
Electrical Engineering Department, University of Applied Sciences Crete (TEI of Crete), Greece

Short biography:
Emmanuel Kymakis is a full Professor and Head of Department of Electrical Engineering at the University of Applied Sciences (TEI of Crete). He received the B.Eng. (First Class Honours) degree in Electrical Engineering & Electronics from Liverpool University in 1999 and the Ph.D. degree in Electrical Engineering from Cambridge University in 2003. He and Prof. Gehan Amaratunga are the inventors of the polymer-nanotube solar cell. His research is focused on the synthesis and solution processing of graphene and other two-dimensional materials with tailored properties, for the development of next generation, solution processed electronic and photovoltaics, compatible with roll-to-roll large area manufacturing methods. He has 100 SCI publications and over 6.500 citations with an h-index of 41. He has been an honorary lecturer at UConn and a recipient of an Isaac Newton and an EPSRC studentship. He was named as a 2014 ChemComm Emerging Investigator and has received two National Excellence Awards. He has served as a member of the general assembly of the Greek Foundation of Research & Innovation. He is currently the deputy leader of the Energy Generation WP of the FET-Flagship Initiative Graphene and a member of Engineering sectoral scientific council of the National Council for Research & Innovation of Greece.
Google Scholar Profile: https://scholar.google.gr/citations?user=AWrgzokAAAAJ&hl=el
Group website: http://nano.teicrete.gr/

Abstract:
Over the last years and after Tsutomu Miyasaka 2009 first demonstration of perovskite application as a solar cell device, implausible advances have been made in the field of perovskite photovoltaics (PePV), offering great prospects for high efficient, low cost and flexible power generators. The power conversion efficiency (PCE) of PePV devices underwent a rapid progress, showing a record high PCE value higher than 23%, within only six years. This is the fastest progress rate a scientific topic has experienced rivalling the current market leader silicon. However, the long-term stability is the most important hurdle that impedes perovskite PVs commercialization, given the achieved record efficiency in on parity with that of commercial silicon PVs. The observed degradation under prolonged illumination arises from external issues, such as chemical decomposition due to the presence of water, thermal stress, UV, electrochemical reactions at the interfaces and intrinsic issues in the halide perovskite itself.
Recently, both the performance and stability of PSCs have been enhanced through the utilization of graphene and related 2D materials (GRMs) to fine control the interface properties between the different layers in the PSC structure. In particular, the best recorded operation lifetime of PSCs (T95) is at 1000 hrs at the maximum power point and at 60oC for mesoscopic solar cells, utilizing a reduced graphene oxide spacer layer between copper thiocyanate and the metal electrode, highlighting the importance of interface engineering in the stability improvement.
In this talk, I will give an overview of our recent activities on the GRMs interfacial engineering for the realization of high efficient and stable perovskite solar cells and modules. I will review the progress of the utilization of GRMs in the electron and hole transport layer of PePVs and demonstrate their significant impact in the PVs field. Moreover, I will directly correlate the outdoor stability measurements of GRM based PePVs with environmental parameters, such as temperature, humidity, and intensities of both ultraviolet and visible illumination, while at the same time, compare their PV outdoor characteristics with different PV technology modules, such as organic and silicon solar modules.

Construction of Palladium Selenide Island on Graphene

Xiao Lin
University of Chinese Academy of Sciences, China

Short biography:
Xiao Lin obtained his Ph. D in Physics under the supervision of Prof. Hong-Jun Gao in Institute of Physics, CAS in 2006. After postdoctoral research supported by Humboldt Foundation with Prof. Hans-Joachim Freund in Fritz Haber Institute of Max Planck Society in Berlin, he became a staff scientist in Pacific Northwest National Laboratory in Washington State. Now, he is a professor in University of Chinese Academy of Sciences. His main research interest is focused in the area of two-dimensional atomic crystals with scanning tunneling microscopy.

Abstract:
Palladium selenide islands were constructed on graphene-SiC(0001) substrate by molecular beam epitaxy (MBE). The structural and electronic properties of the islands were studied by scanning tunneling microscopy (STM) and spectroscopy (STS) combined with density functional theory (DFT) calculations. Islands were found growing continuously across monolayer graphene (MLG) - bilayer graphene (BLG) steps, a bandgap of 1.15 ± 0.07 eV has been revealed and a rigid bandgap shift of 0.2 eV is observed on palladium selenide islands on MLG as compared to on BLG.

Acknowledgements:
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Growth and Application of Meter-sized Single-crystal Graphene

Kaihui Liu
Peking University, China

Short biography:

Prof. Kaihui Liu's research efforts resolve around the structures and physics of low-dimensional materials, with focus on the development of advanced techniques to solve the scientific issues in materials sciences. His main contribution includes: (1) The development of joint nano-optical spectroscopy and transmission electron microscopy with high spatial resolution of single atom and high time resolution of 100 fs; (2) quantitative study of the electronic/phonon quantum couplings and ultrafast charge transfer in atomic-layered materials; (3) realization of recorded ultrafast growth and meter-sized epitaxial growth of graphene single crystals. Thus far, Dr Liu. has published 73 peer-reviewed papers (48 with IF>7), including first- or corresponded-authored Nature Nanotechnology (3), Nature Physics, Nature Communications (3), PNAS, Advanced Materials (5), JACS (2), Nano Letters (1), ACS Nano (2). He applied 16 patents with 6 issued. Dr. Liu was awarded the National Science Fund for Excellent Young Scholar of China, National Thousand Talents Plan for Young Scholars of China, Sub-project leader of National Key R&D Plan of China, First-Class Science & Technology Award of Beijing, and Excellent Young Scholar of Beijing. Currently he served as the associate editor of Science Bulletin and advisory board member of IOP Nanotechnology and Nano Future.

Abstract:

Graphene is of only one atomic layer thick and its property is therefore very sensitive to the interfacial interaction with other materials. By designing and utilizing this interfacial interaction, we have lots of opportunity in engineering the growth and properties of graphene. In this talk I will introduce several our recent works on this topic, including ultrafast graphene growth [1, 2], epitaxial meter-sized single-crystal graphene growth [3], perfect anticorrosion by graphene coating [4], and ultrafast broadband charge collection by graphene electrode [5].

Key words: Graphene, Growth, Physics

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Understanding optical absorption and luminescence in hBN: a tool for a characterisation metrics from bulk to the monolayer

Annick Loiseau
Centre National de la Recherche Scientifique, Onera, France

Short biography:
I am a Physicist with a large expertise in Condensed Matter Physics, Nanoscience, and in Transmission Electron Microscopy (TEM) and spectroscopies techniques. My researches were first focused on phase transitions phenomena in metallic alloys studied thanks to dedicated TEM experiments. From 1994, I progressively turned my researches towards the Nanosciences, and I have been leading one of the pioneering teams in France, conducting research on the synthesis, structural, electronic and optical properties of 1D and 2D objects issued from van der Waals materials such as graphene and boron nitride. I published in 1996 the first experimental observation of boron nitride single wall nanotubes and co-authored in 1997 the first paper on large scale synthesis of carbon single wall nanotubes. These skills led me to implement from 1998 at CNRS-Onera interdisciplinary research programs on nanotubes and extended now to graphene and other 2D materials. Main researches have included developing synthesis techniques of various kinds of single wall nanotubes and of 2D materials, understanding and modelling their formation mechanisms, developing optoelectronic devices for metrology applications. Few examples of my main researches achievements include nucleation/growth model of carbon nanotubes used as a reference worldwide, characterization metrics using TEM, electron and optical spectroscopies. Within the Graphene Flagship, I am leading in WP3 the Task on the synthesis and characterization of BN layers and BN based heterostructures. My activity in WP3 is focused on the synthesis of BN films by scalable CVD techniques and understanding of their spectroscopic properties by luminescence and EELS, with the goal of capitalizing them for developing a characterization metrics. This effort is now extended to Black Phosphorus.

Abstract:
hBN layers meet a growing interest for deep UV LED [1] and has become a strategic material for the fabrication of van der Waals heterostructures. Stacked with any other 2D material it can reveal the best of their physical properties [2]. However, hBN optoelectronic properties remain much less characterized and understood than other 2D materials.
In this talk, we review recent advances made thanks to the development of appropriate spectroscopies in the UV range - cathodoluminescence (CL) at 4K and Raman [3,4], angular resolved EELS [5] combined with ab initio simulations and tight binding modeling [6]. Thanks to these tools, a h-BN characterization metrics has been developed on the basis of their original optical properties, governed, in the energy range 5.5 – 6 eV, by strong excitonic effects easily trapped at structural or chemical defects [3]. We shall discuss the interplay between structure, defects and spectroscopic properties and how these properties can be further exploited for sample benchmarking [3, 7]. Beyond this effort, the talk will also address the recent advances made for the understanding of the high luminescence observed although bulk hBN is an indirect band gap material [1,8,9]. To that aim, the efficiency of radiative recombinations has been measured on a reference single crystal using temperature - dependent CL and compared to that diamond and ZnO [10]. The luminescence of hBN is confirmed to be unusually high and is found to remain constant from 10 to 300K. Enlighting analysis of this behaviour is provided by ab initio calculations of the exciton dispersion in bulk hBN. First, the lowest-energy exciton (iX) is found at 5.97eV and to be indirect, as expected for an indirect band gap, with a binding energy equal to 300 meV. This dispersion behavior accounts for an assignation of the luminescence to phonon assisted recombinations of the indirect exciton as proposed in [11] and for the assignation of the tiny peak observed in CL spectra at 5.956 eV to the zero-phonon radiative recombination of iX [10]. Further iX high binding energy is consistent with the temperature behaviour

of the luminescence, the high yield being the signature of a strong exciton phonon coupling. Second, calculations also confirm the direct exciton (dX) with a binding energy of 670 meV [10], an energy which turns to be only 100 meV above the indirect one. It comes out that bulk hBN displays a peculiar behavior where luminescence and optical absorption are due to different excitons, one resonant and one non-resonant [10].

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Selective gas permeation in graphene oxide-polymer self-assembled multilayers

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Short biography:

Vincenzo Palermo is the vice-director of the Graphene Flagship project and former leader of the work package on composites of the Flagship. He holds a joint position as research director of the National Research Council of Italy, and research professor at the university of Chalmers in Goteborg, Sweden.
In his work, he uses nanotechnology and supramolecular chemistry to create new materials for mechanical, electronics and energy applications. In particular, he works on the production of carbon-based composite materials and on the characterization of their structure and charge transport at the nanoscale. He has published >140 scientific articles on international journals in chemistry, nanotechnology and materials science (>5000 citations, h-index=38).
He has won the Lecturer Award for Excellence of the Federation of European Materials Societies (FEMS), the Research Award of the Italian Society of Chemistry (SCI) and the Science dissemination award of the Italian book association. He is actively involved in science dissemination giving seminars to high-school students and laymen on the interplay between science and history. He has published two books on the life and science of Albert Einstein (Hoepli, 2015) and of Isaac Newton (Hoepli, 2016).

Abstract:

The performance of polymer-based membranes for gas separation is currently limited by the Robeson limit, stating that it is impossible to have high gas permeability and high gas selectivity at the same time. We describe the production of membranes based on graphene oxide (GO) and poly(ethyleneimine) (PEI) multilayers able to overcome such limit.
The PEI chains acts as molecular spacers in between the GO sheets, yielding a highly reproducible, periodic multi-layered structure with constant spacing of 3.7 nm, giving a record combination of gas permeability and selectivity. The membranes feature a remarkable gas selectivity (up to 500 for He/CO_2), allowing to overcome the Robeson limit. The permeability of these membranes to different gases depends exponentially on the diameter of gas molecule, with a sieving mechanism never obtained in pure GO membranes, in which a size cut-off and a complex dependence on the chemical nature of the permeant is typically observed.
The tunable permeability, the high selectivity and the possibility to produce coatings on a wide range of polymers represent a new approach to produce gas separation membranes for large-scale applications.

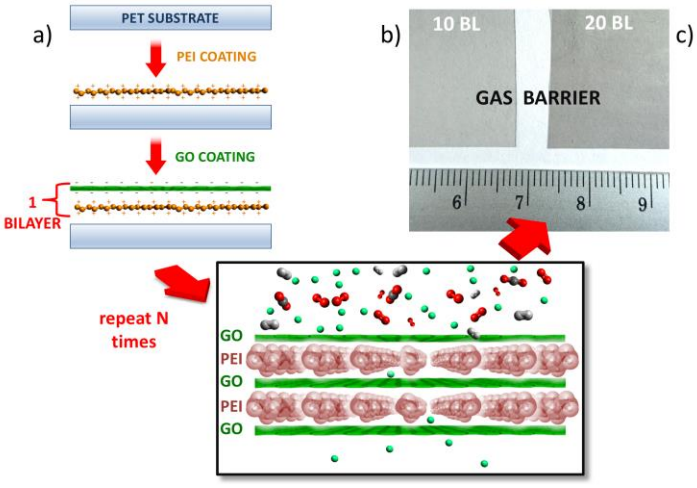

Fig. 1. a) Schematic procedure of the multilayer assembly to form a variable number of GO-PEI bilayers (BL). This is a simplified representation of the real system; b,c) Photograph of PET samples coated by different numbers of GO-PEI bilayers.

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Charge, Thermal and Spin Transport in Graphene Composites & Polycrystalline Heterostructures

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Short biography:
Stephan Roche is ICREA professor at the Catalan Institute of Nanosciences and Nanotechnology (ICN2) and the Barcelona Institute of Science and Technology. He leads the Theoretical and Computational Nanoscience group which focuses on quantum transport in Dirac materials (graphene and topological insulators). He pioneered the development of linear scaling computational approaches for wave packet dynamics, Kubo conductivities, and Landauer–Büttiker conductance in disordered materials. He received, in 2009, the Friedrich Wilhelm Bessel prize from the Alexander von Humboldt Foundation (Germany) in recognition of his outstanding contributions to the field of Computational Nanosciences. Since 2011 he has been actively involved in the European Graphene Flagship project, and currently appointed as the deputy leader of the Graphene Spintronic work package.

Abstract:
I will discuss charge, thermal and spin transport in chemically and structurally complex forms of graphene accounting from substrate effects, polycrystalline morphology of CVD graphene (and hBN), and chemically functionalization; all aspects being of crucial relevance for the development of applications in flexible and transparent electronics, energy harvesting and spintronics. Multiscale simulation and predictive modelling will be shown to enable simulations of physical properties in realistic models of very large system sizes (with up to 1 billion atoms), reaching the experimental and technology scales.

After introducing some challenges about the modelling of graphene composites I will present quantitative analysis of charge and thermal transport properties in graphene materials in presence of structural imperfections as produced during the wafer-scale production of graphene through chemical growth (CVD), the chemical transfer to versatile substrates, and the device fabrication. Fundamental properties of charge mobilities in polycrystalline graphene, accounting the variability in average grain sizes and chemical reactivity of grain boundaries as observed in real samples grown by CVD will be presented, together with their relevance for device optimisation and diversification of applied functionalities such as chemical sensing [1].

In a second part, I will also briefly explain the current state-of-the-art in understanding spin transport in graphene and how spin manipulation can be engineered through the fabrication of van der Waals heterostructures, fostering progress towards the design of non-charge based revolutionary information processing and computing.

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Leveraging the properties of 2D materials: chemical tailoring of multifunctional foams and coatings

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Short biography:

Paolo Samorì (Imola, Italy, 1971) is Distinguished Professor (PRCE) and director of the Institut de Science et d'Ingénierie Supramoléculaires (ISIS) of the Université de Strasbourg (UdS) where he is also head of the Nanochemistry Laboratory. He is also Fellow of the Royal Society of Chemistry (FRSC), fellow of the European Academy of Sciences (EURASC), member of the Academia Europaea (MAE) and junior member of the Institut Universitaire de France (IUF). He obtained a Laurea (master's degree) in Industrial Chemistry at University of Bologna in 1995. In 2000 he received his PhD in Chemistry from the Humboldt University of Berlin (Prof. J. P. Rabe). He was permanent research scientist at Istituto per la Sintesi Organica e la Fotoreattività of the Consiglio Nazionale delle Ricerche of Bologna from 2001 till 2008 and Visiting Professor at ISIS from 2003 til 2008. He has published >290 papers on nanochemistry, supramolecular sciences, materials chemistry, and Scanning Probe Microscopies with a specific focus on graphene and other 2D materials as well as functional organic/polymeric and hybrid nanomaterials for application in opto-electronics, energy and sensing. His work has been awarded various prizes, including the E-MRS Young Scientist Award (1998), the MRS Young Scientist Award (2000), the IUPAC Prize for Young Chemists (2001), the "Vincenzo Caglioti" Award (2006), the "Nicolò Copernico" Award (2009), the "Guy Ourisson" Prize (2010), the ERC Starting Grant (2010), the CNRS Silver Medal (2012), the Spanish-French "Catalán-Sabatier" Prize (2017), the German-French "Georg Wittig - Victor Grignard" Prize (2017), the Surfaces and Interfaces Award of the Royal Society of Chemistry (2018) the Blaise Pascal Medal in Materials Science of the European Academy of Sciences (2018) and the Grand Prix Pierre Süe of the Société Chimique de France (2018). In 2018 he was appointed Advisory Professor at the Shanghai Jiao Tong University, China. He is Associate Editor of Nanoscale and of Nanoscale Advances (RSC) and he is member of the Advisory Boards of Advanced Materials, Small, ChemPhysChem and ChemPlusChem (Wiley-VCH), Chemical Society Reviews, Chemical Communications and Journal of Materials Chemistry (RSC), ACS Nano and ACS Omega (ACS).

Abstract:

During the last decade the scientific community has witnessed a tremendous progress on the production and properties optimization of 2D materials for numerous technological applications in opto-electronics, energy (generation and storage), photonics, etc. Next major steps forward from both fundamental and more technological viewpoint require the fine tuning of the properties of such extraordinary materials, in view of the specific applications. Such a modulation can be achieved by combining the extraordinary characteristics of the single layers with the virtually-infinite variety of molecular systems each holding specific properties, thereby developing advanced hybrid materials exhibiting enhanced or novel functions for the chosen applications.

In my lecture, I will review our recent activity on the covalent and non-covalent functionalization of layered materials with ad hoc (macro)molecules in order to create artificial responsive hetero-structures as well as functional foams and coatings which can operate as selective chemical sensors for ions and polar molecules. I will describe how the same approaches can be exploited to fabricate highly sensitive pressure sensors which can monitor heartbeats, thus holding great potential for their integration in medical diagnostic devices or sport apparatus.

Overall my lecture will offer a hint on the chemist's toolbox to generate multifunctional 2D materials-based nanocomposites with ad-hoc properties to address societal needs in electronics, sensing and energy applications.

Interfacial Interactions in van der Waals Heterostructures of MoS2 and graphene flakes

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Short biography:
Ping-Heng Tan is a Professor at Institute of Semiconductors, Chinese Academy of Sciences. He obtained his B.S. at Peking University and completed his Ph.D. at Chinese Academy of Sciences. His current research focuses on the optical properties of two-dimensional layered materials. He had published over 180 peer-reviewed papers in scientific journals. He was supported by NSFC for Distinguished Young Scholars in 2012 and was awarded Huang Kun prize in Physics in 2015. Now, he is the Editorial Board members of "Journal of Raman Spectroscopy", "Semiconductor Science and Technology", and "npj 2D Materials and Applications". He is also Director of Chinese Light Scattering Committee of Chinese Physical Society (CPS), Member of CPS council, Member of organizing committee of CPS Fall Meeting, Convener of Semiconductor Physics Session of CPS Fall Meeting, international expert of IEC/TC113/WG8 and the member of International Steering Committee of ICORS.

Abstract:
Vertical van der Waals heterostructures (vdWHs) are formed by vertically stacking various two-dimensional materials (2DMs) by van der Waals (vdW) forces but without any constraint of lattice matching and fabrication compatibility. vdWHs offer promising properties and intriguing possibilities for controlling and manipulating charge carriers, excitons, photons, and phonons within these atomic interfaces, facilitating the design of unique electronic and photonic devices. Normally, monolayer graphene (1LG) and transition metal dichalcogenides (TMDs) are two types of essential building blocks for vdWHs. Graphene is not suitable for channelmaterial in transistors owing to the lack of an energy gap. TMDs are not suitable for high-speed electronic devices owing to their low mobility. However, the TMD/graphene vdWHs have been used for various highperformance devices, such as field-effect tunneling transistors, logic transistors, and photovoltaic andmemory devices by taking advantages of the high mobility of graphene and the natural band gap of TMDs. Until now, 1LG and multilayer graphene (MLG) sheets have been widely used as electrodes in vdWH-based devices to achieve higher performance compared to devices with directly deposited metal contacts. An atomically sharp and nondamaging interface in the TMD/graphene vdWHs can be obtained to minimize defects and prevent the Fermi-level pinning, leading to a much lower Schottky barrier height between graphene and TMDs. The van der Waals coupling at the interface of vdWHs is mainly dependent on the distance, twist angle, and stacking order of disparate 2DMs. Therefore, it is very important to investigate the interface interactions in vdWHs for their future high-performance device applications.
Here, we report the ultralow-frequency Raman spectroscopy investigation on interfacial couplings in the vdWHs formed by graphene and MoS2 flakes. [1] Because of the significant interfacial layer-breathing couplings between MoS2 and graphene flakes, a series of layer-breathing modes with frequencies dependent on their layer numbers are observed in the vdWHs, which can be described by the linear chain model. It is found that the interfacial layer-breathing force constant between MoS2 and graphene is comparable with the layer-breathing force constant of multilayer MoS2 and graphene. The results suggest that the interfacial layer-breathing couplings in the vdWHs formed by MoS2 and graphene flakes are not sensitive to their stacking order and twist angle between the two constituents. Our results demonstrate that the interfacial interlayer coupling in vdWHs formed by two dimensional semimetals and semiconductors can lead to new lattice vibration modes, which not only can be used to measure the interfacial interactions in vdWHs but also is beneficial to fundamentally

understand the properties of vdWHs for further engineering the vdWHs-based electronic and photonic devices. [2,3]

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Epitaxial Growth and Properties of 2D Monolayer Antimonene

Yeliang Wang
Beijing Institute of Technology, China

Short biography:
Dr. Yeliang WANG was an undergraduate in material science at the Wuhan University of Technology, after which he moved to Institute of Physics (IOP), Chinese Academy of Sciences (CAS) where he studied condensed matter physics and was awarded a PhD in 2004. He then joined in the nanoscale science department (hosted by Prof. Klaus Kern) as a Humboldt fellow in the Max-Planck-Institute for Solid Research, Germany. He was appointed to an associated professorship in 2008 and a full professorship in 2013 in the Institute of Physics, CAS (in the department hosted by Prof. Hong-jun Gao). He was awarded the distinguished youth scholars by National Scientific Foundation of China in 2017. In 2018, he set up a research group in Beijing Institute of Technology (BIT).
Prof. Wang's research interests focus on the deliberate steering of growth at solid surfaces in ultra-high vacuum conditions(UHV) in aim of fabricating low-dimensional functional nanomaterials, including graphene and its analogues, semiconductor quantum dots, metallic clusters/ films, (bio)molecule and molecular-metallic complex. The physical/chemical properties of these novel systems at a single atomic/molecular level are explored by several advanced techniques like LEED, STM/STS, Raman, XPS and ARPES. He held more than 80 papers published on high-profile journals including one in Nature Materials, one in Phy.Rev.Lett, seven in Nano Letters, three in J.Am.Chem.Soc., and five in Advanced Materials.

Abstract:

The novel properties of graphene honeycomb structure have spurred tremendous interest in investigating other two-dimensional (2D) layered structures beyond graphene for nanodevices. In this talk, I will mention the fabrication and properties of several 2D materials such as graphene, such as, silicene [1], germanene [2] hafnene [3] and antimonene [4], wherein silicon (germanium, hafnium or antimony) atoms are substituted for carbon atoms in graphene. Besides mono-elemental 2D atomic crystals, bi-elemental 2D materials, such as magnetic VSe¬2 monolayer [5], semiconducting PtSe2 monolayer and its intrinsically patterns [6,9], and superconductor transition-metal-trichalcogenide (HfTe3) [7], grown by direct selenization/tellurization of the Pt/Hf substrate, as well as their application exploring in nanoelectronics and valleytronics will also be introduced. In addition, the stacking heterolayers based on several these kinds of 2D materials, for instance, a superconductor-topological insulator layered heterostructure (with a HfTe3/HfTe5 layered configuration) for Majorana bound states will be also presented [8]. The precise structural configurations at atomic-resolution of these materials will also be introduced, based on the measurements by several advanced techniques like LEED, STM/STS and STEM.

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Polymorphism in Elemental 2D Materials

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Short biography:
Kehui Wu is a research group leader in the State Key Laboratory for Surface Physics, Institute of Physics (IOP), Chinese Academy of Science (CAS). He received his Ph.D. degree in condense matter physics from the IOP, CAS in 2000. He was then a postdoctoral fellow at Tohoku Univ., Japan from 2000 to 2004. In 2005 he came back China and joined IOP as a professor. His research field is the growth of low dimensional materials by molecular beam epitaxy, and in-situ, atomic-level characterization of by scanning tunneling microscopy (STM) and related techniques. His recent works include experimental realization of silicene and borophene.

Abstract:
Graphene is a 2D layered material that can be obtained from graphite by cleavage. Silicene and borophene, on the other hand, are non-layered 2D materials that can only be prepared in ultrahigh vacuum (UHV) on appropriate substrates. Interestingly, both silicene and borophene exhibit polymorphism, meaning that a great number of different but similar 2D lattices may exist despite they consist of only single element (Si or B). The polymorphism of silicene arises from the vertical buckling of atomic in a hexagonal lattice, while the polymorphism of borophene arises from periodic hole patterns in a planar, triangular lattice. Both of them are in sharp contrast to graphene where the planar hexagonal lattice allows no polymorphism. In this talk, I will discuss the effects of polymorphism on the properties of silicene and borophene, and the experimental challenges induced by polymorphism in these two systems.

Synthesis and characterizations of graphene and graphene/superconductor hetero-structures

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Shanghai Institute of Microsystem and Information Technology, CAS, China

Short biography:
Xiaoming Xie received his Ph.D degree in 1990 in Shanghai Institute of Microsystem and Information Technology, Chinese Academy of Sciences (SIMIT-CAS). He is a full research Professor at SIMIT and distinguished adjunct Professor at ShanghaiTech University. At the same time, he serves as the vice director of SIMIT and director of the center for excellence in superconducting electronics, Chinese Academy of Sciences. His main research interests include two-dimensional quantum materials, superconducting materials and hetero-structures, development of superconducting devices and applications. He has contributed to 279 publications in scientific journals with 3542 citations and was granted 95 patents, including 5 international patents.

Abstract:
In this talk, I will report our research on the synthesis of graphene and graphene/superconductor hetero-structures. By using local feeding of carbon precursor on Cu85Ni15 foil with moderate carbon solubility, we realized creating single nucleus of graphene and drove its growth up to 1.5” in size. The growth followed a very fast new isothermal segregation mechanism, involving carbon dissolved in the alloy bulk. Single crystalline Cu85Ni15 film can be fabricated on sapphire substrate by magnetic sputtering and appropriate annealing, which enabled the oriented epitaxial growth of ultra-flat single crystalline graphene at much lower temperatures. Epitaxial growth of wafer-sized single crystalline graphene was also realized on Ge (110), thus illuminating the concern for metal contamination. We fabricated graphene/Bi2Sr2Ca1Cu2Ox (BSCCO) hetero-structure with different thickness of BSCCO by mechanical exfoliation. BSCCO is a well-known high temperature superconductor but reported to be insulating when thinned down to unit-cell-thick. With the protection of a graphene layer on top, we confirmed the existence of high temperature superconductivity in graphene/BSCCO hetero-structure down to half-unit-cell-thick of BSCCO. Two magnetic-field-induced quantum critical behaviors were reported by other research group at LaTiO3/SrTiO3 interface and interpreted as the due to coupling of two dimensional electron gas and disordered superconducting puddles at the interface. We deposited superconducting tin islands on graphene/Ge. With magneto-resistivity measurements, we were able to duplicate a very similar phase diagram as that reported in LaTiO3/SrTiO3 interface. The superconductor/graphene hybrid structure offered a unique material platform for the further study of quantum phase transition in two-dimensional system.

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Atomic and electronic structures of transition metal dichalcogenides heterostructures

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Short biography:
Dr. Chendong Zhang got his Ph.D in 2011 from the Institute of Physics, Chinese Academy of Sciences. From 2011 to 2016, he worked in the University of Texas at Austin as a postdoctoral scholar. He joined the School of Physics and Technology of Wuhan University in 2017. He has specialized in the vdW 2D materials, scanning tunneling microscopy and spectroscopy, and thin film growth.

Abstract:

The emerging atomic layer materials offer a remarkably wide range of building blocks of nanostructures. Key advantages of these van der Waals materials include a broad span of energy gaps, flexibility of stacking different types of materials to form heterostructures, tunability in material properties by doping and strain, and the relative ease of integration with other electronic and photonic devices. This talk will be focused on our recent work in probing the atomic and electronic structure of transition metal dichalcogenides (TMDs) heterostructures, including both vertical and lateral structure. I will first show that in vertically stacked MoS2/WSe2 heterostructures, how the interlayer coupling can be used as a new designing parameter to create a lateral 2D electronic superlattices. For lateral WSe2-MoS2 heterostructure, we present a novel method to determine the anisotropic strain based on Moiré pattern imaging. The 2×2 strain tensor is imaged with nanometer spatial resolution. We also determine the band offset across the junction and show that the strain effect converts the otherwise type-II into type-I band alignment. Moreover, a “line interface specific” electronic structure due to the specific bonding configuration is discovered at the interface.

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Scalable monolayer MoS2 for electronic devices

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Education & Working Experience:
1995-1999 Shandong University, BS
1999-2004 Institute of Physics CAS, PhD
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Research interests:
Low dimensional, especially 2D, materials
Quantum transport properties
Novel electronics based on 2D materials

Abstract:

2D semiconductors have potentials to extend the current semiconductor-based sciences and technologies, benefiting from their ultra-thin bodies and the ease of surface and interface modulations. In this presentation, I will introduce our recent progress on scaled-up growth of monolayer MoS2 and engineering of its surface and interface properties towards electronic applications.

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Exploring strain effect at 2D material interfaces at the atomic scale

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Short biography:
Wu Zhou is a Professor in School of Physical Sciences and leads the electron microscopy laboratory at the University of Chinese Academy of Sciences (UCAS) in Beijing, China. Prior to joining UCAS, he was a Staff Scientist at Oak Ridge National Laboratory (ORNL), USA. He received his B.S. degree in 2006 from Tsinghua University (Beijing, China) and his Ph.D. in 2010 from Lehigh University (USA), both in Materials Science and Engineering. Wu's research is focused on understanding the behavior of functional materials at the atomic scale using cutting edge electron microscopy techniques and theoretical modeling, with focuses on 2D materials, battery materials, and catalysts.

Abstract:

Two-dimensional (2D) materials have attracted intense research efforts in the past decade due to many unique properties and promising applications of these atomically thin layered materials. Their physical properties can be further tailored by lattice strain, which provides new means to create new functionalities in 2D materials via strain engineering. In this presentation, I will discuss two examples from our recent studies to explore the interplay of strain and lattice structure at 2D semiconductor interfaces, using a combination of low-voltage aberration corrected scanning transmission electron microscopy (STEM) imaging and density-functional theory studies.

First, I will show that the van der Waals (vdW) interaction between two transition metal dichalcogenide (TMDC) layers can significantly modify the atomic arrangement in a mirror twin boundary (MTB) in bilayer TMDC films, leading to the development of a local strain field of a few nanometers in the vicinity of the MTB [1].

When stitching two different monolayer materials with lattice mismatch side-by-side, e.g. a selenide monolayer (WSe2 or MoSe2) and a sulfide monolayer (WS2 or MoS2), strain relaxation at the lateral mismatched interfaces often leads to misfit dislocation arrays, which are highly active during the high temperature chemical vapor deposition growth for the heterostructures. Insertion of metal and S atoms into the dislocation cores induces dislocation climb while concomitant selective substitution of Se atoms around the dislocation core by S atoms, driven by the local strain field, leads to the growth of WS2 and MoS2 quantum-well arrays embedded in the WSe2 and MoSe2 monolayers. Preliminary monochromatic electron energy-loss spectroscopy (EELS) analysis shows that the optical properties of such quantum well superlattices are considerably different from their parent 2D components. This misfit-dislocation-driven growth mechanism should be applicable to different combinations of 2D monolayers with lattice mismatch for the fabrication of a wide range of 2D lateral superlattices with width smaller than 5 nm, a regime where quantum size effect would come into play [2].

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Theoretical Design of 2D Ferroelectric and Multiferroic Materials

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Short biography:
Prof. Wenguang Zhu received his B.S. in physics at Peking University in 1999 and Ph.D. in condensed matter physics at the Institute of Physics, Chinese Academy of Sciences in 2004. After a postdoc appointment at Harvard University, he joined University of Tennessee in 2006 as a research assistant professor and then promoted to a research associate professor in 2011. He has been a full professor at University of Science and Technology of China since 2012.

Abstract:

In this talk, we will first present a discovery of a 2D ferroelectric materials family, rooted in III2-VI3 van der Waals materials and distinctly characterized by exhibiting versatile ferroelectricity with both in-plane and out-of-plane electric polarization [1]. This prediction has recently been confirmed experimentally by several research groups. The device potentials of these new 2D ferroelectric materials will be demonstrated using the van der Waals heterostructures. Based on these discovered 2D ferroelectric materials, we further propose a design of 2D multiferroic materials via doping a small amount of magnetic ions into the 2D ferroelectric material. This design provides a novel multiferroic system based on van der Waals 2D materials, and these 2D multiferroic materials are expected to have strong coupling between the ferroelectric polarization and the magnetic order.

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Rational Design 2D Porous Organic Materials for Energy Storage and Conversion

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Abstract:
Two-dimensional (2D) porous carbons and their composites have attracted tremendous attention from both science and industry communities due to their wide applications for energy storage and conversion. Surface area, dopants and dimensionality have been recognized to be the main features determining the performance of these porous materials. However, the rational synthesis of carbon-rich 2D porous materials with controlled porosity, heteroatom dopants and dimensionality still remain great challenge. Porous polymers, which are one kind of rising porous carbon precursors, can rational synthesized at molecular level due to the widely commercial available and designable heteroatom-containing monomers and different high yield polymerization methods. Most importantly, the 2D dimensionality can be controlled by using 2D materials, e.g. graphene, MXene and MoS2, as templates. Beyond 2D templates, both layered C=C bond linked covalent organic framework and single layered coordination polymer frameworks can be rational designed and synthesized. In this presentation, the energy related applications of 2D porous polymers and their derived porous carbons will be introduced, e.g., as electrodes for supercapacitors, as electrocatalysts for oxygen reduction reaction and hydrogen evaluation reaction, and as air-cathodes for Zn-air batteries.

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