

## Scientific Program

July 1 <sup>st</sup> , Monday, IOP Building M234	
9:00–9:10	<b>Opening Ceremony and Welcome Remarks</b> <b>Hong-Jun Gao</b> ( <i>Institute of Physics, CAS, China</i> )
9:10–9:20	<b>Photo</b>
9:20–10:20	<b>Session 1</b> <i>Chair: Karl-Heinz Ernst</i>
9:20–9:50	<b>Stephen J. Pennycook</b> ( <i>National University of Singapore, Singapore</i> ) “Designing Energy Materials via Atomic-resolution Microscopy and Spectroscopy”
9:50–10:20	<b>Katharina Uta Schlickum</b> ( <i>Institute for Applied Physics, Technical University Braunschweig, Germany</i> ) “High Resolution Characterization of Surface Products”
10:20–10:30	Coffee Break
10:30–12:00	<b>Session 2</b> <i>Chair: Stephen J. Pennycook</i>
10:30–11:00	<b>Karl-Heinz Ernst</b> ( <i>EMPA, Swiss Federal Laboratories for Materials Testing &amp; Research, Switzerland</i> ) “On-Surface Topochemistry of Helicenes”
11:00–11:30	<b>Andrew Wee</b> ( <i>National University of Singapore, Singapore</i> ) “The Molecule-2D Interface”
11:30–12:00	<b>Matthias Batzill</b> ( <i>University of South Florida, USA</i> ) “Properties of Monolayer Vanadium Dichalcogenides”
12:00	Lunch

14:00–15:30	<b>Session 3</b> <i>Chair: Jiandi Zhang</i>
14:00–14:30	<b>Werner Hofer</b> ( <i>Newcastle University, UK</i> ) “Many-body physics in real space”
14:30–15:00	<b>Thomas Jung</b> ( <i>Paul Scherrer Institute, Switzerland</i> ) “Thermally-activated Self-assembly and <i>In Situ</i> Oxidation of a Reduced Decaazapentacene”
15:00–15:30	<b>Changgan Zeng</b> ( <i>University of Science and Technology of China, China</i> ) “Flat Band, Magnetism and Topological Properties of Kagome Lattices”
15:30–15:40	Coffee Break
15:40–17:10	<b>Session 4</b> <i>Chair: Thomas Jung</i>
15:40–16:10	<b>Feng Wang</b> ( <i>University of California, Berkeley</i> ) “Engineering Correlated Physics in Two-Dimensional Moiré Superlattices”
16:10–16:40	<b>Guozhen Shen</b> ( <i>Institute of Semiconductors, CAS, China</i> ) “Growth of well-aligned Nano/Microwires for flexible photodetectors and image sensors”
16:40–17:10	<b>Lei Fu</b> ( <i>Wuhan University, China</i> ) “Precise Synthesis of 2D Atomic Crystals @ Liquid Metal”

**July 2<sup>nd</sup>, Tuesday, IOP Building M234**

9:00–10:30	<b>Session 5</b> <i>Chair: Zhichuan Xu</i>
9:00–9:30	<b>Jingcheng Li</b> ( <i>Nanoscience Cooperative Research Center, Spain</i> ) “Spintronic Devices Based on Graphene Nanoribbons”
9:30–10:00	<b>Aitor Mugarza Ezpeleta</b> ( <i>Catalan Institute of Nanoscience and Nanotechnology, Spain</i> ) “Nanostructuring graphene from 0D to 2D”
10:00–10:30	<b>Oliver Gröning</b> ( <i>EMPA, Swiss Federal Laboratories for Materials Testing &amp; Research, Switzerland</i> ) “Engineered Quantum States in Graphene Nanoribbons”
10:30–10:45	<b>Oxford Instruments</b>
10:45–11:45	Lab Tour
11:45	Lunch

14:00–15:30	<b>Session 6</b> <i>Chair: Matthias Batzill</i>
14:00–14:30	<b>Thomas Greber</b> ( <i>University of Zürich, Switzerland</i> ) “Functional Large Scale, Single Layer Hexagonal Boron Nitride”
14:30–15:00	<b>Zhichuan Xu</b> ( <i>Nanyang Technological University, Singapore</i> ) “Oxygen Electrocatalysis on Transition Metal Spinel Oxides”
15:00–15:30	<b>Chonglin Chen</b> ( <i>University of Texas at San Antonio, USA</i> ) “Direct Observation of Ultrafast Room Temperature Oxygen Redox Dynamics in Oxide Thin Films”
15:30–15:40	<b>Coffee Break</b>
15:40–17:10	<b>Session 7</b> <i>Chair: Chonglin Chen</i>
15:40–16:10	<b>Min Ouyang</b> ( <i>University of Maryland, USA</i> ) “Colloidal Spin Quantum Bits”
16:10–16:40	<b>Jiandi Zhang</b> ( <i>Louisiana State University, USA</i> ) “Can Ferroelectrics Get Along with Metallicity?”
16:40–17:10	<b>Yuyang Zhang</b> ( <i>School of Physics, UCAS, China</i> ) “The Observation of Majorana Zero Mode and Conductance Plateau in an Iron-based Superconductor”

**July 3<sup>rd</sup>, Wednesday, IOP Building M234**

9:00–10:30	<b>Session 8</b> <i>Chair: Andrew Wee</i>
9:00–9:30	<b>Francois Peeters</b> ( <i>University of Antwerp, Belgium</i> ) “Atomic Collapse and Flat Bands in Graphene”
9:30–10:00	<b>Qihua Xiong</b> ( <i>Nanyang Technological University, Singapore</i> ) “Ultrafast Charge Transfer in 2D Semiconductors and Heterostructures”
10:00–10:30	<b>Zheng Liu</b> ( <i>Nanyang Technological University, Singapore</i> ) “TMDs: Towards Electrochemical Electronics”
10:30-10:45	Coffee Break
10:45–11:45	<b>Session 9</b> <i>Chair: Qihua Xiong</i>
10:45-11:15	<b>Feng Miao</b> ( <i>Nanjing University, China</i> ) “Electronic Transport and Device Applications of 2D Materials”
11:15-11:45	<b>Lihong Bao</b> ( <i>Institute of Physics, CAS, China</i> ) “Observation of Weak Antilocalization Effect in Few-Layer VSe <sub>2</sub> ”
11:45	Lunch

14:00–15:30	<b>Session 10</b> <i>Chair: Thomas Greber</i>
14:00–14:30	<b>Hao Zeng</b> ( <i>Department of Physics, University at Buffalo, the State University of New York, USA</i> ) “Proximity Effects in Magnetic/TMD Heterostructures”
14:30–15:00	<b>Jian Shen</b> ( <i>Fudan University, China</i> ) “Complex magnetic domain structures in oxides: physical origin and device application”
15:00–15:30	<b>Ling Li</b> ( <i>Institute of Microelectronics, CAS, China</i> ) “Dimensionality Induced Crossover from Coulomb Blockade to Luttinger-Liquid in the Nonlinear Transport of Conducting Polymers”
15:30–15:40	<b>Coffee Break</b>
15:40–17:10	<b>Session 11</b> <i>Chair: Jian Shen</i>
15:40–16:10	<b>Liang Zhang</b> ( <i>The University of Manchester, UK</i> ) “To Tie or Not To Tie”
16:10–16:40	<b>Wu Zhou</b> ( <i>School of Physics, UCAS, China</i> ) “Low voltage aberration corrected STEM for 2D materials”
16:40-17:10	<b>Geng Li</b> ( <i>Institute of Physics, CAS, China</i> ) “Construction of graphene/silicene heterostructure by Si intercalation”

# Designing Energy Materials via Atomic-resolution Microscopy and Spectroscopy

Stephen J. Pennycook

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In recent years, the sensitivity of the electron microscope for imaging and spectroscopy has dramatically improved due to aberration correction, greatly assisting the correlation of atomic-scale structure and bonding to materials' properties. Trial and error materials' development is increasingly being replaced by atomic scale engineering, informed by the powerful combination of microscopy and theoretical calculations.

In catalysis for example, it has become almost routine to image single atoms and probe their coordination by spectroscopy, greatly aiding the development of so-called single atom catalysts (SACs). Their unique coordination can impart exceptional activity and selectivity, and much effort is ongoing to replace platinum group metals by cheaper, earth abundant metals such as cobalt or nickel. One example is the synthesis of graphene-supported cobalt SACs with a tunable high loading using atomic layer deposition that show exceptional activity and selectivity for the hydrogenation of nitroarenes to azoxy aromatic compounds.[1] Single Co atoms are visible in the Z-contrast image, and electron energy loss (EEL) spectra from them show that whenever Co is detected, so also is O; theory then shows that these proximal O atoms expose partially-filled Co-d orbitals, resulting in the excellent catalytic activity. Another example of a cobalt SAC uses porous nitrogen-doped carbon nanoflake arrays as support. These SACs show a lower oxygen evolution reaction (OER) overpotential and higher oxygen reduction reaction (ORR) saturation current than Co nanoparticle catalysts, showing that Co metal clusters are actually redundant for both the OER and ORR reactions.[2] The well-dispersed Co single atoms are the active sites, attached to the carbon network through N-Co bonding. The electrocatalyst was used as the air cathode in a solid-state Zn-air battery, achieving good cycling stability (2500 min, 125 cycles) and a high open circuit potential (1.411 V).

Single atom sensitivity is also important for developing thermoelectric materials. Whereas nanostructuring has been well appreciated, recently the key role of interstitials and interstitial clusters on thermal and electrical transport properties has also been elucidated.[3] In piezoelectrics, gradual atomic-scale polarization rotation among co-existing phases has been recently found in lead-free piezoelectrics,[4] a feature that seems common to all high-performance piezoelectric systems at phase boundaries.

## **References:**

- [1] H Yan et al., Nature Communications DOI: 10.1038/s41467-018-05754-9 (2018).
- [2] W Zang et al., ACS Catal, **8**, (2018) p. 8961.
- [3] Y Xiao et al., J Am Chem Soc, **139**, (2017) p. 18732.

## **characterization of surface products**

Uta Schlickum

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Molecular systems carry intriguing intrinsic functionalities that often come along with complex and dynamic structures. Here we present applications of high-resolution characterization by scanning tunnelling microscopy (STM) and atomic force microscopy (AFM) in ultra-high vacuum revealing structural details of biological relevant systems such as peptides as well as of reactants and products involved in on surface reactions. To be able to fabricate and image highly pure samples we employ Electrospray Ion Beam Deposition (ES-IBD) and an ultra-high vacuum suitcase to transfer the samples insitu into the low temperature scanning probe microscopes.

We can trigger a desulfurization reaction by the electric field confined in the tunnel junction of a scanning tunnelling microscope. The precise control of the external stimulus allows resolving the elementary reaction steps of this direct desulfurization process. An atomically precise reconstruction of the reactant and product was possible with the help of density functional theory calculations [1].

The Reichardt's dye molecule undergoes fragmentation reactions on a Cu surface. High resolution STM and AFM images clearly reveal the structure of the reactants, present on the surface after soft-landing, and reacted products created by thermal treatment or after an impact in the hyperthermal energy regime (5-100 eV) during ES-IBD. Our analysis allows the extraction of abundances as a function of collision energy, which hints towards a reaction mechanism in which the kinetic energy of the collision directly drives the reaction. As a consequence, we observe products that cannot be reached through thermal routes, which makes ES-IBD a unique tool for novel chemistry [2].

Combing ES-IBD with low temperature STM even allows determining under well controlled conditions structural properties of biologically relevant macromolecular systems like peptides. We investigate the self-assembly of peptides on surfaces and probe the interaction between specific amino acids at sub-molecular length scales. Our results show, how specific changes of the sequence can influence the self-assembly pattern due to the high conformational freedom of these molecular systems.

[1] B. Borca, T. Michnowicz, R. Pétuya, M. Pristl, V. Schendel, I. Pentegov, U. Kraft, H. Klauk, P. Wahl, R. Gutzler, A. Arnau, U. Schlickum, and K. Kern, *Electric field driven direct desulfurization*, ACS Nano 11, 4703 (2017).

[2] S. Rauschenbach, M. Ternes, L. Harnau & K. Kern, *Mass Spectrometry as a Preparative Tool for the Surface Science of Large Molecules*, Annu. Rev. Anal. Chem. 9, 16.1–16.26 (2016).



# On-surface topochemistry of helicenes

Anais Mairena<sup>1</sup>, Christian Wäckerlin<sup>1</sup>, Milos Baljovic<sup>1</sup>, Kevin Martin<sup>2</sup>, Narcis Avarvari<sup>2</sup>, Andreas Terfort<sup>3</sup>, Karl-Heinz Ernst<sup>1,4\*</sup>

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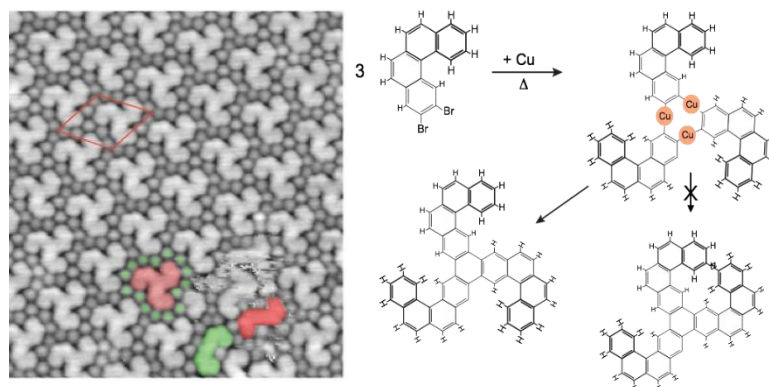
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**Keywords:** Helicene, On-surface chemistry, STM

Surfaces functionalized with helicenes are also of interest for chiroptical electronic devices or for electron-spin filtering. While self-assembled layers facilitate studying interesting phenomena, covalently linked chiral modified materials would be much more robust and therefore better suited for applications.

We report the stereoselective chemistry of different helicene species on noble metal surfaces. The stereochemical analysis of diastereoisomers formed on the surface is performed by scanning tunneling microscopy (STM). The Ullmann coupling reaction of 9-bromo[7]helicene proceeds with a high probability for heterochiral product, while homochiral products are favoured in C-C coupling dimerization and trimerization of 2-bromo[4]helicene and 2,3-dibromo-[4]helicene (Fig. 1). The diastereoselective chemistry is explained by topochemical effects due to the surface alignment of the helicenes during reaction.



**Fig. 1.** STM image of homochiral tris[4]helicene (trisphenanthro[3,4; 3',4'; 3'',4'']-b,h,n]triphenylene) after Ullmann coupling of dibromo[4]helicene. Each molecule is surrounded by bromine atoms (green dots) that were released in the C-C coupling reaction.

- [1] A. Mairena et al., *Chemical Science* 10, in press (2019)
- [2] A. Mairena et al., *J. Am. Chem. Soc.* 140, 15186 (2018)
- [3] A. Mairena et al., *J. Am. Chem. Soc.* 140, 7705 (2018)
- [4] A. Mairena et al., *Chem. Comm.* 54, 8757 (2018)
- [5] J. Li et al. *Chem. Comm.* 54, 7948 (2018)

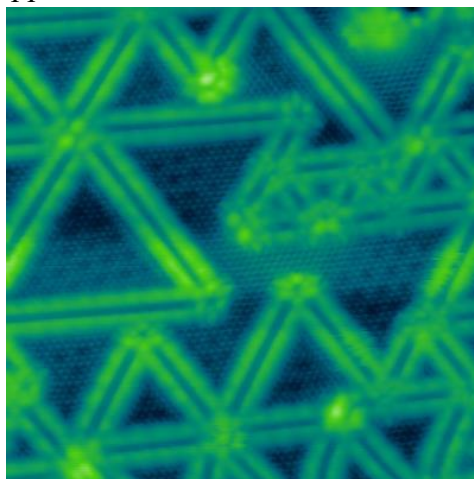
# The Molecule-2D Interface

Andrew Wee

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In this talk, Prof. Wee will introduce the research at the Surface Science Laboratory at NUS. In particular, he will present some recent work on the molecule-2D interface. In our laboratory, we use high resolution scanning tunneling microscopy/spectroscopy (STM/STS) and non-contact atomic force microscopy (nc-AFM) to study the atomic structure and local electronic properties of 2D graphene and transition metal dichalcogenides (TMDs) monolayers, e.g. MoS<sub>2</sub>, WSe<sub>2</sub>, MoSe<sub>2</sub>. Using monolayers of adsorbed organic molecules, we demonstrate the surface transfer doping of epitaxial graphene and TMDs. We also investigated the fabrication and electronic properties of a lateral doped/intrinsic heterojunction in 2D WSe<sub>2</sub>, partially covered with a molecular acceptor C<sub>60</sub>F<sub>48</sub>. Recent results of the self-organisation of DAP molecules on MoSe<sub>2</sub> (Fig. 1) will also be introduced. Our work shows the use of organic-2D hybrid heterointerfaces is a promising approach to manipulate the electronic properties for flexible and wearable applications.



**Fig. 1.** High resolution STM image of MoSe<sub>2</sub>

## **About the speaker:**

Professor Andrew Wee is a Professor of Physics, and Vice President (University and Global Relations) at the National University of Singapore (NUS). He is director of the Surface Science Laboratory, Fellow of the Singapore National Academy of Science (SNAS), Institute of Physics UK (IoP) and Institute of Physics Singapore (IPS), and an academician of the Asia-Pacific Academy of Materials (APAM). His research interests include scanning tunneling microscopy (STM) and synchrotron radiation studies of the molecule-substrate interface, graphene and 2D materials. He co-teaches an undergraduate class “Science at the Nanoscale”, and is a co-author of a textbook of the same title. He is an Associate Editor of ACS Nano, and on the Editorial Boards of several other journals. He holds a BA (Hons) and MA from the University of Cambridge, a DPhil from the University of Oxford, and a PGCE from the University of London.



# Properties of Monolayer Vanadium Dichalcogenides

Matthias Batzill

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Layered transition metal dichalcogenides (TMDCs) exhibit a wide range of electronic and many body properties, making them exciting materials for studying fundamental properties in the 2D-materials limit and/or to combine them into van der Waals heterostructures. In this talk we discuss the synthesis of monolayer TMDCs by van der Waals epitaxy and their characterization by mainly scanning tunneling microscopy (STM) and angle resolved photoemission spectroscopy (ARPES). Here we focus on the layer dependent variations of the properties of VSe<sub>2</sub> [1] and VTe<sub>2</sub>. For both materials we observe a charge density wave (CDW) behavior in the monolayer limit compared to their bulk properties. From ARPES and DFT we can also show that CDW competes with ferromagnetic ordering in monolayer VSe<sub>2</sub> [2]. In VTe<sub>2</sub> we observe a structural transition from a distorted-1T structure in the bulk to a simple hexagonal 1T structure in the monolayer. This structural transition is accompanied by a CDW instability for the monolayer that gives rise to a 4x4 CDW at low temperatures, in contrast to bulk VTe<sub>2</sub> that does not exhibit a CDW instability.

[1] M Bonilla et al. Strong room-temperature ferromagnetism in VSe<sub>2</sub> monolayers on van der Waals substrates. *Nat. Nanotechnol.* 13, 289 (2018).

[2] P Coelho et al. Charge Density Wave State Suppresses Ferromagnetic Ordering in VSe<sub>2</sub> Monolayers. *J. Phys. Chem. C* in press.

# Many-body physics in real space

Werner A Hofer and Thomas Pope

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For the last eighty years it has been the conventional wisdom in condensed matter theory that systems of  $N$  electrons have to be described by a mathematical framework involving  $3N$  coordinates and a many-electron wavefunction of the same complexity. However, as established in our work in the last eight years [1-3], such a framework is not only unnecessary, but also extremely inefficient. We show that general many-electron systems can be described in real space by two density functions, which combine to an effective wavefunction of three, instead of  $3N$  coordinates. Spin in this model is described by a complex vector field, which encodes the spin properties of electrons in an elementary manner. The method has been implemented in the routines of a standard density functional theory code and is shown to yield the same level of accuracy as our best Kohn-Sham methods today. In the final part of the talk we demonstrate that this level of description is in itself an approximation, and we derive a four component model which we think represents correlated electron systems in an exact manner.

[1] Werner A Hofer, Unconventional Approach to Orbital-Free Density Functional Theory Derived from a Model of Extended Electrons, *Foundations of Physics*, 41, 754-781 (2011).

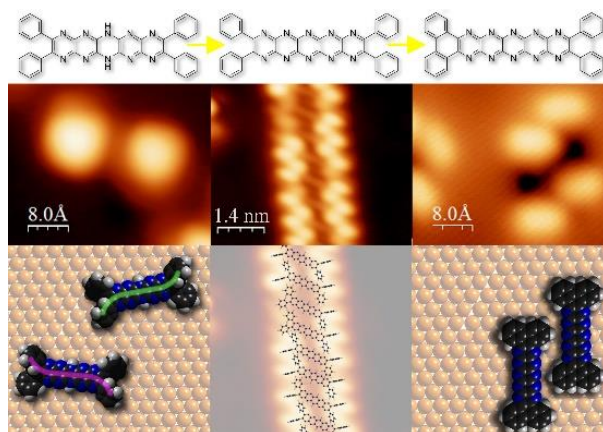
[2] Thomas Pope and Werner Hofer, Spin in the extended electron model, *Frontiers of Physics* 12, 128503 (2017).

[3] Thomas Pope and Werner Hofer, A two-density approach to the general many-body problem and a proof of principle for small atoms and molecules, *Frontiers of Physics* 14, 23604 (2019).

# Thermally-activated Self-assembly and In Situ Oxidation of a Reduced Decaazapentacene

D. Miklik, F. Mousavi, A. Ahsan, A. Middleton, Y. Matsushita, J. Labuta, P. Karr, P. Svec, F. Bures, G. Richards, F. Souza, T. A. Jung and J. Hill  
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The higher pyrazinacenes are a newly synthesized class of molecules which may take an important role in organic semiconductors. This is due to their expected n-type behaviour which complements to the already important p-type pentacene derivatives with their closely related molecular structure. We report on the supra-molecular interactions and self-assembly of octaazatetracene and decaazapentacenes, two different lengths molecules in this class. On atomically clean Cu(111) the initially achiral compounds take a chiral conformation upon adsorption. Both compounds are imaged individually and form structurally related chains. Dehydrogenation occurs upon thermal activation as recognized by its stronger adsorption in the form of individual units. This on-surface reaction is compared to the dehydrogenation in solution. Experimental evidence is provided by Scanning Tunneling Microscopy and X-ray Photoelectron Spectroscopy.



**Fig. 1.** Putting more ‘N’s in pentacene. Octaazatetracene and decaazapentacene chromophores have been successfully synthesized and their self-assembly and other properties studied. By scanning tunneling microscopy, self-assembly and disassembly of molecular nanowire structures is coupled with the oxidation state of the oligoazaacene molecules.

# **Flat Band, Magnetism and Topological Properties of Kagome Lattices**

Changgan Zeng

*University of Science and Technology of China*

Based on the electronic band theory, various exotic band structures can be realized by proper design of the lattice structures. For example, Dirac band hosting massless fermions and flat band hosting superheavy fermions are expected to be established in the kagome lattices. In this talk, I will present our recent progresses on the flat band, ferromagnetism, and topological properties in Fe-based kagome compounds. Collectively, these findings help to shed new light on the exploitation of emergent physics in the nontrivial lattice geometries by design.

# **Engineering Correlated Physics in Two-Dimensional Moire Superlattices**

Feng Wang

*University of California, Berkeley*

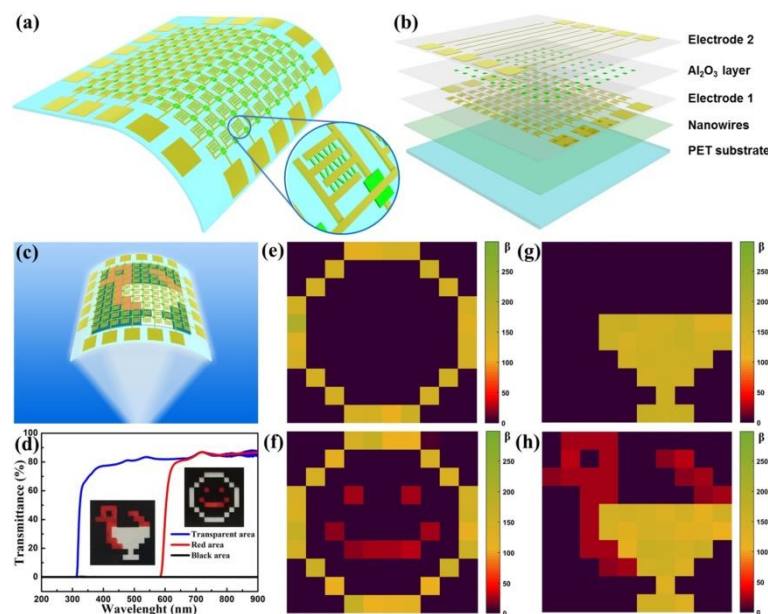
Van der Waals heterostructures of atomically thin crystals offer an exciting new platform to design novel electronic and optical properties. In this talk, I will describe a general approach to engineer correlated physics using moire superlattice in two dimensional heterostructures. One example is the tunable Mott insulator realized in the ABC trilayer graphene (TLG) and hexagonal boron nitride (hBN) heterostructure with a moiré superlattice, where the moiré leads to narrow electronic minibands and allows for the observation of gate-tunable Mott insulator states at  $1/4$  and  $1/2$  fillings. In addition, signatures of superconductivity are observed at low temperature near the  $1/4$  filling Mott insulator state in the TLG/hBN heterostructures. Another example is the WS<sub>2</sub>/WSe<sub>2</sub> heterostructure, where the moire superlattice leads to flat exciton subbands and emerging excitonic transitions.

# Growth of well-aligned Nano/Microwires for flexible photodetectors and image sensors

Guozhen Shen

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As one of the most important flexible electronic devices, flexible photodetectors have gained great research interests in recent years due to their potential applications in flexible image sensors, artificial intelligent, and smart homes. With large surface area, special geometry and quantum effect, one-dimensional (1D) semiconducting nanostructures are thought to be excellent candidates for high performance flexible photodetectors. In this talk, we will briefly introduce our recent work on developing high performance flexible photodetectors and image sensors using 1D semiconductor nanostructures. We will start our talk from single nanowire devices, followed with the procedures to improve the performance of nanowire devices, including using 0D-1D heterostructures, and nanowires arrays, etc. By forming flexible photodetectors arrays, we then fabricated flexible image sensors response to lights with different wavelength. An interesting artificial flexible visual memory system was also developed by integrating microwire PDs with oxide memristor.



## References

- [1] S. Chen, Z. Lou, D. Chen,\* G. Shen,\* *Adv. Mater.* **2018**, *30*, 1705400.
- [2] L. Li, Z. Lou, G. Shen,\* *Adv. Funct. Mater.* **2018**, *18*, 1705389.
- [3] L. Li, L. Gu, Z. Lou, Z. Fan,\* G. Shen,\* *ACS Nano*, **2017**, *11*, 4067.



# Precise Synthesis of 2D Atomic Crystals @ Liquid Metal

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Due to the confinement of the charge, spin, and heat transport in the plane, two-dimensional (2D) atomic crystals have been demonstrated to own many unique and excellent properties and witnessed many breakthroughs in physics. However, a bottleneck to widespread applications is precise and reliable fabrication of 2D atomic crystals. As compared to traditional solid metal catalysts, the emergence of liquid metal catalysts has brought a brand-new perspective and contributes to a huge change and optimization in the fabrication of 2D atomic crystals. Here we report our recent work on precise synthesis of 2D atomic crystals on liquid metals. The atoms in the liquid metal tend to move intensely and arrange in an amorphous and isotropic way. The liquid surface is smooth and isotropic, and the vacancies in the fluidic liquid phase enable the embedding of heteroatoms. The phase transition from liquid to solid will facilitate the unique control of the mass-transfer path, which can trigger new growth mechanisms. On the other hand, the excellent rheological properties of liquid metals allow us to explore self-assembly of the 2D atomic crystals grown on the surface, which can activate new applications based on the derived collective properties, such as the integrated devices.

**Key words:** 2D atomic crystals; precise synthesis; liquid metal; CVD

## Author CV



Prof. Lei Fu received his B.S. degree in chemistry from Wuhan University in 2001. He obtained his Ph.D. degree from the Institute of Chemistry, Chinese Academy of Sciences in 2006. After obtaining his Ph.D., he worked as a Director's Postdoctoral Fellow at the Los Alamos National Laboratory, Los Alamos, NM (2006~2007). Thereafter, he became an Associate Professor of Peking University. In 2012,

he joined Wuhan University as a Full Professor. His research interests cover two-dimensional materials and energy devices. He has published more than 100 papers. He has been awarded several prizes, including Chinese Chemical Society Award for Outstanding Young Chemist (2012), Outstanding Young Scholars of National Science Foundation (2013), Outstanding Young Scientists of Wuhan City (2014) and Yangtze River Young Scholar of Chinese Ministry of Education (2016).

# Spintronic devices based on graphene nanoribbons

Jingcheng Li

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The realization of spintronic devices relies on the precise strategy to embed individual spins into electrical circuits, and on the existence of efficient electron-spin interaction enabling writing and reading information. Graphene and graphene nanoribbons are ideal systems for realizing such functions as they can act as electrodes with high electron mobility and structural stability, and they can even be magnetic sources themselves.

In the first part of my talk, I will summarize our last results about the construction and magnetic characterization of a fully functional hybrid molecular system composed of a single magnetic porphyrin molecule bonded to graphene nanoribbons [1, 2]. These systems are created through on- surface synthesis route on an Au(111) substrate. By means of inelastic tunneling spectroscopy, we prove the survival of the magnetic functionality of the contacted porphyrin. Furthermore, we show that the spins of magnetic porphyrin in such a hybrid system can be electrically addressed in the transport measurements.

Predictions also state that graphene structures with specific shapes can spontaneously develop magnetism driven by Coulomb repulsion of  $\pi$ -electrons, so they can behave as functional components in spintronic devices. In the second part of my talk, I will show our recent work on the observation and manipulation of magnetic moments in graphene nanostructures [3]. Using scanning tunneling spectroscopy, we detect the presence of electron spins localized around certain zigzag sites of the nanostructures. I will also show that in the follow-up experiments, the exchange coupling between localized spins can be engineered by precise controlling over the size and edge topology of the nanostructure, which can be used as spin filters.

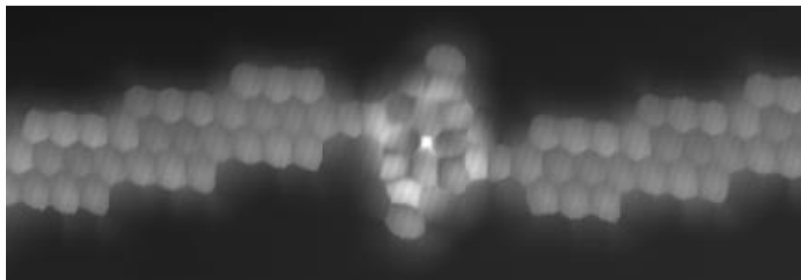


Figure: Fusing magnetic porphyrine into chiral (3,1) graphene nanoribbons.

## References

1. J.Li et al, Sci. Adv. 4: eaaq0582 (2018)
2. J.Li et al, Nano Lett. 19,3288-3294 (2019)
3. J.Li et al, Nat. Commun. 10, 200 (2019).

# Nanostructuring graphene from 0D to 2D

Aitor Mugarza Ezpeleta

*Catalan Institute of Nanoscience and Nanotechnology*

Nanostructuring graphene confers multiple functionalities to this material, making it attractive to very diverse applications in electronics, molecular sensing and filtering. For instance, semiconducting gaps can be induced by reducing its dimensions to the nanometer scale, whereas introducing pores of similar sizes turns impermeable graphene into the most efficient molecular sieve membrane. In both cases, the interesting scale for applications is below 3-5 nm, a regime where bottom-up synthesis can be particularly efficient.

Here I report different on-surface methods to grow graphene quantum dots with controlled shape and edge structure (1, 2), periodic arrays of nanoribbons with lengths exceeding 100 nm (3, 4), and nanoporous graphene sheets that combine 1nm size ribbons and pores (5). Their novel electronic states are correlated with the particular atomic structures by using STM. Their potential application in devices is illustrated by gate modulated transport measurements in nanoporous graphene sheets.

## References:

1. A. Garcia-Lekue *et al.*, *J. Phys. Chem. C* **119**, 4072–4078 (2015).
2. S. O. Parreiras *et al.*, *2D Mater.* **4**, 025104 (2017).
3. C. Moreno *et al.*, *Chem. Commun.* **54**, 9402–9405 (2018).
4. C. Moreno *et al.*, *Chem. Mater.* **31**, 331–341 (2019).
5. C. Moreno *et al.*, *Science (80-. )*. **360**, 199–203 (2018).

# Engineered Quantum States in Graphene Nanoribbons

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Graphene provides an ideal platform to create materials with diverse electronic properties by rational control of its nanoscale structure. Quantum confinement effects can be exploited in strictly planar 2D (e.g. porous graphen) or 1D (graphene nanoribbon GNR) graphene structures. However, in order to achieve well defined electronic properties with high electron motilities the nanostructures need to be synthesized with atomic precision[1].

Very recently, it has been found theoretically that localized zero energy modes can be obtained at the junctions of topologically dissimilar graphene nanoribbons (GNR)[2]. We have experimentally realized such GNR junctions using on-surface synthesis, i.e. by the polymerization of molecular precursors rationally designed to yield the desired final GNR on single crystal surfaces. By creating well defined periodic sequences of these topological electronic modes, one-dimensional electronic bands can be created, which are described by the Su-Schrieffer-Heeger (SSH) Hamiltonian representing the dimerized atomic chain [3]. By manipulating the intra- and inter-cell coupling strength we could further create SSH analogs with different Chern number and therefore topological class. The topological class distinction is evidenced by presence, respectively absence of zero energy end states at the termini of the corresponding GNR or their junctions to structurally dissimilar GNRs.

We will discuss the concept of topological boundary states in GNR junctions and the creation of 1D SSH-type electronic bands by their periodic arrangement on a host GNR. The theoretical basis of attributing  $Z_2$  topological invariants to these structures will be discussed. We then present the experimental synthesis of different structures exhibiting different topological classes. The structural characterization and atomic precision of these GNR was achieved by low-temperature scanning tunneling microscopy (STM) and high resolution non-contact atomic force microscopy (nc-AFM) [3]. The electronic properties are elucidated by scanning tunneling spectroscopy (STS), where we invoke the bulk-boundary correspondence to determine the topological properties.

## References

- [1] Cai, J. et al. Atomically precise bottom-up fabrication of graphene nanoribbons. *Nature* 466, 470–473 (2010)
- [2] Cao, T., Zhao, F. & Louie, S. G. Topological Phases in Graphene Nanoribbons: Junction States, Spin Centers, and Quantum Spin Chains. *Phys. Rev. Lett.* 119, 076401 (2017)
- [3] O. Gröning, et al., Engineering of robust topological quantum phases in graphene nanoribbons. *Nature* 560, 209 (2018)

# Functional large scale, single layer hexagonal boron nitride

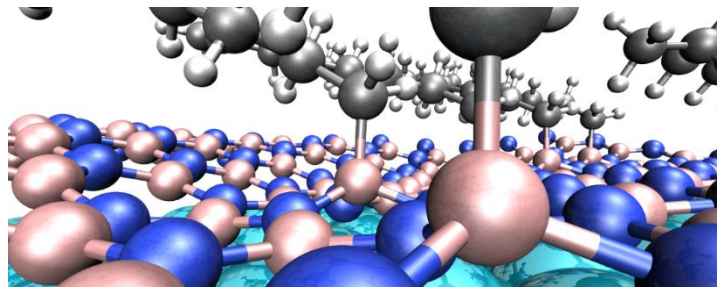
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Two-dimensional (2D) van der Waals materials may be stacked layer by layer and thus allow for the realization of unprecedented properties of condensed matter systems. This perspective relies on the availability of inert 2D materials, where boron nitride is expected to play the first violin.

I will report on our recent progress on the exfoliation of centimeter sized single orientation, single layer boron nitride from its metal growth substrate [1]. To demonstrate the quality of the material on a large scale, it was employed as a packing-layer to protect a germanium wafer from oxidation in air at high temperature. A second set of experiments involved the nanoscale engineering of the h-BN layer with the “can opener effect” [2] prior to the transfer. This allowed the realization of boron nitride membranes with 2 nm voids, across which we measured ion transport in aqueous solutions [1].



**Fig.** Boron nitride on a Rh(111) surface functionalized with hydrocarbons. (Density functional theory results by Tocci and Iannuzzi, UZH [3].)

The new BN exfoliation process involves in the first step the application of tetraoctylammonium (TOA) from a water free electrochemical reaction with the h-BN/Rh(111) substrate before the standard hydrogen bubbling. With high-resolution x-ray photoelectron spectroscopy, atomic force microscopy and density functional theory we identify the proximity of the metal substrate to enable covalent functionalization of h-BN with TOA constituents [3].

[1] Centimeter-Sized Single-Orientation Monolayer Hexagonal Boron Nitride With or Without Nanovoids, H. Cun et al., *Nano Letters* 2018,18,1205.

[2] Two-Nanometer Voids in Single-Layer Hexagonal Boron Nitride: Formation via the “Can-Opener” Effect and Annihilation by Self-Healing, H. Cun et al., *ACS Nano* 2014, 8, 7423.

[3] Catalyst proximity induced functionalization of h-BN with quat-derivatives, A. Hemmi et al., submitted.

# Oxygen Electrocatalysis on Transition Metal Spinel Oxides

Zhichuan J. Xu (徐桂川)

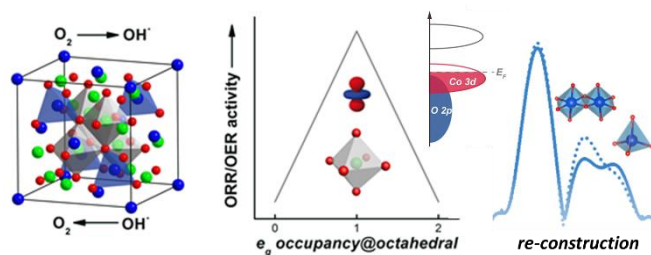
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Exploring efficient and low cost oxygen electrocatalysts for ORR and OER is critical for developing renewable energy technologies like fuel cells, metal-air batteries, and water electrolyzers. This presentation will presents a systematic study on oxygen electrocatalysis (ORR and OER) of transition metal spinel oxides. Starting with a model system of Mn-Co spinel, the presentation will introduce the correlation of oxygen catalytic activities of these oxides and their intrinsic chemical properties. The catalytic activity was measured by rotating disk technique and the intrinsic chemical properties were probed by synchrotron X-ray absorption techniques. It was found that molecular orbital theory is able to well-explain their activities. The attention was further extended from cubic Mn-Co spinels to tetragonal Mn-Co spinels and it was found that the molecular theory is again dominant in determining the catalytic activities. This mechanistic principle is further applied to explain the ORR/OER activities of other spinels containing other transition metals (Fe, Ni, Zn, Li, and etc.). The talk further gives insight on surface reconstruction on spinel oxides and how the bulk properties affect such reconstruction during OER.



**Fig. 1.** A simple demonstration of spinel structure, the activity descriptor, and bulk thermodynamics determined surface reconstruction.

## Reference

- [1] Wei C, Feng Z, Scherer G, Barber J, Shao-Horn Y, Xu Z, Adv. Mater. 2017, DOI: 10.1002/adma.201606800.
- [2] Suntivich J, May KJ, Gasteiger HA, Goodenough JB, Shao-Horn Y, Science 334 (2011) 1383.
- [3] Zhou Y, Sun S, Xi S, Duan Y, Sritharan T, Du Y, Xu Z, Adv. Mater., 2018, DOI: 10.1002/adma.201705407
- [4] Zhou Ye, Sun S, Song J, Xi S, Chen B, Du Y, Fisher A, Cheng F, Wang X, Zhang H, Xu Z, Adv. Mater. 2018, DOI: 10.1002/adma.201802912
- [5] Yan Duan, Shengnan Sun, Yuanmiao Sun, Shibo Xi, Xiao Chi, Qinghua Zhang, Xiao Ren, Jingxian Wang, Samuel Jun Hoong Ong, Yonghua Du, Lin Gu, Alexis Grimaud, Zhichuan J. Xu, Adv. Mater., 2019, 1807898
- [6] Shengnan Sun, Yuanmiao Sun, Ye Zhou, Shibo Xi, Xiao Ren, Bicheng Huang, Hanbin Liao, Luyuan Paul Wang, Yonghua Du, Zhichuan J. Xu, Angewandte Chemie International Edition, 2019, DOI: 10.1002/anie.201902114

## Photograph and brief introduction of speaker

Zhichuan is an associate professor in School of Materials Science and Engineering, Nanyang Technological University. He received his PhD degree in Electroanalytical Chemistry at 2008 and B.S. degree in Chemistry at 2002 from Lanzhou University, China. His PhD training was received in Lanzhou University (2002-2004), Institute of Physics, CAS (2004-2005), and Brown University (2005-2007). Since 2007, he worked in State University of New York at Binghamton as a Research Associate and from 2009 he worked in Massachusetts Institute of Technology as a Postdoctoral Researcher. Dr. Xu is member of International Society of Electrochemistry (ISE), The Electrochemistry Society (ECS), and American Association for the Advancement of Science (AAAS). He was awarded Fellow of Royal Society of Chemistry (FRSC) in Nov. 2017. He served as a guest editor for the special issue ICEI2016 of *Electrochimica Acta* and an associate editor for *Nano-Micro Letters*. He is also the development editor for *Current Opinion in Electrochemistry* and the vice president of ECS Singapore Section. Dr Xu is 2018 Highly Cited Researcher by Clarivate Analytics, Web of Science.



# **Direct Observation of Ultrafast Room Temperature Oxygen Redox Dynamics in Oxide Thin Films**

Chonglin Chen

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Control of oxygen vacancy and redox dynamics are of great interest in functional oxides for enormous practical applications, such as fuel cells, batteries, sensors, smart windows, etc. In situ examination of oxygen redox dynamics is a key technique to gain direct information for understanding the reactive mechanisms and the surface catalytic principles. However, the room temperature chemical redox dynamics are limited by the catalytic surface potential that results in the irreversible atomic process. Our directly in situ observation of the nonvolatile nano-scale expansive and contractive topographic deformations using electrochemical strain microscopy technique provides a platform for understanding the room temperature chemical dynamics nature. The deformations are attributed to oxygen vacancy dynamics that the oxygen vacancies can be reversibly injected into and pumped out rapidly at room temperature from  $\text{PrBa}_{1-x}\text{Ca}_x\text{Co}_2\text{O}_{5+\delta}$  film by bias tip potential. This is the first time to validate the ultrafast, reversible, and reproducible topographic deformations in the complex oxide system at the standard atmosphere condition. Our finding may pave a new way for material genetic designs and novel material multifunctionality manipulations.



# Colloidal Spin Quantum Bits

Min Ouyang

*University of Maryland*

In this talk, I will present a few recent advances from my group, centering on exploration of semiconductor based colloidal nanostructures as spin quantum bits. I will particularly focus on optical spin measurement and control of this emerging class of colloidal nanostructures. Development of emerging colloidal hybrid nanostructures and their assembly make it feasible to achieve desirable integration of multiple functionalities in one single nanoscale unit to create novel synergistic interactions. By combining ultrafast optical spectroscopy with this new materials advance, precise control of quantum optical interactions can thus be achieved at the nanoscale, including spin coherence dynamics. This has further led to all optical spin manipulation and spin echo achievable in colloidal semiconductor nanostructures, uncovering microsecond long spin coherence lifetime for the first time. Observation of long spin coherence lifetime should pave the way to develop colloidal quantum bits as an alternative to the existing candidates. If time allowed, application of such colloidal spin quantum bits will also be presented, including development of colloidal central spin system for probing many body physics.

**Brief Biography:** Min Ouyang is professor in Physics department with affiliate appointment in the Department of Materials Science and Engineering in the University of Maryland at College Park. Min Ouyang received his B.S. (1996) and M.S. (1997) in Electronics from Peking University, M.S. (1999) and Ph.D (2001) in Chemistry from Harvard University, followed by postdoctoral research in Physics at the University of California in Santa Barbara (2002-2004). Professor Ouyang has broad interest in areas that intersect emerging materials chemistry, nanoscale ultrafast and single photon optics, and technology applications at the nanoscale, and has led to significant scientific impacts as recognized by numerous high profile publications and awards, including Alfred P. Sloan Fellowship, NSF CAREER award, Ralph E. Powe award, ONR Young Investigator award, Beckman Young Investigator award, University of Maryland CMPS Discovery award, and Scialog Fellow of the Research Corporation.

# Can Ferroelectrics get along with metallicity?

Jiandi Zhang

*Louisiana State University*

Ferroelectric (FE) distortion in a metallic state has long been thought experimentally inaccessible because itinerant electrons screen the long-range Coulomb interactions that favor a polar structure. *In 1965, Anderson and Blount [1] hypothesized that ferroelectricity can appear in a metal if the electrons at the Fermi level is decoupled to the unstable phonon which results in the FE transition. Such a FE metal would require a continuous structural transition accompanied by the removal of an inversion center and the emergence of a unique polar axis. A breakthrough has been achieved with the recent discovery of LiOsO<sub>3</sub>, which has been identified as a clear example of a FE-like metal [2]. Furthermore, it is possible to create interface with polar metal phase [3-5] and even magnetic polar metal phase [6] through fabrication of oxide heterostructures. In this talk, I will discuss our recent studies on the bulk polar metal LiOsO<sub>3</sub> with Raman scattering [5]. we reveal an unusual 2<sup>nd</sup>-order order-disorder type FE phase transition with the participation of itinerant electrons in LiOsO<sub>3</sub>. Recognizing that the interplay between FE dipoles and itinerant electrons is essential to understand this unusual transition. we suggest that the weak coupling between *itinerant electrons and the FE distortion, originally proposed by Anderson and Blount [3], may not be an essential prerequisite for searching for polar/FE metals.**

1. Anderson PW, Blount EI (1965) Symmetry Considerations on Martensitic Transformations: "Ferroelectric" metals? *Phys Rev Lett* **14**:217-219.
2. Shi YG, et al. (2013) A ferroelectric-like structural transition in a metal. *Nat Mater* **12**:1024-1027.
3. Kim, T. H. et al. Polar metals by geometric design. *Nature* **533**, 68–72 (2016).
4. Cao, Y. et al. (2018) Artificial two-dimensional polar metal at room temperature. *Nat. Commun.* 9:1547.
5. Meng M., *et al*, Interface-induced Magnetic Polar Metals in Correlated Oxides, *Nat. Commun.*, in review.
6. F. Jin, *et al*, Raman interrogation of the ferroelectric phase transition in polar metal LiOsO<sub>3</sub>, *PNAS*, in review

# The Observation of Majorana Zero Mode and Conductance Plateau in an Iron-based Superconductor

Yu-Yang Zhang<sup>1</sup>, Dongfei Wang<sup>1</sup>, Shiyu Zhu<sup>1</sup>, Lingyuan Kong<sup>1</sup>, Peng Fan<sup>1</sup>, Hui chen<sup>1</sup>, Wenyao Liu<sup>1</sup>, Lu Cao<sup>1</sup>, Yuqing Xing<sup>1</sup>, Yujie Sun<sup>1</sup>, Shixuan Du<sup>1</sup>, John Schneeloch<sup>2</sup>, Ruidan Zhong<sup>2</sup>, Genda Gu<sup>2</sup>, Liang Fu<sup>3</sup>, Hong Ding<sup>1</sup>, Hong-Jun Gao<sup>1</sup>.

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Majorana bound states (MBSs) are spatially-localized zero-energy fractional quasiparticles with non-Abelian braiding statistics that hold great promise for topological quantum computing. By using scanning tunneling microscopy/spectroscopy (STM/STS), here we report the observation of MBSs in a single material platform of high- $T_c$  iron-based superconductors, FeTe<sub>0.55</sub>Se<sub>0.45</sub>, which combined advantages of simple material, high- $T_c$ , and large ratio of  $\Delta/E_F$ . We observed a sharp zero-bias peak inside a vortex core that does not split when moving away from the vortex center. The evolution of the peak under varying magnetic field, temperature, and tunneling barrier is consistent with the tunneling to a nearly pure MBS, separated from nontopological bound states [1]. We further investigated the MBS and observed a conductance plateau feature, which is protected by the Majorana particle-hole symmetry [2]. The observations not only prove a strong evidence of MBSs in this iron-based superconductor, but also offer a single-material platform for Majorana braiding at relatively high temperature.

References:

[1] D. F. Wang et al, *Science*. **362**, 333 (2018).

[2] S. Y. Zhu et al, arXiv: 1904.06124 (submitted to *Science* on February 15, 2019)

# Atomic Collapse and Flat Bands in Graphene

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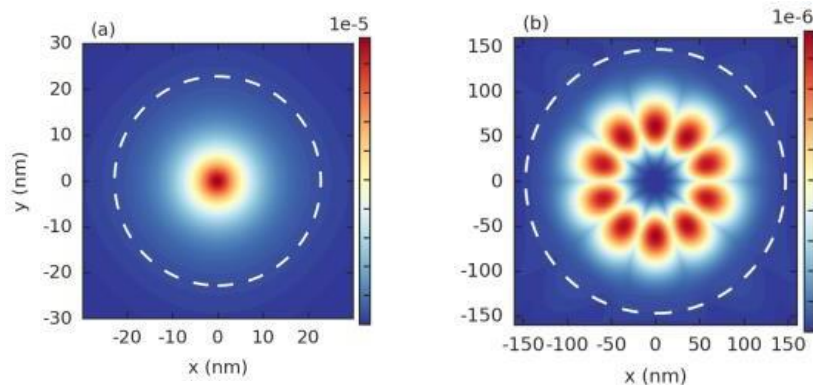
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Quantum electrodynamics predicts that heavy atoms ( $Z > Z_c \sim 170$ ) will undergo the process of *atomic collapse* where electrons sink into the positron continuum and a new family of so-called *collapsing* states emerges. This phenomenon has never been confirmed experimentally. The wonder material graphene has made it possible to investigate<sup>1</sup> similar physics in two dimensions using vacancies with tunable charge where the ‘atomic’ collapse occurs at a much lower critical charge ( $Z_c \sim 1$ ).

The transition from sub-critical to the supercritical regime is accompanied by trapping of electrons in quasi- bound states which are the condensed matter analogue of the long sought after phenomenon of atomic collapse in super-heavy nuclei. The quasi-bound electron-states show up as a strong enhancement of the density of states within a disc centered on the vacancy site. We find that these states are surrounded by a circular halo of hole states which are interpreted as the analogue of positron production in atomic collapse. We further show that the quasi-bound states at the vacancy site are gate tunable and that the trapping mechanism can be turned on and off, providing a new paradigm to confine, control and guide electrons in graphene.

Recently<sup>2</sup>, we found that a sharp STM tip is able to induce similar atomic collapse states (see Fig. a). For large tip potentials a sub- micrometer scale p-n junction is induced that



exhibits *whisper gallery modes* (see Fig. b). Thus, the STM tip allows us to tune a circular p-n junction in graphene from quantum confinement to optical guiding.

We realized<sup>3</sup> a periodic buckling structure of a single graphene layer. Because of the periodic strain the electrons are subject to a periodic *pseudomagnetic field* that does not break time reversal symmetry. Through a detailed STM spectrum mapping and tight binding calculations, we reveal the possibility of generating a robust flat band. This buckling method should enable us to design flat bands with different superlattice symmetry which is inaccessible by the moiré superlattices method that was recently realized for magic angle twisted bilayer graphene<sup>4</sup>.

*References:*

1. J. Mao et al., *Nat. Phys.* **12**, 545 (2016).
2. Y. Jiang et al., *Nat. Nanotechnology* **12**, 1045 (2017).
3. Y. Jiang et al, (to be published).
4. Y. Cao et al, *Nature* **556**, 43 (2018); *ibid.* **556**, 80, (2018).

# Ultrafast Charge Transfer in 2D Semiconductors and Heterostructures

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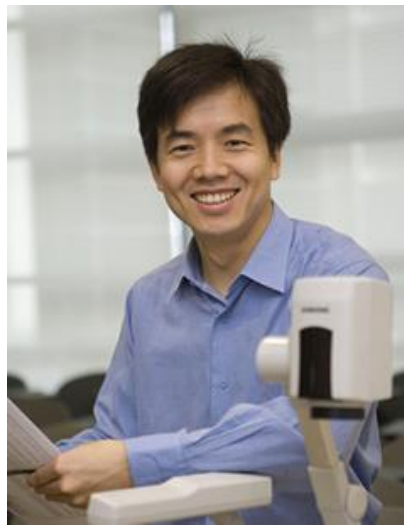
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2D semiconductors, such as transitional metal chalcogenides and black phosphorus, have attracted considerable attention due to fascinating physical properties a wide range of applications in valleytronics, optoelectronics and superconductivity. The interlayer interaction is particularly important in both homogenous few-layer systems and heterogeneous structures formed by “lego” fashion, which underpins the foundation for rational engineering towards unprecedented functionality. In this talk, I will introduce our work on unique interlayer charge transfer mechanism in 2D semiconductor monolayer heterostructures leads to an interesting blinking phenomenon, whereby a bright state emission occurs in one monolayer while a dark state emission occurs in the other, and vice versa. Such correlated blinking can be probed in detail by steady-state and transient spectroscopy measurements, which uncovered an ultrafast charge transfer process  $\sim 120$  fs, providing new platform to study the long-standing puzzling blinking phenomenon in nanomaterials. Secondly, I will present how the charge transfer by a gate modulation breaks the symmetry in a bilayer sample such that a charge-induced second harmonic generation is produced, due to a confined charging in W-atomic plane and a screening effect. This bilayer system can be further modulated by introducing plasmonic structures, from which an ultrafast plasmonic hot carrier injection ( $\sim$  ps) can lead to symmetry breaking, as such a second harmonic generation is produced. Our study creates opportunity for the ultrafast all-optical control of SHG in an all-optical manner that may enable a variety of applications.

## References

1. X.L. Wen, W.G. Xu, W.J. Zhao, J.B. Khurgin and **Q.H. Xiong\***, “Plasmonic hot carriers controlled second harmonic generation in WSe<sub>2</sub> bilayers”, *Nano Lett.*, DOI: 10.1021/acs.nanolett.7b04707 (2018)
2. W.G. Xu, W.W. Liu, J. F. Schmidt, W.J. Zhao, X. Lu, T. Raab, C. Diederichs, W.B. Gao, D. V. Seletskiy, and Q.H. Xiong\*, “Correlated fluorescence blinking in two-dimensional semiconductor heterostructures”, *Nature*, Doi:10.1038/nature20601 (2017)
3. H.K. Yu, D. Talukdar, W.G. Xu, J.B. Khurgin\* and **Q.H. Xiong\***, "Charge-Induced Second-Harmonic Generation in Bilayer WSe<sub>2</sub>", *Nano Lett.* **15**(8), 5653-5657 (2015)
4. Y.Y. Zhao, X. Luo, H. Li, J. Zhang, P.T. Araujo, C.K. Gan, J. Wu, H. Zhang, S.Y. Quek, M.S. Dresselhaus, and Q.H. Xiong, “Interlayer breathing and shear modes in few-trilayer MoS<sub>2</sub> and WSe<sub>2</sub>”, *Nano Lett.* **13**, 1007-1015 (2013)

**Biography:** Qihua Xiong is currently Professor of Physics and Electrical Engineering at Nanyang Technological University. He received his B.S. degree in physics from Wuhan University in 1997, and then obtained his M.Sc. degree from the Shanghai Institute of Applied Physics, Chinese Academy of Sciences in 2000. He received his Ph.D. degree from The Pennsylvania State University in 2006. After three years postdoctoral experience in Prof. Charles M. Lieber's group at Harvard University, he joined Nanyang Technological University as an assistant professor in 2009 and promoted to Nanyang Associate Professor with tenure in 2014. He was promoted to full Professor in 2016. He is a Fellow of Singapore National Research Foundation (NRF) awarded in 2009 and the inaugural NRF Investigatorship Award in 2014. He is the recipient of IPS Nanotechnology Physics Award (2015) and Nanyang Award for Research Excellence of NTU (2014). Prof. Xiong's research focuses on light-matter interactions of emergent quantum matter by optical spectroscopy approaches, such as semiconductor nanomaterials, 2D transitional metal chalcogenides and halide perovskite materials. He has more than 200 papers published, which attracted >10000 citations with an H-index of 59. Starting from this year, he serves as the associate editor for Optics Express, the flagship open access journal of Optical Society of America. He is APS Fellow elected in 2018.



# TMDs: Towards Electrochemical Electronics

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Two-dimension (2D) transition-metal dichalcogenides (TMDs) have recently provided a rich source of research opportunity, revealing interesting physical phenomena including quantum-spin Hall effect (QSH), valley polarization, 2D superconductivity, and potential applications for functional devices. Here, we demonstrate that molten salt-assisted chemical vapor deposition can be broadly applied for the synthesis of a wide variety of 2D TMDs [1]. We demonstrate the synthesis of 47 compounds, including 32 binary (Ti-, Zr-, Hf-, V-, Nb-, Ta-, Mo-, W-, Re-, Pt-, Pd- and Fe-based), 13 alloys (including 11 ternary, 1 quaternary and 1 quinary), and 2 heterostructured compounds. We elaborate the general growing mechanism of this method, demonstrating that the salt decreases the melting point of reactants and facilitates the formation of intermediate products.

Based on the 2D materials, we have recently revisited the semiconductor-electrolyte interface and unraveled a universal self-gating phenomenon through micro-cell based in-situ electronic/electrochemical measurements [2]. We unveiled a surface conductance mechanism under self-gating that dominates the charge transport in semiconductor electrocatalysts, and demonstrate the strong correlation between them. Then we demonstrate that the type of semiconductor catalysts strongly correlates and their electrocatalysis, i.e., n-type semiconductor catalysts favor cathodic reactions such as hydrogen evolution reaction (HER), p-type ones prefer anodic reactions such as oxygen evolution reaction (OER), and bipolar ones tend to perform both anodic and cathodic reactions. Our study provides a new insight into the electronic origin of semiconductor-electrolyte interface during electrocatalysis, paving the way for designing high-performance semiconductor catalysts.

## References:

- [1] Jiadong Zhou, *et al.*, A library of atomically thin metal chalcogenides, *Nature* 556, 355, 2018
- [2] Yongmin He, *et al.*, Self-gating in semiconductor electrocatalysis, *Nature Materials*, 2019



## Biography – Liu, Zheng

Dr. Zheng LIU is currently an associate professor in Nanyang Technological University, Singapore. He works on following topics: 1) Synthesis of high-quality and large-size novel 2D monolayers, especially, transition metal dichalcogenides (TMDs); 2) Engineering of 2D materials such as lateral/vertical 2D heterostructure and alloy; 3) Physical properties of 2D monolayers such as 2D superconductivity, 2D ferroelectricity, 2D ferromagnetism and 2D Wyle semi-metals; 4) Applications of 2D materials such as novel semiconducting electronics. He has published > 190 papers including 28 papers in Nature and Science serial journals; 26 in Adv Mater; 24 in Nano Lett; 16 in ACS Nano, 4 in JACS, with total citations > 20,000 and H-index of 66 (GoS, as to 1 June 2019). He was the finalist of the World Technology Award in Energy category in 2012. In 2013, he was awarded the prestigious Singapore NRF Fellowship and the elite Nanyang Assistant Professorship. He was awarded ICON-2DMAT Young Scientist Award and the prestigious Singapore Young Scientist Award in 2018. He was highly cited researcher in 2018 in the category of Materials Science. He was named Materials Research Society of Singapore Chair in 2019.



# Electronic Transport and Device Applications of 2d Materials

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Two-dimensional (2D) materials have emerged as promising candidates for post-Moore electronics due to their unique electronic properties and atomically thin geometry. Our group at Nanjing University have been focused on exploring electronic transport properties and device applications of novel 2D semiconductors and semimetals, as well as their heterostructures. I will start with our studies on atomically thin semiconducting material rhenium disulfide (ReS<sub>2</sub>) and type-II Weyl semimetal (WSM) tungsten ditelluride (WTe<sub>2</sub>). We observed interesting in-plane anisotropic transport and mechanical properties of ReS<sub>2</sub>, together with its potential electronic and optoelectronic applications.[1] In thin tungsten ditelluride (WTe<sub>2</sub>) flakes, we observed notable angle-sensitive negative longitudinal magnetoresistance (MR) and strong planar orientation dependence which reveal important transport signatures of chiral anomaly and type-II Weyl fermions. By applying a gate voltage, we further demonstrated that the Fermi energy can be tuned through the Weyl points via the electric field effect; this is the first report of controlling the unique transport properties *in situ* in a WSM system.[2]

By stacking layers of different 2D materials together, van der Waals (vdW) heterostructures offer unprecedented opportunities to create materials with atomic-level precision by design, and combine superior properties of each component. In the second part of my talk, I will show that robust memristors with good thermal stability, which is lacking in traditional memristors, can be created from a vdW heterostructure composed of graphene/MoS<sub>2-x</sub>O<sub>x</sub>/graphene.[3] Our latest results on the observation of ballistic avalanche phenomena in thin vdW heterostructures made of black phosphorus and Indium Selenide (InSe), as well as its high-performance electronic and optoelectronic device applications will also be presented.[4]

## References

- [1] Liu, *et al.*, *Nat. Comm.* **6**, 6991 (2015); *Adv. Func. Mater.* (2016); Wang, *et al.*, *ACS Nano* (2018).
- [2] Wang, *et al.*, *Nat. Comm.* **7**, 13142 (2016); *Nano Lett.* (2019); Li, *et al.*, *Nano Lett.* (2018).
- [3] Wang, *et al.*, *Nat. Electronics* **1**, 130 (2018).
- [4] Gao, *et al.*, *Nat. Nano.* **14**, 217 (2019).

## Observation of Weak Antilocalization Effect in Few-layer VSe<sub>2</sub>

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With strong spin-orbit coupling (SOC), ultrathin two-dimensional (2D) transitional metal chalcogenides (TMDs) are predicted to exhibit weak antilocalization (WAL) effect at low temperatures. The observation of WAL effect in VSe<sub>2</sub> is challenging due to the relative weak SOC and three-dimensional (3D) transport nature in thick VSe<sub>2</sub>. In this talk, I will present the observation of quasi-2D transport and WAL effect in sublimed-salt assisted low temperature chemical vapor deposition (CVD) grown few-layered high-quality VSe<sub>2</sub> nanosheets. The WAL magnitudes in magnetoconductance can be perfectly fitted by the 2D Hikami-Larkin-Nagaoka (HLN) equation in the presence of strong SOC, by which the spin-orbit scattering length  $l_{SO}$  and phase coherence length  $l_{\phi}$  have been extracted. The phase coherence length  $l_{\phi}$  shows a power law dependence with temperature,  $l_{\phi} \sim T^{-1/2}$ , revealing an electron-electron interactions dominated dephasing mechanism. Such sublimed-salt assisted growth of high-quality few-layered VSe<sub>2</sub> and the observation of WAL paves the way for its future spintronic and valleytronic applications.

### References

[1] H. T. Liu et al, *Nano Letters* (submitted).

# Proximity Effects in Magnetic/TMD Heterostructures

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The broken inversion symmetry together with strong spin orbit coupling leads to two degenerate yet inequivalent valleys K and K' in monolayer transition metal dichalcogenides (TMDs), with opposite spin characters. The spin-locked valley states have been proposed for classical and quantum information applications. For such applications, one needs to create, manipulate and switch valley polarization. Valley polarization can be realized by applying a magnetic field to Zeeman split the band edge states. However, the splitting value of  $\sim 0.2$  meV/T is small, making valley control difficult. In this talk I will discuss an approach of using the proximity effect from a ferromagnetic substrate to enhance the valley splitting in monolayer TMDs. Using magnetic semiconductor EuS as a substrate in the WSe<sub>2</sub>/EuS heterostructure, we have achieved a valley splitting of 2.5 meV/T, an order of magnitude higher than that by an external field. In WS<sub>2</sub>/EuS, the splitting value is increased to  $\sim 16$  meV/T, which is an enhancement by nearly two orders of magnitude. More interestingly, the valley splitting of the two materials have opposite signs, suggesting the complex exchange interactions between the TMD and magnetic substrates. At the end of this talk, I will discuss a theoretical proposal to realize robust valley exciton emission with long lifetime and nearly 100% valley polarization at room temperature.

# **Complex magnetic domain structures in oxides: physical origin and device application**

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Physics of magnetic domains of conventional magnetic materials can be well described by minimization Landau-Lifshitz free energy. However, for magnetic oxides, competition between various types of exchange interactions has often led to complex magnetic domain structures that are far from being understood. One of the most typical examples is the domain structure in colossal magnetoresistive manganites, which is featured by spatial coexistence of ferromagnetic, antiferromagnetic and even spin glass domains. These domains are not only in different magnetic states, but are also in different conducting states. By studying the effect of spatial ordering of the chemical dopants, we conclude that the dopants-induced disorder is the key reason for the formation of the complex domain structures in magnetic oxides. Based on the understanding of the physical origin of the complex magnetic domains in oxides, we have developed various methods to control the domain patterns in oxides and fabricated multi-bit memory device that can also carry out logic operations.

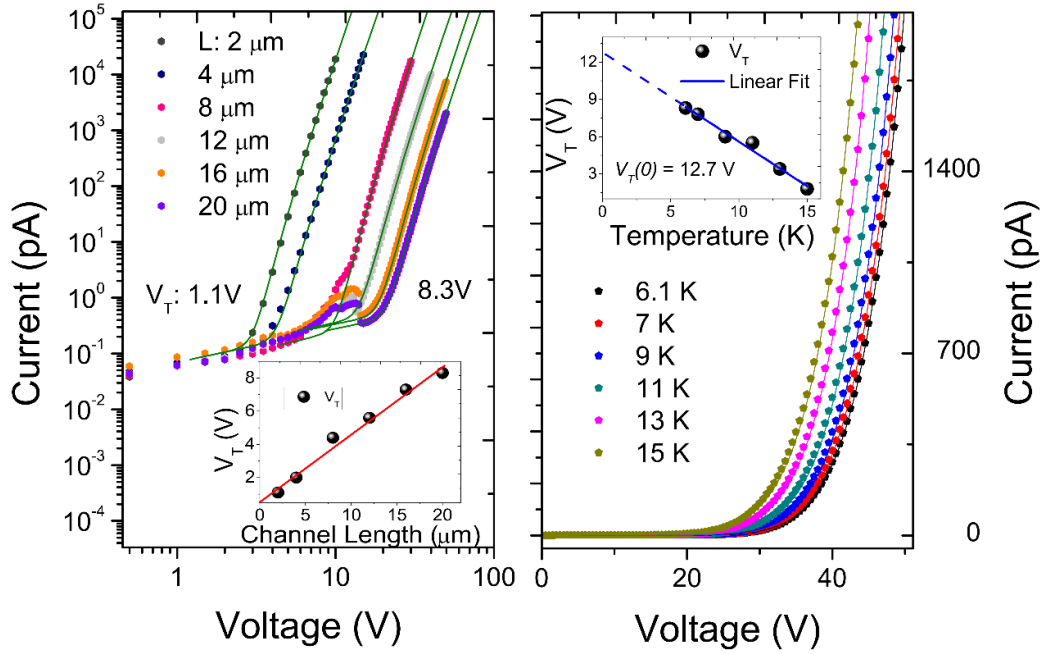
# Dimensionality Induced Crossover from Coulomb Blockade to Luttinger-Liquid in the Nonlinear Transport of Conducting Polymers

Ling Li, Jiawei Wang, and Ming Liu

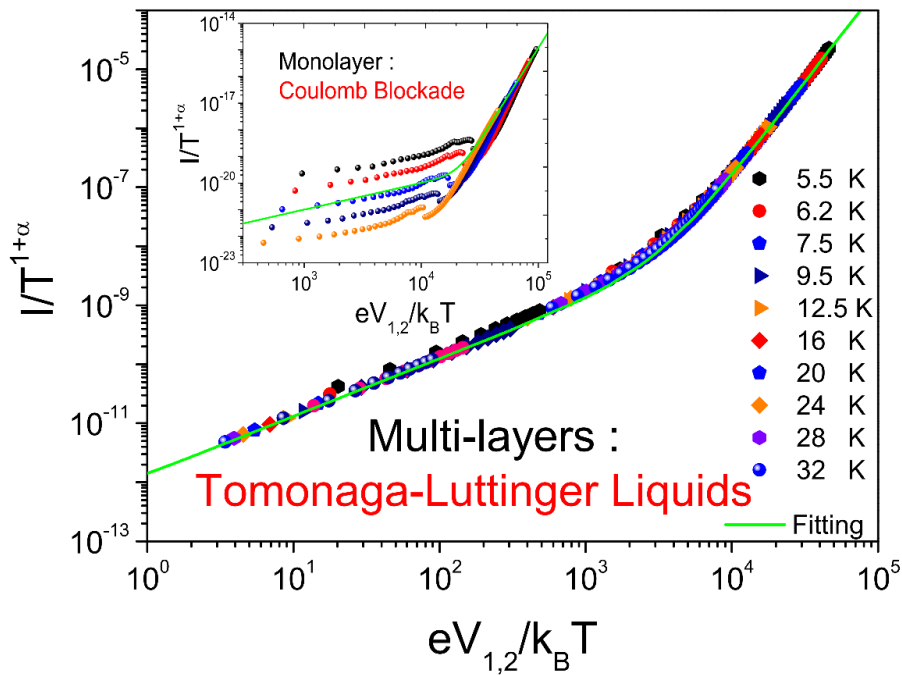
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Charge transport in the disordered organic conducting/semiconducting system has always been a topic that draw much interests and attentions, the most heated discussions in recent ten years mainly focused on the nonlinear transport phenomenons for conducting polymers. Various theories have been employed to model the power-law behavior ( $I \propto V^\beta$ ) in the nonlinear IV relations observed in different polymer materials, among which, Coulomb blockade (CB) and Luttinger liquid (LL) models, both involving the electrons coulombic correlations effect, are the most promising ones, though the topic is still under disputes with more new models being proposed.

In this study, we observe a crossover from Luttinger liquid to Coulomb blockade when we thinning the 3D bulk layer to single molecular layer --- a pure 2D system, it's for the first time that two mechanisms are simultaneously observed in one kind polymeric material, just depending on the dimensionality. A universal random quantum resistive networks related to the microstructures of the polymer film is proposed to model the coexistence of the CB and LL mechanisms, in which the crystalline grains and amorphous intergrains are respectively related to coulomb islands and 1D tie-bridges. In 2D limits, the charging energy  $E_c$  in the coulomb islands is much larger than the Bosonization correlation energy  $E_b$  in the 1D chains, leading to the domination of CB effect; while thickening the film to 3D situation, increase of the capacitance of coulomb islands, due to the multi-layers' grains fusion under a percolation scenario, would make the  $E_c$  less influenced, consequently the tunneling into Luttinger liquids with power-law density of states (DOS) occurred in the 1D tie-chains would determine the linear transport.



**Fig.1** Coulomb blockade effect in the nonlinear transport of single molecular layer conducting polymer.



**Fig. 2** Luttinger liquid dominant nonlinear transport in multi-layer polymer film, scaling with the LL tunneling formula. The inset is the failure when using the LL model to fit the 2D nonlinear transport.

### Reference

- [1] Nonlinear transport in semiconducting polymers at high carrier densities, Jonathan D. Yuen et.al, Nat. Mater, 8, 2009.
- [2] Universal Scaling in Highly Doped Conducting Polymer Films, A. J. Kronemeijer et. Al, Phys. Rev. Lett, 105, 156604, 2010.
- [3] Coulomb Blockade in a Two-Dimensional Conductive Polymer Monolayer, M. Akai-Kasaya et.al, Phys. Rev. Lett, 115, 196801, 2015.

# To Tie or Not To Tie

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Knots are important structural features in DNA and some proteins, and are thought to play a significant role in the physical properties of both natural and synthetic polymers.<sup>1</sup> Although billions of prime knots are known to mathematics, few have succumbed to chemical synthesis.<sup>1</sup> Here we will discuss the latest progress from our laboratory in this field, including the synthesis of the most complicated molecular composite knot, chiral knots and links (catenanes) made to date, and the properties that knotting at the molecular level can induce.<sup>2-5</sup>

## References

- (1) Fielden, S. D. P.; Leigh, D. A.; Woltering, S. L.; *Angew. Chem. Int. Ed.* **2017**, *56*, 11166.
- (2) Zhang, L.; Stephens, A. J.; Nussbaumer, A. L.; Lemonnier, J.-F.; Jurček, P.; Vitorica-Yrezabal, I. J.; Leigh, D. A. *Nature Chem.* **2018**, *10*, 1083.
- (3) Zhang, L.; August, D. P.; Zhong, J.; Whitehead, G. F. S.; Vitorica-Yrezabal, I. J.; Leigh, D. A. *J. Am. Chem. Soc.* **2018**, *140*, 4982.
- (4) Leigh, D. A.; Pirvu, L.; Schaufelberger, F.; Tetlow, D. J.; Zhang, L. *Angew. Chem. Int. Ed.* **2018**, *57*, 10484.
- (5) Zhang, L.; Lemonnier, J.-F.; Acocella, A.; Calvaresi, M.; Zerbetto, F.; Leigh, D. A. *Proc. Natl. Acad. Sci. USA* **2019**, *116*, 2452.

## Biography

Liang Zhang was born in Lanzhou, Gansu (China). He obtained his Bsc and Msc from Fudan University and then joined Prof. David Leigh's group for a PhD degree in 2015 funded by President's Doctoral Scholar (PDS) Award from the University of Manchester. He recently completed his PhD on synthesis and studying of topologically complex molecules and won the RSC Macrocyclic and Supramolecular Chemistry PhD Thesis Award. He is now continuing his research as a postdoctoral research associate in Prof. David Leigh's group in Manchester and team leader in Leigh's East China Normal University.





# Low voltage aberration corrected STEM for 2D materials

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Aberration-corrected scanning transmission electron microscopy (STEM) operated at low accelerating voltage can now provide real space imaging and spectroscopy analysis at the atomic scale with single atom sensitivity. This opens new opportunities for quantitative study of the structure and chemistry in 2D materials and monitoring of their dynamical behavior under e-beam irradiation or in-situ heating. Such studies, especially when combined with first-principles calculations, serve as an important step to correlate the atomic structure with their local properties, unveil the atomic growth mechanism for new quantum-structures, and help to create new functionalities in these 2D materials via defect engineering.

Using low-voltage aberration corrected STEM imaging, we show that for epitaxial grown 2D lateral heterostructures where the two monolayer components have similar crystal structure but different lattice constants, such as  $WS_2/WSe_2$  or  $MoS_2/MoSe_2$ , strain relaxation at lateral interfaces due to lattice mismatch often lead to misfit dislocation arrays. We demonstrate that such misfit dislocations can induce the formation and growth of sub-2-nm quantum-well arrays in semiconductor monolayers, driven by dislocation climb [1]. This misfit-dislocation-driven growth can be applied to different combinations of 2D monolayers with lattice mismatch, paving the way to a wide range of 2D quantum-well superlattices with controllable band alignment and nanoscale width.

By performing in-situ annealing experiments in STEM, we found that stacking faults and rotational disorders in multilayered 2D crystals can be healed by grain boundary (GB) sliding, which works like a “wiper blade” to correct all metastable phases into thermodynamically stable phase along its trace [2]. The driving force for GB sliding is the gain in interlayer binding energy as the more stable phase grows at the expense of the metastable ones. Density functional theory calculations show that the correction of 2D stacking faults is triggered by the ejection of Mo atoms in mirror twin boundaries, followed by the collective migrations of 1D GB. The study highlights the role of the often-neglected interlayer interactions for defect repair in 2D materials and shows that exploiting these interactions has significant potential for obtaining large-scale defect-free 2D films.

## References

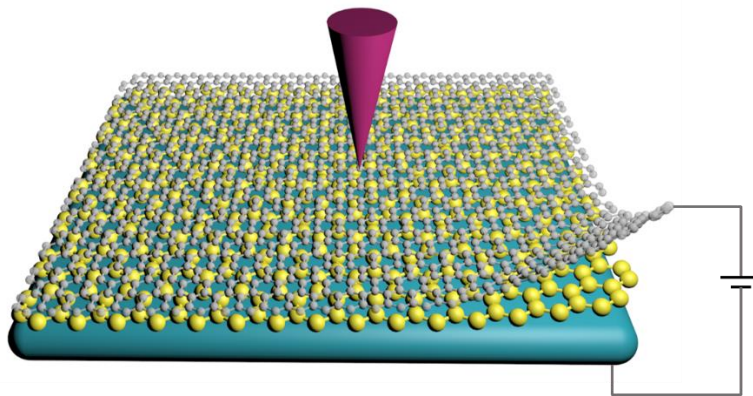
- [1] W. Zhou et al., *Science Advances* 4, eaap9096 (2018).
- [2] X. Zhao et al., *Advanced Materials* 31, 1900237 (2019).

# Construction of graphene/silicene heterostructure by Si intercalation

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The easy oxidation of silicene in air limits its applications in device design and fabrication. Here we report the experimental fabrication of silicene protected by a graphene overlayer. The graphene layer is grown first on a Ru(0001) substrate and silicene is grown under it by Si intercalation. By controlling the amount of silicon, ordered arrays of pseudomorphic silicene nano flakes as well as single layers and multilayers of silicene can be successfully fabricated under graphene that is epitaxially grown on Ru(0001). Density-functional-theory calculations show weak interactions between graphene and silicene layers, indicating that the fabricated structures are silicene/graphene van der Waals heterostructures. The as-prepared silicene-based structures show no observable damage after air exposure for two weeks. The vertical graphene/silicene/Ru heterostructure shows rectification behavior with an ideality factor of  $\sim 1.5$ .



## References

- [1] J. H. Mao et al., *Appl. Phys. Lett.* 100, 093101 (2012).
- [2] Y. Pan et al., *Adv. Mater.* 21, 2777 (2009).
- [3] G. Li, et al., *J. Am. Chem. Soc.* 137, 7099 (2015).
- [4] G. Li, et al., *Adv. Mater.* 30, 1804650 (2018).
- [5] G. Li, et al., *Chem. Soc. Rev.* 47, 982 (2018)