Abstracts
Tuesday 11 December

PLENARY

Smart interfacial materials from super-wettability to binary cooperative complementary systems

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Learning from nature and based on lotus leaves and fish scale, we developed super-wettability system: superhydrophobic, superoleophobic, superhydrophilic, superoleophilic surfaces in air and superoleophobic, superareophobic, superoleophilic, superareophilic surfaces under water [1]. Further, we fabricated artificial materials with smart switchable super-wettability [2], i.e., nature-inspired binary cooperative complementary nanomaterials (BCCNMs) that consisting of two components with entirely opposite physiochemical properties at the nanoscale, are presented as a novel concept for the building of promising materials [3-4].

The smart super-wettability system has great applications in various fields, such as self-cleaning glasses, water/oil separation, anti-biofouling interfaces, and water collection system [5].
The concept of BCCNMs was further extended into 1D system. Energy conversion systems that based on artificial ion channels have been fabricated [6]. Also, we discovered the spider silk's and cactus's amazing water collection and transportation capability [7], and based on these nature systems, artificial water collection fibers and oil/water separation system have been designed successfully [8]. Learning from nature, the constructed smart multiscale interfacial materials system not only has new applications, but also presents new knowledge: Super wettability based chemistry including basic chemical reactions, crystallization, nanofabrication arrays such as small molecule, polymer, nanoparticles, and so on [9].

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PLENARY

2D materials for high-performance electronics

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The layered crystals are an extremely rich family of materials spanning from superconductors to insulators with a bandgap over 6 eV, from magnets to ferroelectrics, while boasting an atomically thin dimensionality that was difficult to access previously without expensive equipment. Furthermore, number of layers coupled with the crystal structure allows one to explore the impact of controlled symmetry on electronic, optical and magnetic properties. The facile processes to prepare layered materials and heterostructures have enabled an unprecedented number of scientists and engineers in history to interrogate this material group, aiming to answer what new physics can be found and what new applications can be explored. To this end, our group has focused on one type of applications: high-performance electronics. Is it possible to build new electronic switches that at least rivals the prevalent Si CMOS transistor with a population orders of magnitude higher than human being? Is it possible to ever exceed the performance of today's switches thus offering possible pathways to extend "more Moore" or offer "more than Moore"? As electronics are intimately integrated with our lives, we need sensors to collect signal, amplifiers to boost signal strength, transmitters and receivers to communicate signals, logic blocks to process information and memory blocks to store information. While an electronic switch is an important building block to all the above, these applications all have their own unique figures-of-merits. In this talk, I will discuss a few examples on high-performance electronics built on 2D materials including steep transistors [1], THz modulators [2], RF oscillators [3], and memories as well as our effort on growing 2D materials by molecular beam epitaxy [4].

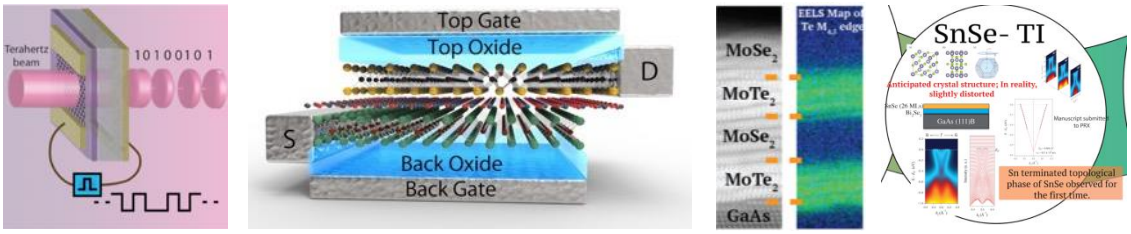

Fig. 1. From left to right: graphene THz modulator, Thin-TFET (two-dimensional heterojunction interlayer tunnel field effect transistor), layered heterostructures and crystalline topological insulator by MBE

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SYMPOSIA 1 – PHYSICS

Van der Waals heterostructures: from commensurate superlattice to incommensurate quasicrystal

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Two-dimensional (2D) materials provide an important playground for exploring fundamental physics and potential applications. By stacking simple 2D materials together to form heterostructures, we can use the band structure engineering at the interface to obtain new properties that are not otherwise possible in a single material. In this talk, I will present our recent progress in the band structure engineering of two prototypical examples of van der Waals heterostructures, a commensurate graphene/BN heterostructure with Moire pattern [1], and an incommensurate 30° twisted bilayer graphene which shows symmetries similar to a quasicrystal [2].

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Cavity polaritons in strongly-correlated two-dimensional materials

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Following the recent success of realizing exciton-polariton condensates in cavities, I will discuss the hybridization of cavity photons with collective modes in interacting two-dimensional materials. First, I will discuss how the Higgs mode in various symmetry-broken states of matter can be stabilized and excited by resonantly coupling it to cavity photons. Next, I will examine the closest analog of excitons within a superconductor, states called Bardasis-Schrieffer modes. Though Bardasis-Schrieffer modes do not typically couple directly to light, one can engineer a coupling with an externally imposed supercurrent, leading to the formation of hybridized Bardasis-Schrieffer-polariton states. These new excitations have nontrivial overlap with both the original photon states and d-wave superconducting fluctuations, implying that their condensation could produce an exotic s±id superconducting state. In conclusion, I will discuss how cavities can be used to enhance coherent quantum states in strongly correlated materials.

Room temperature in-plane ferroelectricity in β'-In_2Se_3

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Ferroelectrics are important elements for non-volatile memory and low-power electronic and optoelectronic switches [1]. Van der Waals (vdW) layered materials are promising candidates to achieve ultrathin ferroelectrics. We here reported the discovery of in-plane ferroelectricity in a widely investigated vdW layered material, β'-In_2Se_3 [2]. A monolayer In_2Se_3 consists of 5 layers of atoms, see Fig. 1A. The in-plane ferroelectricity is strongly tied to the formation of one-dimensional superstructures aligning along one of the threefold rotational symmetric directions of the hexagonal lattice in the c plane, owing to the shift of the middle Se atoms. Fig. 1B indicates the micro-low energy electron diffraction patterns corresponding to the domains shown in Fig. 1C. The superstructures and ferroelectricity are stable to 200 ℃ in both bulk and thin exfoliated layers. Due to the in-plane nature of ferroelectricity, the domains exhibit a strong linear dichroism, enabling novel polarization-dependent optical properties.

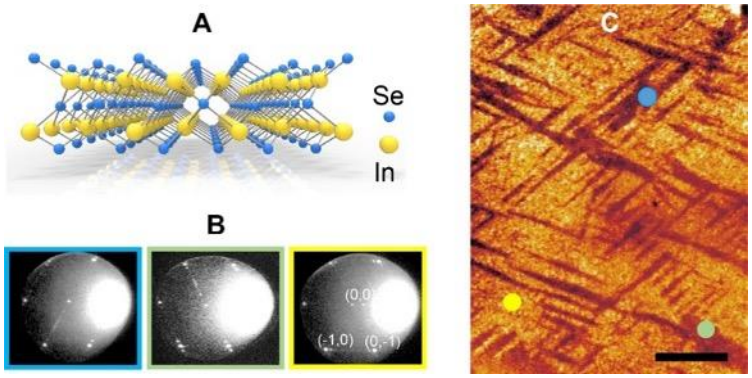

Fig. 1. (A) Crystal structure of layered β-In_2Se_3. (B) Low energy electron diffraction patterns of the three domains shown in the low energy electron microscopy image (C) taken at 9.9 eV. Scale bar: 1.5 µm.

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Helicity dependent photocurrent in transition metal dichalcogenide van der Waals heterostructures

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In transition metal dichalcogenide monolayers, photogalvanic effect can be induced by an obliquely incident polarized excitation owing to spin-orbit coupling and broken symmetry[1-3]. Transition metal dichalcogenide van der Waals heterostructures, which have lower symmetry than monolayers, exhibit ultra-long valley polarization lifetime [4] and optical spin pumping [5] in the presence of a magnetic field. Here we report on the generation of helicity dependent photocurrent in van der Waals heterostructures with a normally incident polarized excitation in the absence of an external magnetic field. We suggest that the helicity dependent photocurrent originates from the C_1 symmetry when two heterogenic monolayers are coupled together. The spin-charge conversion makes spin detection and amplification more efficient, which will ease the application of valleytronic devices.

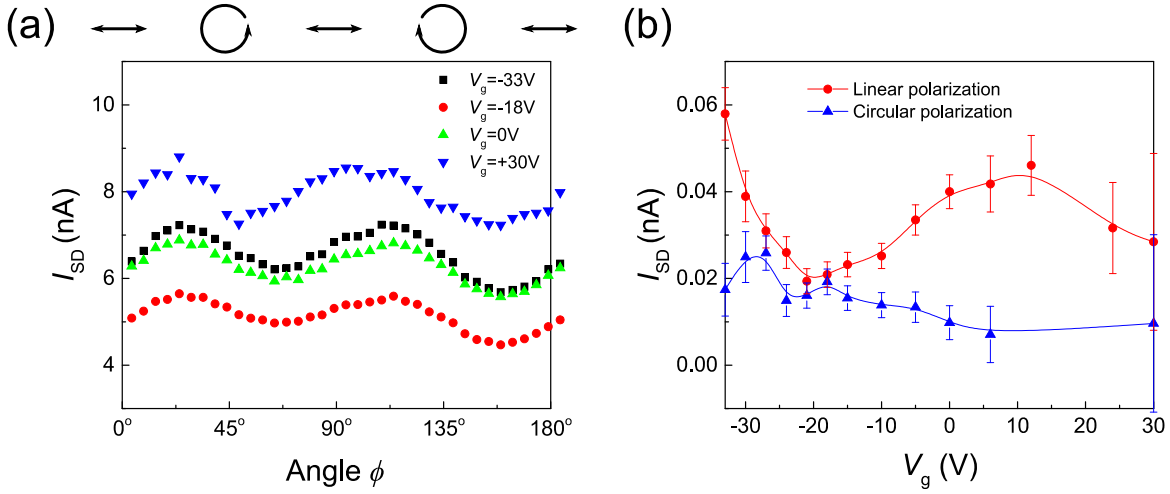

Fig. 1. Circular and linear photogalvanic effect at normal incidence in WSe_2-$MoSe_2$ heterostructure. (a) Photocurrent versus photon helicity at different back gate voltage. (b) Linear and circular photogalvanic effect as a function of back gate voltage.

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Conventional and in-situ quantum transport measurement of two-dimensional materials

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Due to the very large surface to bulk ratio, two-dimensional (2D) materials has a greatly enhanced response to stimulus from the environment. This presentation will focus on our recent progress in quantum transport measurement of 2D mesoscopic devices in controlled environment. By encapsulation of the 2D materials, we ensure high quality and stability of our devices for conventional transport measurements, which revealed rich physics and a variety of potential applications for 2D materials. By in-situ manipulation of sample surface during a single experimental run, we can continuously tune the interactions of the 2D electronic systems and observe the resultant changes in their electronic states. As an example, magneto-transport experiment with *in-situ* cobalt adsorption and hydrogenation of graphene will be discussed, and the stark contrast of the electronics states between metal decorated graphene and covalently modified graphene is demonstrated.

SYMPOSIA 1 – DEVICES

The organic-2D transition metal dichalcogenide interface

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We use high resolution scanning tunneling microscopy/spectroscopy (STM/STS) to study the atomic structure and local electronic properties of 2D MoS2 and WSe2 monolayers on HOPG substrates, and show that the electronic bandgaps can be tuned by strain at grain boundaries and dislocations [1,2]. Using PTCDA as a prototype semiconductor organic molecule, we show that a monolayer TMD can effectively screen an organic-inorganic heterointerface [3]. We demonstrate the fabrication and unravel the electronic properties of a lateral doped/intrinsic heterojunction in 2D WSe2, partially covered with a molecular acceptor C60F48 [4].

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Atomic layer 2D nanoelectromechanical systems (NEMS) with ultra-broad electrical tunability

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Atomically thin crystals have rapidly emerged to enable two-dimensional (2D) nanostructures with unusual electronic, optical, mechanical, and thermal properties. While graphene has been the forerunner and hallmark of 2D crystals, new elemental and compound 2D semiconductors (with various bandgaps), high-k dielectric crystals, and their van der Waals heterostructures also offer wide spectra of fascinating attributes. This presentation will focus on reporting and updating some latest highlights on exploring device physics and engineering of nanoelectromechanical systems (NEMS) based upon suspended, mechanically active atomic layer semiconductors and their vertically stacked heterostructures, toward realizing ultrasensitive transducers and ultralow-power signal processing devices at radio frequencies (RF). We will describe electrically tunable multimode resonant 2D NEMS using atomic layer transition metal dichalcogenides (TMDCs) and black phosphorus crystals, and their van der Waals heterostructures with graphene and hexagonal boron nitride (h-BN), and high frequency 2D NEMS resonators with ultra-broad tunability (>300%) of their resonance frequencies. We employ both analytical and computational approaches to reveal the device physics, and the unusually strong and efficient electromechanical coupling that underlies such ultra-broad electrical tuning. We then describe ongoing explorations toward fully on-chip integration and scaling of such device technologies, and their emerging applications in fundamental physics and nanosystems.

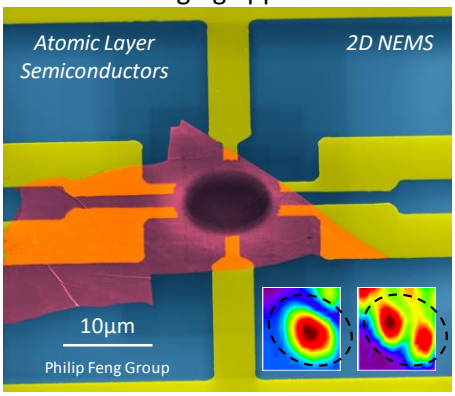

Fig. 1. A representative 2D NEMS resonator with broad electrical tuning.

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Band structure engineering of atomically thin PbI_2 with monolayer transition metal dichalcogenides

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To explore new components in two-dimensional material family and to combine their best in van der Waals heterostructures provides an essential engineering platform for modern electronics. Here we fabricate PbI_2 crystals down to atomic scale, and further mechanically assemble them with transition metal dichalcogenides (TMDs) monolayers, in realization of designing different types of band alignment and interlayer interactions. The photoluminescence of MoS_2 is enhanced in MoS_2/PbI_2 heterojunction, while a dramatic photoluminescence quenching of TMDs was revealed in WS_2/PbI_2 and WSe_2/PbI_2 stacks. This is attributed to the effective heterojunction formation between PbI_2 and TMDs materials, but type I band alignment in MoS_2/PbI_2 and type II in both WS_2/PbI_2 and WSe_2/PbI_2 stacks, as confirmed by first-principles calculations and interlayer exciton lifetime. Our results demonstrate that MoS_2, WS_2, WSe_2 monolayers with very similar electronic structures themselves, show distinct charge transfer process and optical properties when in incorporation with atomically thin PbI_2 crystals, which opens a new window to heterostructure engineering that potentially applied in two-dimensional lasers, light-emitting diodes, photodetectors and photovoltaic devices.

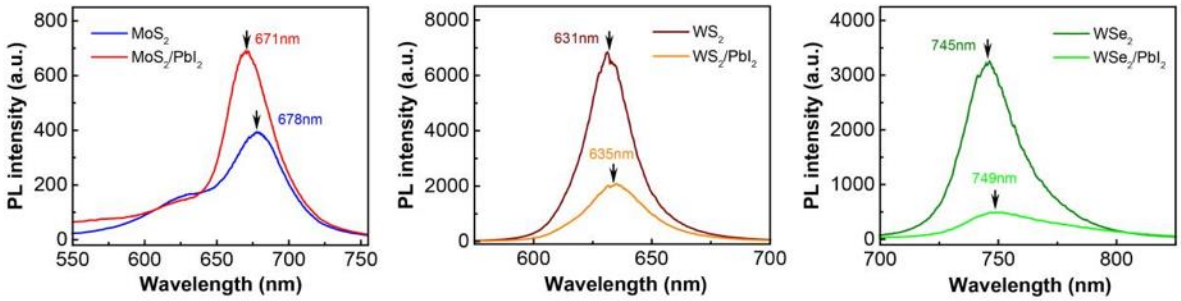

Fig. 1. Photoluminescence measurement of MoS_2/PbI_2, WS_2/PbI_2, WSe_2/PbI_2 heterostructures.

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Phosphorene: an alternative elemental analog of graphene

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Black-phosphorus (BP) has emerged as a material of interest owing to its high carrier mobility and the presence of an intrinsic direct bandgap. Few-layer BP has been a focus of several studies and is promising for applications in electronics, optoelectronics, energy storage, gas sensing, catalysis and chemical/biosensing. However, the ambient instability of BP remains the biggest hurdle in its progress. The fact that the material has to be stored and handled in an inert environment renders it to be unfavourable for practical implementation. Our work with BP involves understanding the origins of degradation and developing a surface treatment based approach to prevent ambient deterioration. [1-4] We have also explored how defect doping can be used to manipulate the electronic and optical properties of BP to create applications in UV sensing and artificial synaptic emulation. A combination of these studies opens opportunities to practically implement BP and other environmentally-sensitive two-dimensional (2D) materials for electronic applications.

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Ultralow power MoS_2 negative capacitance field-effect transistors

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2D semiconductors are promising candidates for future electronic device applications due to their immunity to short-channel effects, but many important issues regarding mobility, contact, interface and power consumption still remain. Recently, negative capacitance field-effect transistors (NCFETs) with ferroelectric gate stack provides a viable solution to break the thermodynamic limitation of the subthreshold slope (SS) of 60 mV/dec and realize ultra-low power transistors. Here, we realize 2D NCFETs using ferroelectric $HfZrO_x/AlO_x$ as dielectric layer and MoS_2 as channel material. The MoS_2 NCFETs exhibit ultra-low SS of 23 mV/dec, sub-60mV/dec over 6 orders of I_D, nearly hysteresis-free, and 10^7 on/off ratio under V_{dd}=0.5V. We further study high frequency performance and show that sub-60mV/dec is maintained at least to 10 kHz without signs of degradation. Our results demonstrate the potential of 2D NCFETs for ultralow-power electronics applications.

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SYMPOSIA 1 – CHEMISTRY

Electrocatalysis for water splitting and CO2 conversion

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The oxygen evolution reaction (OER) and hydrogen evolution reaction (HER) are two important processes in the electrocatalytic water splitting. Replacement of precious metal catalysts by commercially available alternatives is of great importance among both fundamental and practical catalysis research. Nanostructured carbon-based and transition metal materials have demonstrated promising catalytic properties in a wide range of energy generation/storage applications. Specifically engineering carbon with guest metals/metal-free atoms can improve its catalytic activity for electrochemical OER and HER, thus can be considered as potential substitutes for the expensive Pt/C or IrO_2 catalysts in water splitting process. In this presentation, I will talk about the synthesis of nonprecious metal and metal free elements-doped graphene, and their application on electrocatalysis [1-6]. The excellent OER and HER performance (high catalytic activity and efficiency) and reliable stability (much better than the commercial Pt/C or IrO_2) indicate that new materials are promising highly efficient electrocatalysts for clean energy conversion. I will also present some research results of CO2 electrocatalytic reduction conducted in my research group [7,8]. We explored the fundamental role of the secondary active site (metal or carbon) in Cu-based electrocatalysts for CO2 reduction, focusing on how these active sites affect the selectivity of the CO2 reduction products. We found a trend that exists in a long time yet never has been discovered.

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Nicklel-iron based 2D materials for electrocatalytic water splitting

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The increasing demands for clean energy have triggered tremendous research interests on electrochemical energy conversion and storage systems with minimum environmental impact. Electrolytic water splitting holds the promise for global scale storage of renewable energy, e.g., solar and wind in the form of hydrogen fuel, enabling the continuous usage of these diffusive and intermittent energy sources when used together with fuel cells.[1,2] Nevertheless, the widespread application of water splitting technology has been severely constrained by the use of precious metal catalysts, such as oxides of ruthenium and iridium for the anodic oxygen evolution reaction (OER), and platinum for the cathodic hydrogen evolution reaction (HER). This presentation concerns our recent progress in developing low cost, Ni and Fe-based 2D materiasl as electrocatalysts for OER and HER, as well as our strategies for enhancing the efficiency of these catalysts by 2D nanostructuring to a level comparable to that of precious metal catalysts.[3-7] The commercialisation of some 2D materials in water electrolysis industry also will be discussed.

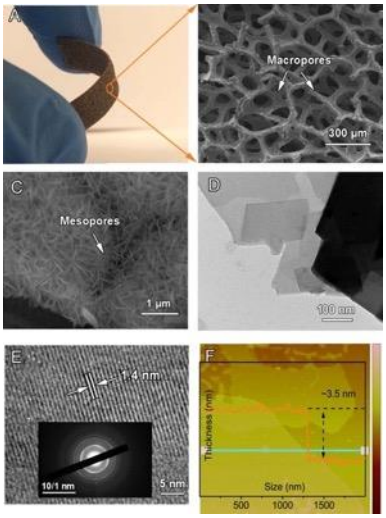

Fig. 1. Ultrathin 2D NiFe metal-organic framework (MOF) array for electrocatalytic water splitting.[10]

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Coordination-engineering cobalt on phosphorized carbon nitride for water splitting

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Two-dimensional (2D) nanomaterial have emerged as promising candidates for energy conversion technologies due to their unique electronic properties. Here, we utilized interfacial coupled and confined approach to modulate Cobalt species with selectable form and coordination environment, to be efficient and durable photocatalyst and electrocatalyst. At first, we achieve a strategy via constructing the single site to simultaneously promote charge separation and catalytic activity for achieving robust overall water splitting. As a prototype, the single Co_1-P_4 site confined on g-C_3N_4 2D nanosheets was accessed by a facile phosphidation method, as identified by electron microscopy and X-ray absorption spectroscopy. Thus, the developed single-site photocatalyst delivers steady and high-efficient water splitting activity with H_2 evolution rate up to 410.3 μmol h^{-1} g^{-1}, and quantum efficiency as high as 2.2% at 500 nm.[1] Furthermore, we increased the size and altered coordination environment of Co species simultaneously to obtained a CoO_x clusters with uniform size range 1.5 nm on the phosphorized carbon nitride (PCN). X-ray absorption spectroscopy and theoretical insights demonstrate that coordinatively unsaturated surface and strongly coupling effect of PCN tailor the electronic structure of Co active sites with optimized OH^- adsorption energy for oxygen evolution. The resulting hybrid catalyst exhibits excellent water oxidation activity, reaching 10 mA cm^{-2} current by applying a low overpotential of 250 mV for continuous operation of 10 h. Remarkably, the CoO_x possesses outstandingly intrinsic activity, delivering turnover frequency of 1.69 O_2 s^{-1} at overpotential of 300 mV, which are the best among those catalysts reported for water oxidation. [2]

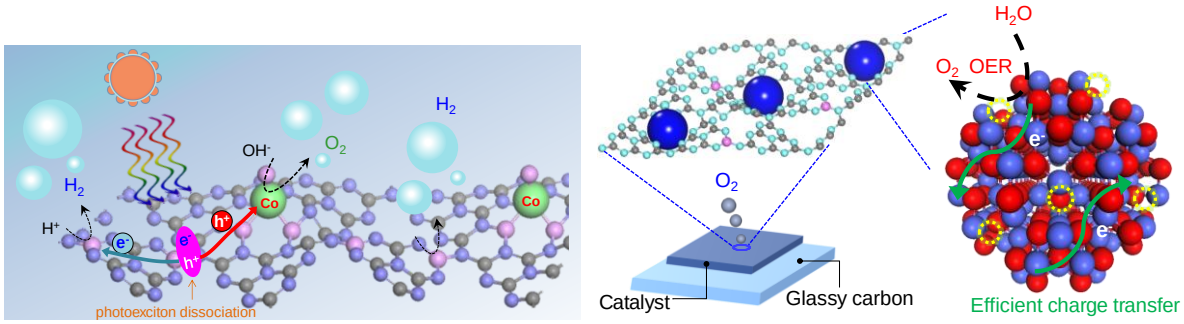

Fig. 1. Schematic illustration of coordination-engineering Co on phosphorized carbon nitride for water splitting.

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Enhanced properties of the high internal phase water-in-oil emulsion using graphene oxide-based additives

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The two peculiar properties of graphene oxide (GO) viz. stabilizing interfaces and additive for electrical and thermal percolation have been the areas of interest for research. Exploring these properties in combination can enable thermal interface materials derived from a two-phase system. GO, partially-reduced GO (prGO) and amine-functionalized GO (fGO) are used to enable high-internal phase water-in-oil emulsion (HIPE) with improved rheology and thermal conductivity. The change in hydrophilic-to-lipophilic balance (HLB) in prGO enables HIPE without the use of long-chain additives. The droplet size, polydispersity and the viscoelasticity of the resultant HIPE can be tuned by participating phases and prGO concentration. The aging characteristics of the HIPE has been affected by metastability which is limited by non- dispersion of GO in the continuous phase. The amine-functionalisation of GO significantly enhances the stability of HIPE synthesized using conventional emulsifier. The dispersion of fGO in the continuous phase improves processibility by acting as a lubricant investigated using rheological properties, nullifies the competitive action of the surfactant-GO with the emulsifier at the interface and enhances the thermal conductivity of HIPE. The fGO thermally percolates at a critically low volume fraction of 0.0002%, with maximum enhancement of 21% in the thermal conductivity at 0.0004%. The results are compared and contrasted with literature so far on the thermally conducting emulsions. This is the lowest volume fraction of additives ever reported to enhance the thermal conductivity of a two-phase system.

Graphene as playground for molecules: from chemisorption to catalysis

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The chemical functionalization of graphene has been intensely pursued in the last years. A significant part of the research efforts from the wet chemistry trench have focused on the covalent attachment of molecular fragments to graphene. This lack of selectivity is a major drawback if the objective of the covalent modification is to modulate the electronic properties of graphene. The periodic landscape is provided by a single monolayer of graphene grown on Ru(0001) that presents a moiré pattern due to the mismatch between the carbon and ruthenium hexagonal lattices. The moirè contains periodically arranged areas where the graphene−ruthenium interaction is enhanced and shows higher chemical reactivity. This phenomenon is demonstrated by the attachment of cyanomethyl radicals ($CH_2CN^{\bullet}$) produced by homolytic breaking of acetonitrile (CH_3CN), which is shown to present, under appropriate conditions t a nearly complete selectivity (>98%) binding covalently to graphene on specific atomic sites with an extremely high yield, 92% of the reactive atomic sites are occupied by CH_2CN. The key to maintaining selectivity while increasing the yield is to increase the temperature of the sample during functionalization, to prevent the CH_2CN attaching at local minima over the chemisorption energy surface (see Figure 1). This method has been extended to other organic nitriles, paving the way for the attachment of functional molecules.
Finally I will discuss how epitaxial graphene become a catalyser that promotes the reversible formation of a C-C bond between two organic molecules. The reaction is fully reversible as demonstrated by single molecule manipulation by injecting electrons with the STM tip on the empty molecular orbitals.

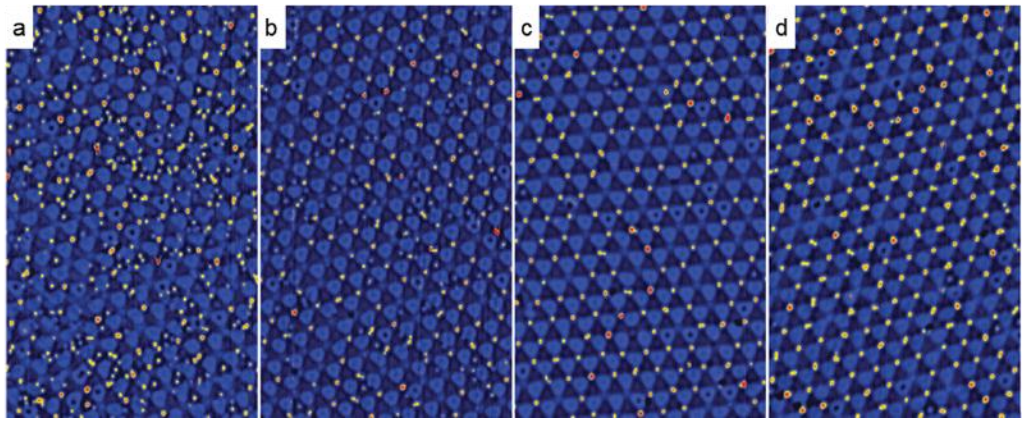

Fig. 1. (a) STM image (56×34 nm^2, V_b = +1.7 V, I_t = 10 pA) acquired after exposing the sample at 300 K to 720 L of CH_3CN. (b) STM image (70×40 nm^2, V_b = +1.7 V, I_t = 10 pA) acquired after exposing the sample at 354 K to 720L of CH_3CN. (c) STM image (69×40 nm^2, V_b=+1.7 V, I_t = 10 pA) acquired after exposing the sample at 374 K to 720 L of CH_3CN. (d) STM image (61×32 nm^2, V_b = +1.7 V, I_t = 15 pA) acquired after exposing the sample at 374 K to 1080 L of CH_3CN. All images acquired at 78 K.

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SYMPOSIA 1 – SYNTHESIS

Magnetic and physical properties of new 2D materials

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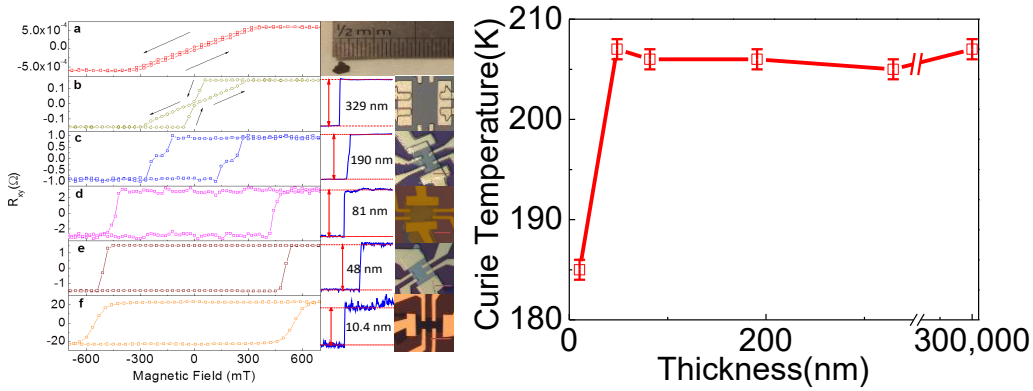
The representative 2D materials, graphene, h-BN, and MoS_2, have interesting mechanical, electrical and optical properties and have exhibited fascinating physical phenomena so far. However, they mostly lack one important physical property in physics, magnetism. The new 2D materials such as CrSiTe3, CrI3, and FePS3, which began to be studied recently, possess ferro- or antiferro-magentic properties even in atomic level thickness and are expected to reveal deep level of physics in 2-dimensional confinement. In this talk, our recent works on thickness dependence of magnetic and optical properties of ternary 2D materials, Fe3GeTe2 and CrPS4, which are ferromagnetic and antiferromagnetic 2D materials, will be presented. Fe3GeTe2 was studied with hall measurement[1] and STM methods[2]. From the hall measurement, it exhibited the anomalous hall effect due to its intrinsic ferromagnetism. Interestingly, the magnetic properties such as coercivity changed significantly with decreasing thickness changing from weak ferromagnet to strong ferromagnet (Figure 1). STM study revealed some magnetic domains on the surface. The domain structures barely changed below Curie temperature, but disappeared above the critical temperature, which suggests they are magnetic structures. CrPS4, which is an antiferromagnet, was characterized with Raman and PL spectroscopies[3]. Its bandgap was measured to be roughly 1.3 eV and its structure showed strong in-plane optical anisotropy.



(a) (b)

Fig. 1. Thickness dependent magnetic properties of Fe3GeTe2 (a) thickness dependent coercivity (b) thickness dependent Curie temperature

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Nanoscopic redox governing charge carriers in two-dimensional crystals

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Controlling extra charge carriers in two-dimensional (2D) crystals has played an important role in manipulating their various material properties. Intense efforts via chemical charge doping have been devoted to not only enhancing electrical conductivity, opening bandgap and tuning optical transparency of graphene, but also inducing superconducting phase and manipulating exciton dynamics of transition metal dichalcogenides. Despite these, the mechanistic details of their spontaneous hole doping in ambient air and acidic solution are not well understood [1~4]. Here we show the essence is a redox reaction that involves oxygen and water molecules using environment-controlled photoluminescence imaging of WS_2 and Raman spectroscopy of graphene [5]. In particular, the 2D nanoscopic space between 2D crystals and substrates accommodates otherwise labile water species that plays a second role as a solvent. We also confirm HCl-driven doping is tuned by dissolved O_2 and can be described by the Nernst equation. These results will be important for efficient control of charge density in various 2D materials and devices.

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Investigating novel synthesis, optical properties and applications of model 2D semiconducting nanocrystals

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This research explores the synthesis and fundamental properties of model two dimensional (2D) metal oxides and transition metal chalcogenides, specifically 2D tin (II) oxide (SnO) and tungsten disulphide (WS_2). These materials are extensively characterised, leading to the discovery of laser-induced, localised reduction in the PL of 2D WS_2; enhanced photocatalytic efficacy of 2D WS_2 nanoflakes when hybridised with carbon dots (CDs); and a facile method for producing p-type semiconducting SnO as centimetre sized large-area monolayers. Recently, we describe the morphology and compositional characteristics of tin oxides, obtained *via* the liquid metal based van der Waals exfoliation technique, at distinct stages of growth on molten tin at 300°C in ambient atmospheric conditions (Fig. 1).[1] We show that the 2D skin on the surface of molten tin gradually evolves into different stoichiometries and thickens over time. This will provide a roadmap for gaining a better control and understanding as to how tin oxides of a desired thickness and stoichiometry can be reliably and consistently obtained.

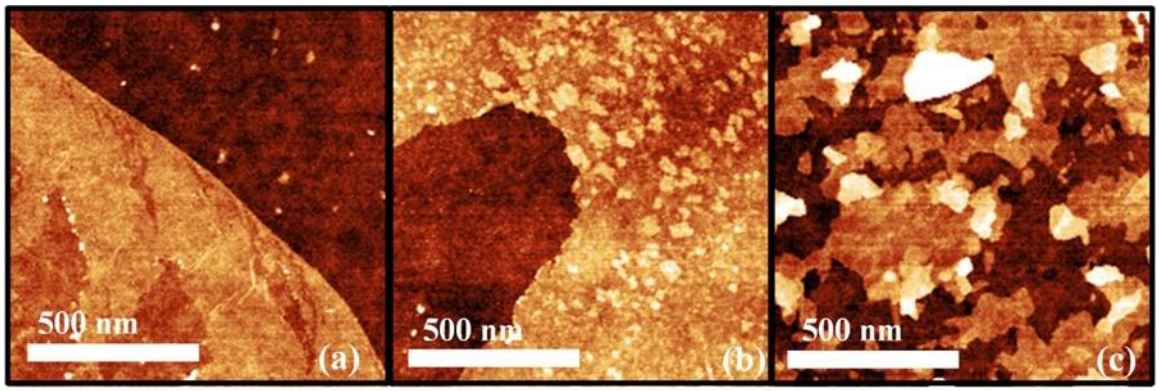

Fig. 1. AFM images of (a) fresh, (b) yellow and (c) pink tin oxides. In the fresh oxide sample (a), a flat nanosheet is observed with a large region of increased thickness at the edge; the height profile (d) confirms this to be a SnO monolayer, with the edge folded back on itself to form a large bilayer region. The yellow oxide shown in (b) consists of a section of large-area folded bilayer with smaller sheets of variable area and orientation across its surface

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Edge optical scattering of two-dimensional materials

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Rayleigh scattering has shown powerful abilities to study electron resonances of nanomaterials regardless of the specific shapes. In analogy to Rayleigh scattering, here we demonstrate that edge optical scattering from two-dimensional (2D) materials also has the similar advantage. Our result shows that, in visible spectral range, as long as the lateral size of a 2D sample is larger than 2 μm, the edge scattering intensity distribution of the high-angle scattering in k space is nearly independent of the lateral size and the shape of the 2D samples. The high-angle edge scattering spectra are purely determined by the intrinsic dielectric properties of the 2D materials. As an example, we experimentally verify this feature in single-layer MoS_2, in which A and B excitons are clearly detected in the edge scattering spectra, and the scattering images in k space and real space are consistent with our theoretical model (Fig. 1). This study shows that the edge optical scattering is a highly practical and efficient method for optical studies of various 2D materials as well as thin films with clear edges. It is also promising for a variety of characterizations in 2D systems such as heterojunctions, interlayer coupling, grain/domain boundaries, phase separation/transition, topological edge states, and so on, as long as the discontinuity of dielectric properties exists [1].

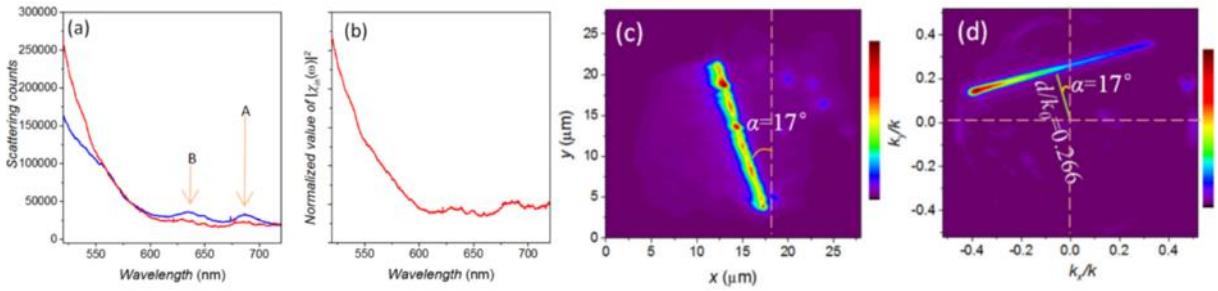

Fig. 1. (a) s wave (red line) and p wave (blue line) edge scattering spectra from a single flake of monolayer MoS_2. (b) Relative normalized value of $|\chi_{in}(\omega)|^2$. (c) and (d): The high-angle scattering images of a flake in real space (c) and k space (d).

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Motions induced by interface strain in nano-layered structures

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Interface strain exist very commonly in layered structures, particularly at a hetero-interface between two different materials. Dynamic change of the strain could induce various types of motions such as bending, rotating, or buckling, which exhibit new features in some novel functional materials. Here the motions induced by interface strain in two types of layered hetero-structures, which are based on a phase-change material and 2-dimensional (2D) crystals (MoS_2, ReS_2, etc), respectively, will be presented. In the former, the drastic interface strain delivers a powerful mechanical actuation with an ultra-high work density, while in the latter, it causes dynamic buckling of semiconducting films with new functionality. The exploration of these systems not only provides mechanical insight to the understanding of functions and interface physics of layered hetero-structures, but also potentially allows engineering of layered structures as desired.

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SYMPOSIA 2 – PHYSICS

An orbitally driven single atom magnetic memory on black phosphorus

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Single-atom memory represents the ultimate limit in high-density storage and a route toward quantum coherent manipulation. Of particular interest are single magnetic atoms on surfaces, which can represent a bit employing the bi-stability of the magnetic moment, as they offer tunable interatomic coupling and bottom-up design. While atomic spins can have long-lived lifetimes, the key challenge has been to decrease fluctuations induced by spin-sensitive readout or scattering mechanisms utilizing robust magnetic anisotropy. We demonstrate a single-atom magnetic memory derived from bi-stability in the orbital configuration or so-called valency of a single Co atom on semiconducting black phosphorus, yielding two stable and distinct total magnetic moments. Utilizing scanning tunneling microscopy and *ab initio* calculations, we detail the effect of the local tip-induced gate potential and spatially anisotropic wavefunctions on the switching behavior. I will also detail the electronic properties of black phosphorus and intrinsic defects as seen with tunneling spectroscopy. This opens up the possibility of utilizing the orbital degree of freedom for robust single-atom magnetic information storage without requiring spin-sensitive detection, as well as understanding the effect of gating a single atomic bit with an anisotropic charge distribution.

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How robust is the metallicity of two-dimensional gallium?

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Atomically thin gallium layers have been experimentally produced via solid-melt exfoliation, and have been shown to have promise as robustly metallic 2D materials for electronic applications [1]. However the extent to which the experimental technique can be extended to other metals relies on understanding how the 2D structures relate to the bulk form of gallium, which is itself unique as an elemental 'molecular metal' (Fig. 1). We relate the experimentally formed 2D materials to the theoretically predicted 'bilayer gallium' which has previously been shown to be stable in vacuum at the nanoscale, via density functional theory calculations [2]. We also study the variation of electronic structure with lattice strain to confirm that the metallicity will indeed be robust on a wide range of substrate materials.

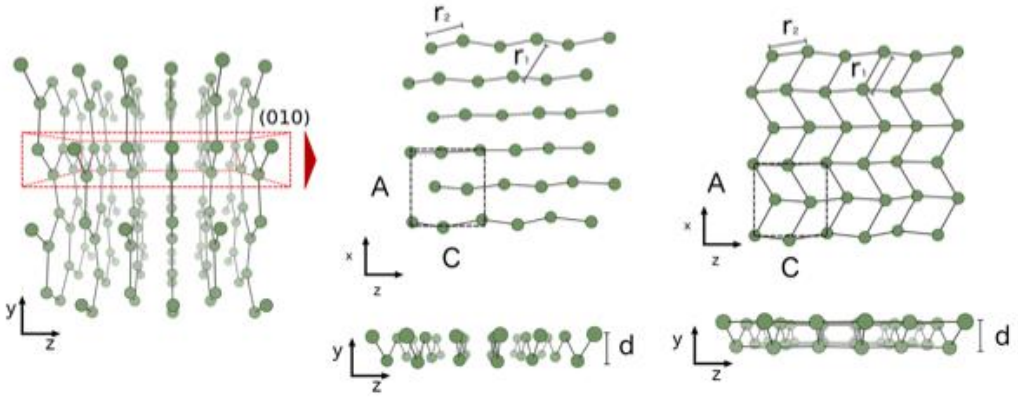

Fig. 1. The relationship between the bulk structure of gallium (under standard conditions) and the two-dimensional structure obtained by isolating the buckled metallic planes and cutting through the covalent bonds in the structure is shown.

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Black-phosphorous-like bismuthene and antimonene in topological van der Waals heterostructures

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The experimental investigation of topological materials has been a highly active research field for more than a decade. One of the earliest confirmed topological materials was the Bi1-xSbx alloy [1]. Subsequently, bismuth-(111) bilayers [2] were reported to be topologically nontrivial, as well as atomically thin black phosphorous-like (110)-oriented alpha-bismuthene [3] and even bulk bismuth [4]. The (111)-oriented antimonene, on the other hand, is a trivial semiconductor that potentially becomes nontrivial only under substantial strain [5]. There is significant interest in these 2-dimensional topological materials as they could be combined with other functional materials in specifically tailored van der Waals heterostructures in which they retain their characteristic properties due to the weak interaction. Moreover, when combining these ultrathin sheets of material moiré patterns can arise due to different lattices and rotation angles. Such moiré patterns can have a marked effect on the electronic band structure [6] and constitute yet another way to tune the properties of the heterostructure. When growing atomically thin Sb on top of alpha-bismuthene nano-islands [7,8], it forms the known (111) phase, as well as (110)-antimonene which has not been experimentally studied before. Also, moiré patterns emerge inevitably on both antimonene phases. We present our joint study [9] of alpha-antimonene, in which we combined scanning tunnelling microscopy experiments and DFT calculations. Our results show that this new material is topologically nontrivial. Geometric modelling of the layers is used to understand the moiré patterns and support the determination of the lattice parameters.

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Electromechanical actuation properties of group IV monochalcogenides

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The intrinsic nanosized thickness and superior flexibility render 2D materials indispensable candidates for flexible nano-electromechanical system (NEMS) devices, integrating the electrical and mechanical functionality at the nanoscale for applications such as energy conversion, soft robotics, and bioengineering. In most NEMS devices, electromechanical actuators are the key components, which converts electric energy to mechanical motion. Group IV monochalcogenide (prototyped as black phosphorene) is a 2D material family with unique puckered atomistic structure and remarkable physical and chemical properties. In this talk, we report density functional theory computational study of an unexpected shape memory effect and giant piezoelectricity in this material family. We find two stable phases in a two-dimensional (2D) phosphorene with adsorbed Li adatoms (P_4Li_2). Applying an external electric field can turn on or off the unique adatom switches in P_4Li_2 crystals, leading to a reversible structural phase transition and thereby the shape memory effect with a tunable strain output as high as 2.06%. Our results demonstrate that multiple temporary shapes are attainable in one piece of P_4Li_2 material, rendering programmability that is particularly useful for device designs. Additionally, the P_4Li_2 displays superelasticity that can generate a pseudoelastic tensile strain up to 6.2%. We also find with appropriate surface adatom adsorption, some group IV monochalcogenide exhibits the highest piezoelectric coefficient. The atomic thickness, superior flexibility, excellent electromechanical strain output, the special shape memory phenomenon, and the programmability feature endow P_4Li_2 with great application potential in high-efficient energy conversion at nanoscale and flexible nanoelectromechanical systems.

Spin transport studies in graphene and black phosphorus

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The electric field effect in 2D materials is crucial for many novel device concepts including spintroncis. They are also ideal to induce complementary properties by means of the proximity effect. For example, the combination of Rashba interaction, magnetic moments and electric field control of the density, is akin to dilute magnetic semiconductors. Thus, this opens a route toward electric field control of magnetism and engineering topological magnetic states. In the first part of my talk I will discuss efforts in inducing a large spin orbit coupling in graphene and spin transport studies in black phosphorus. Pristine graphene has negligible spin-orbit coupling (SOC). However, strong SOC can be induced, e.g. by hybridization with heavy metals. I will discuss experiments where this has been achieved with Au intercalated van der Waals heterostructures of graphene and hexagonal boron nitride [1]. The SOC of pristine black phosphorus (bP) is equally weak. In the second part of my talk I will show, based on measurements in the non-local spin valves geometry, that the spin relaxation times can be as high as ~ 4ns with spin relaxation lengths exceeding 6 μm [2]. In principle this should make bP an equally exciting material platform for proximity effect studies in 2D. I will conclude my talk with a brief discussion on potential applications of graphene explored in my group.

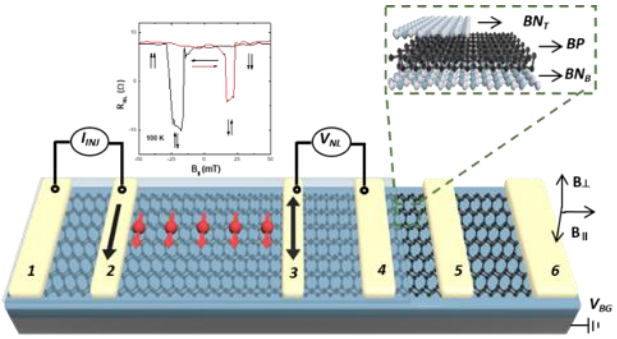

Fig. 1. A lateral spin valve with semi-conducting black phosphorus [2].

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SYMPOSIA 2 – DEVICES

Advanced in situ TEM on manipulation of nanostructure and probing new properties at atomic scale

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Transmission electron microscopy (TEM), with its high spatial resolution and versatile external fields, is undoubtedly a powerful tool for the static characterization and dynamic manipulation of nanomaterials and nanodevices at the atomic scale. The rapid development of thin-film and precision microelectromechanical systems (MEMS) techniques allows 2D layered materials and nanodevices to be probed and engineered inside TEM under external stimuli such as thermal, electrical, mechanical, liquid/gas environmental, optical, and magnetic fields at the nanoscale. Such advanced technologies leverage the traditional static TEM characterization into an in situ and interactive manipulation of 2D layered materials and nanodevices without sacrificing the resolution or the high vacuum chamber environment, facilitating exploration of the structure–property relationship of 2D layered materials and nanodevices [1]. Here, taking advantage of advanced in situ transmission electron microscopy, we manipulated interfacial defects in Ⅲ-Ⅴ devices [2] and RRAM [3]. We also observed the whole growth process of the monolayer graphene and MoS_2 nanoribbon at real time. The progress of the in situ TEM paves the way to future high-speed and high-reliability devices [4,5].

Fig. 1. In situ transmission electron microscopy, with its versatile external field stimuli, is a powerful tool for the static characterization and dynamic manipulation at the atomic scale.

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Detection and modulation of light wave with graphene

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Graphene is a member of two-dimensional materials demonstrating very extraordinary electronic, optical, thermal, and mechanical properties. Significant progress has been made in the past decade, which shed convincing light on the possible applications from visible to terahertz (THz) light waves. In order to enhance the performance of conventional graphene-based optoelectronic devices by enlarging the length of light-matter interaction beyond a single-atomic scale, we explore several avenues towards high-performance optoelectronic devices (namely, photodetectors (from visible to the near- and mid-infrared regions) and THz modulators), by exploiting the unique electronic and optical properties of graphene and its intrinsic transition attributes. We highly anticipate that similar techniques are applicable to other two-dimensional transition metal dichalcogenides (TMDs) and the related heterostructures.

Acknowledgement: The work is in part supported by Research Grants Council of Hong Kong, particularly, via Grant Nos. AoE/P-02/12, 14207515, 14204616, and CUHK Group Research Scheme.

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Engineering the 2D hole gas on diamond by surface transfer doping and its device applications

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Despite being a bona-fide bulk insulator, diamond develops an intriguing two-dimensional (2D) *p*-type surface conductivity when its surface is terminated by hydrogens and exposed to appropriate surface adsorbate layer such as atmospheric water as a result of the surface transfer doping process. Consequently, the surface of diamond presents a versatile platform for exploiting some of the extraordinary physical and chemical properties of diamond, leading to applications such as chemical/biological sensing and the development of high-power and high-frequency field effect transistors (FETs)[1].

In this talk, I will describe our work on the surface transfer doping of diamond by a variety of solid-state acceptors[2,3]. I will show that by interfacing diamond with suitable materials a 2D hole conducting layer with metallic transport behaviours arises on diamond. Magnetotransport studies at low

temperature reveal phase coherent transport in the 2D channel represented in the form of weak localisation and antilocalisation, and are analysed in the context of spin-orbit coupling induced by Rashba effect. We demonstrate that this surface conducting channel can be exploited to build diamond surface electronic devices such as metal-oxide semiconductor FETs (MOSFETs). Lastly, the prospects for constructing novel quantum devices on diamond surface by making use of this highly tunable 2D conducting layer on diamond are also explored.

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Multi-functional sensor based on rGO/SWCNT fabric with high durability and waterproofing for human-motion detection

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Wearable strain-pressure sensors with 2D carbon fabric materials for detecting electrical signals generated by human activities are being widely investigated because of their diverse potential applications, from human motion detection to healthcare monitoring. Herein, we demonstrated a rGO/SWCNT fabric-based multi-functional strain−pressure sensor with a simple solution fabrication process. The structural and chemical features of the rGO/SWCNT fabric were characterized by SEM, Raman, and XPS analysis. Complex networks containing rGO and SWCNT were homogeneously formed on the cotton fabric. The device performance was evaluated by measuring the effects of bending strain and pressure. When the SWCNT content upto 0.04 wt% was increased, the change in relative resistance decreased, while durability was significantly improved. Especially, the rGO/SWCNT fabric sensor exhibited remarkable mechanical stability during 100,000 pressure and bending tests at an applied pressure of 254 kPa and the bending strain of ~12% (small bending radius of 3.5 mm), respectively. Moreover, the rGO/SWCNT fabric sensor exhibited excellent water resistant properties after ten washing cycles due to its hydrophobic nature. Finally, we also demonstrated a motion glove with the distinguishable characteristics of movement for detecting human hand movements, including pressing, bending, grabbing, and wrist actions.

Directional valley-locked emission from a monolayer transition metal dichilcogenide enabled by plasmonic nanoantenna

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Two-dimensional (2D) transition-metal dichalcogenides (TMDCs) with intrinsically crystal inversion-symmetry breaking have shown many advanced optical properties [1]. In particular, the optically addressable valley polarization, namely, the photoluminescence emission from monolayer TMDCs has the same helicity as the pumping light due to strong spin-orbit coupling, has enabled lots of new physical phenomena and showed great potential for applications in valleytronics [2]. It can be envisioned that the dynamic excitation and control of carriers in different valleys is crucial for future valley-based information technologies and applications.

Here, we propose a TMDCs-nanoantenna system that could effectively enhance and separate emission from different valleys in monolayer TMDCs into opposite directions. By mimicking the emission from valleys in a monolayer WSe_2 (TMDCs) as circular dipole emitters, we demonstrate that the emission from different valleys goes into opposite directions when coupling to a two-bar plasmonic nanoantenna. The directionality derives from the interference between the dipole and quadrupole modes excited in the two bars, respectively. Thus, we could tune the emission direction from the TMDCs-nanoantenna system by simply tuning the pumping without changing the nanoantenna structure. The scheme we propose here could potentially serve as an important components for valley-based applications such as non-volatile information storage and processing.

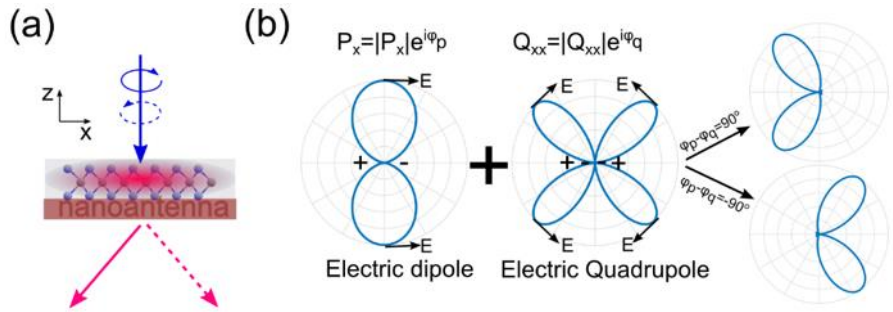

Fig. 1. (a) The proposed scheme to separate emission from different valleys through integrating with properly designed nanoantennas, the directions of the emission from monolayer TMDCs depend on the polarization states of the excitation (different valleys are addressed). (b) The working principle of the nanoantenna is based on the interference between the electric fields radiated from an electric dipole and an electric quadrupole; the direction of constructive interference depends on the relative phase difference between the dipole and quadrupole.

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SYMPOSIA 2 – CHEMISTRY

Hybrid composites of graphene and polymers for 3D printing

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Electrically conductive polymer composites can potentially be used in electronics and 3D printing. Graphene-based composites show promise; however, there are several challenges with properties and product design. In this study, we have developed a novel class of composites by hybridising conductive polymers with graphene in thermoplastic matrices to overcome some of those barriers. Eventually, 3D printing applications are also investigated with these as an alternative to expensive printable conductive inks. The analyses of the composites have shown to form a synergistic relationship with the graphene fillers by lowering the percolation threshold and therefore achieving significant electrical conductivity values at relatively low filler loadings [1]. The achieved highest conductivity was 8.5 $S.cm^{-1}$ with samples that contained 10 wt.% polypyrrole, 10 wt.% graphene in PMMA matrix. The relationship between crystallinity and electrical conductivity has also been examined, and it has been observed that there is a definite correlation between the sample conductivity and the method of production. By observing I_D/I_G ratio from the Raman spectroscopy study, it can be seen that the electrical conductivity of the samples is positively correlated with their structural quality. Moreover, proportions of individual components, particularly the graphene content, and the production method can explain the diversion from the relationship between the intensity ratio and the electrical conductivity. A similar relationship has been reported by Mohan *et al*. [2]. In general, it was found that in the melt blending process, particles tend to be insulated to a higher level than what happens in the solvent casting method. SEM images of cross-sections of some samples are shown in Figure 1.

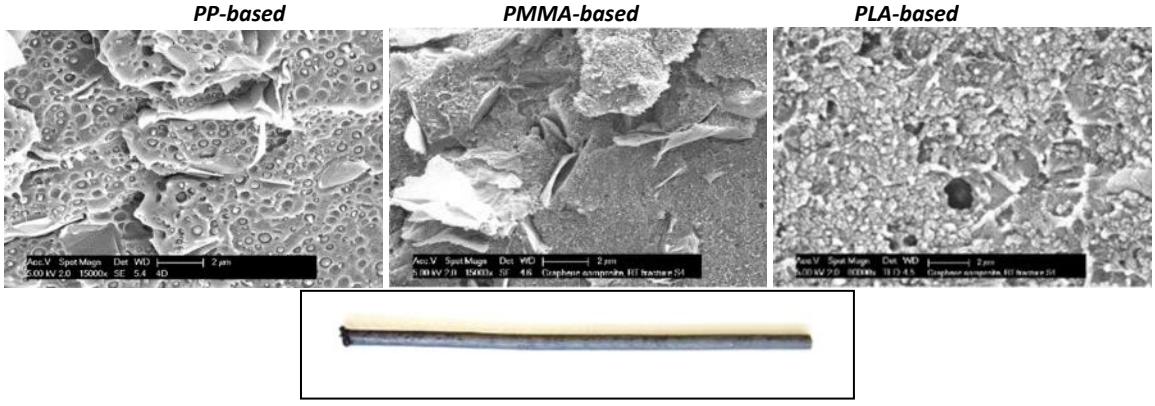

Fig. 1. SEM images of hybrid composite materials- inset- Composite strand

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Mass production of electrochemically-derived graphene oxide in a packed bed reactor and its application in nanocomposites

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Electrochemistry has become an increasingly attractive alternative to traditional chemical approaches to synthesizing graphene oxide (GO). Although electrochemistry promises to provide a greener and more cost effective route towards GO, it remains unclear how electrochemical techniques may be used to produce GO on a large scale from natural graphite precursors. The current study addresses this issue by developing a packed bed reactor model for electrochemical-derived graphene oxide (EGO) synthesis. Graphite particles were galvanostatically charged and the resulting amperometric curves were examined. At the end of the charging, the product was purified and the effect of various experimental variables on material properties were assessed using multiple characterisation techniques (e.g. XRD, XPS, FTIR, etc.) It was shown, for instance, that higher charging densities led to higher voltages, an inhibition of the oxidation reaction and a reduction of the reaction time. XPS data showed that significant oxygen functionality was imparted to the graphite electrode. The controllable oxidation level of the EGO makes it an attractive precursor for many applications, such as electronics and nanocomposites. The 3D printing of multifunctional devices would accelerate the development of various wearable electronics, including smart sensor and human–machine interfaces. Polydimethylsiloxane (PDMS) elastomer is widely used in a wide range of wearable electronics. However, it has proved challenging to 3D print PDMS based electronics with complex structures and multifunctionality, due to its low elastic modulus and need for support during the printing process. Herein a facile, cost-effective and efficient method is presented for 3D printing conductive PDMS ink containing PDMS nanoballs and EGO. Due to the unique hybrid structure of PDMS and EGO, with low volume percentage, the EGO/PDMS nanocomposite has demonstrated linear and reproducible sensitivity to tensile strains which is able to detect various human motions from finger bending to pulse. The strain sensor is then interconnected via printed conductive traces to yield soft electronic devices that may find potential application in wearable sensor, soft robotics, and biomedical devices.

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On-chip micro-supercapacitors integrated gas sensor based on three dimensional graphene networks

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Micro-supercapacitors (MSCs) is a promising power storage integrated with wearable electronic electronics such as gas/strain sensors[1,2] and solar cells[2]. In this work, we presented three dimensional (3D) graphene networks based MSCs with interdigital structure by CVD methods and microelectronics technology. We discussed the effect of different interdigital width and intersperse for the MSCs. In order to improve the device capacitance and energy density, we prepared 3D graphene/Ni(OH)2 MSCs by depositing Ni(OH)2 nanoplates on graphene MSCs. Combining conductive graphene networks and hydroxide redox reaction, the device displays a high capacitance of 0.75mF/cm2(1.37F/cm3), energy density of 0.52mWh/cm3 and power density of 9.4mW/cm3, and it also exhibited stable electrochemical performances with flexible substrate under various bending degree. Then a gas sensor based on the 3D graphene networks was fabricated and integrated with MSCs arrays to demand the integrated sensing and self-powering application.

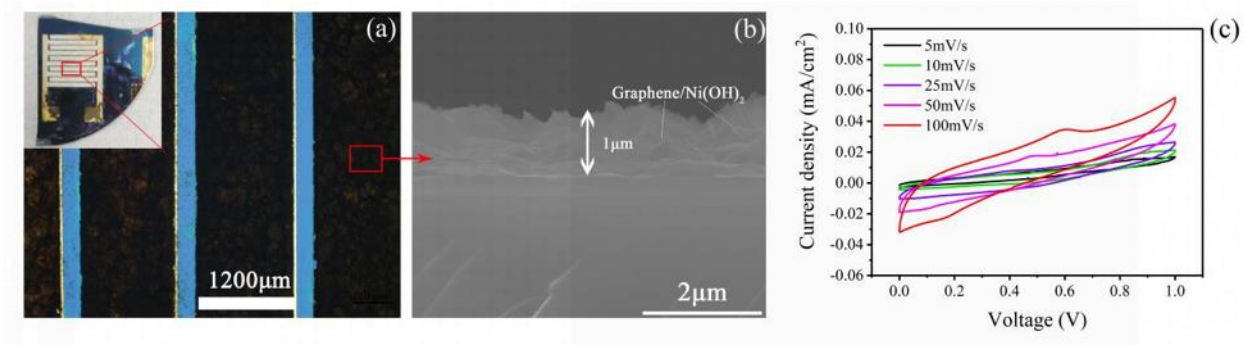

Fig. 1. 3D graphene/Ni(OH)2 MSCs.(a)Optical images of the MSCs.(b)SEM image of the 3D graphene/Ni(OH)2 materials. (c) CV curves of the MSCs.

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Graphene oxide-silica hybrid capsulee for sustained fragrance release

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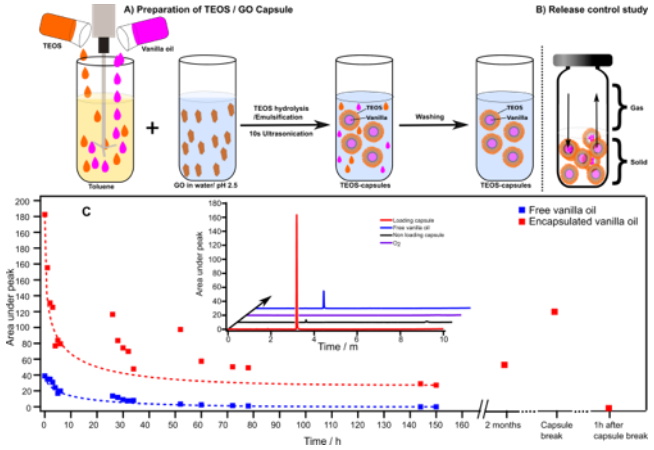
Hybrid colloidal capsules are obtained using a Pickering emulsification route in which the interface is stabilised by graphene oxide (GO) and silica particle composite materials that form a shell. Two methods are proposed to fabricate these capsules using both pre-grown silica particles and solution phase growth of silica from an organic precursor. The GO/SiO_2/oil hollow capsule system is characterized using atomic force microscopy (AFM) and scanning electron microscopy (SEM).



Exploration of the mechanical properties using AFM, rheology measurements and compression–expansion techniques support the existence of hard shells surrounding the droplet contents, with the mechanical strength depending greatly on the concentration of the materials and the density of the shells. This capsule system has potential applications for the delivery of fragrances, pesticides and fertilizer materials. The capsule efficiency as a carrier has been determined by monitoring the release of loaded materials as a function of time using headspace gas chromatography.

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SYMPOSIA 2 – SYNTHESIS

Synthesis and properties of magnetic atoms doped MoS_2

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MoS_2, as a typical transition metal dichalcogenide, has drawn intensive attentions owing to its high on/off ratio, high mobility and inversion broken symmetry for applications in photodetector, field-effect transistor and valley spintronics. However, synthesis and properties of doped MoS_2 monolayer is rarely reported. Here, the magnetic atoms (Co, Fe, V and Cr) are successfully doped into MoS_2 via chemical vapor deposition [1]. The techniques such as STEM, XPS are used to confirm the magnetic element substitution in the MoS_2 lattice. Furthermore, the doped MoS_2 monolayer exhibits excellent properties, such as enhanced valley splitting, and superior HER performance. Our studies open a way to synthesize doped TMDs and also shed light to explore the novel physical properties in MoS_2.

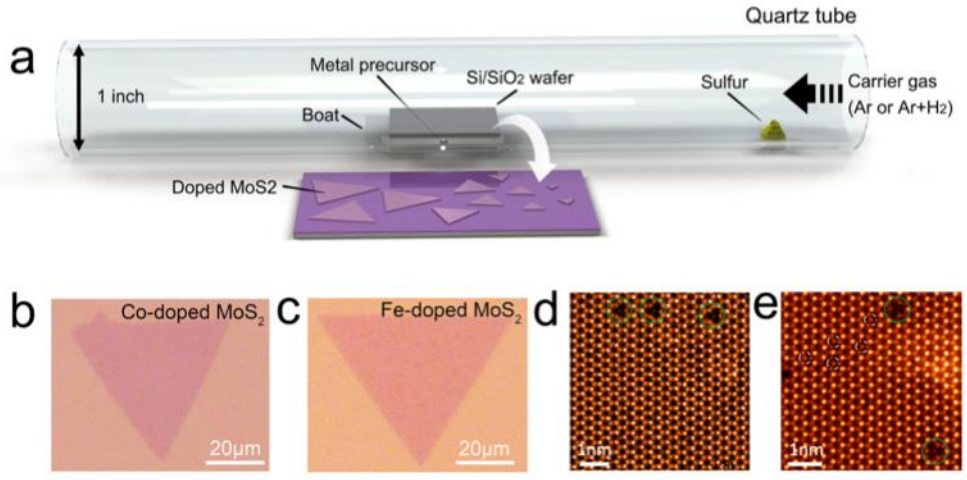

Fig. 1. a, The growth setup used for the synthesis of pure MoS_2 and doped MoS_2. b and c, Optical images of Co- and Fe-doped MoS_2 monolayer. d and e, ADF-STEM imaging of Co- and Fe-doped MoS_2 monolayer, revealing the presence of isolated single dopants in all samples and tri-dopant clusters in Co and Fe doped MoS_2.

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Synthesis of a library of atomically-thin metal chalcogenides

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Two-dimension (2D) transition-metal chalcogenides (TMCs) 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 TMCs [1-3]. 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.

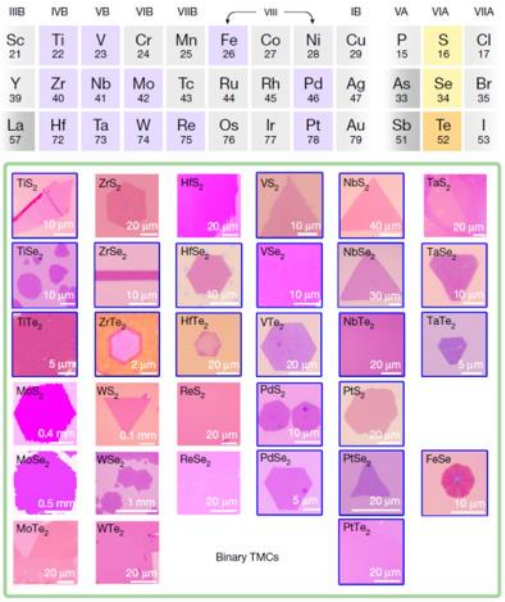

Fig. 1. The transition metals and chalcogens used, and optical images of the resulting different atomically thin TMCs.

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Tailoring photocarrier dynamics in 2D materials and heterostructures

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Transient photocarrier excitation and relaxation processes are fundamental factors that govern the performance of a range of photonic devices, including LEDs, optical modulators and photodetectors [1]. 2D semiconductors, including transition metal dichalcogenides and black phosphorus, exhibit rich photo-physics and have the potential to become the basic building block for next-generation optoelectronics. However, strategies developed for conventional III-V bulk materials are not directly applicable to the emerging 2D platform due to the ultra-thin nature of TMDs and BPs. Here, we present our recent results on controlling the photocarrier lifetimes in TMD/oxide and TMD/BP hybrid systems, where we find interfacial electron-coupling and Coulomb effects can serve as effective knobs for tailoring the exciton dynamics in these 2D semiconductor systems. Ultrafast spectroscopy investigation of other emerging low-dimensional materials including 3D Dirac semimetal Cd_3As_2 and high-mobility material Bi_2O_2Se will also be discussed.

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Van der Waals crystal for battery applications

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Wetting liquid metal on the solid electrolyte of a liquid-metal battery determines the battery's operating temperature and performance. Liquid sodium electrodes are particularly attractive because of their low cost, natural abundance, and geological distribution, but wet poorly on a solid electrolyte near its metaling temperature, limiting their widespread suitability for low-temperature batteries used for large-scale energy storage systems. We present (1) an isolated metal island and (2) sparked two-dimensional (2D) material strategy that can improve sodium wetting in sodium-beta alumina batteries that allows operation at lower temperatures. Our results suggest that in situ heat treatment of a solid electrolyte followed by metal deposition effectively eliminates oxygen and moisture from the surface of the solid electrolyte, preventing the formation of an oxide layer on liquid sodium, leading to enhanced wetting. We also show that employing isolated metal islands and 2D material significantly improves cell performance, retaining 94% charge after the initial cycle, an improvement over cells without such materials. These results suggest that coating isolated metal islands and 2D material is a promising but simple strategy for the development of low-temperature sodium-beta alumina batteries.

Liquid-phase exfoliated semiconducting transition metal dichalcogenide 2D nanoflakes for large-area optoelectronic applications

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Given their established robustness and favorable optoelectronic properties, the semiconducting transition metal dichalcogenides (TMDs, e.g. MoS_2 and WSe_2) are attractive for optoelectronic applications including solar energy conversion (photovoltaic and photoelectrochemical solar fuel production).[1] Recent advances in the liquid-phase exfoliation (LPE) of semiconducting TMDs into mono- or few-layered 2D nanoflake dispersions suggests that inexpensive roll-to-roll processing can be used to prepare TMD-based devices inexpensively over large area.[2] However, the high concentration of defects in these materials act as recombination sites for photogenerated carriers and limit the performance. In this presentation the challenges with charge transport, separation, recombination, and interfacial transfer in LPE TMD nanoflake thin film devices will be discussed with respect to the 2D flake size and defect passivation/charge extraction treatments.[3] Our results give insight into the roles of both edge and internal defects (Fig. 1) and suggest routes for improvement. Overall it is shown that LPE semiconducting TMDs with suitable defect mitigation can achieve internal quantum efficiency for photon harvesting similar to bulk single crystal samples. Specifically, we show that WSe_2 nanoflake thin films achieve absorbed-photon-to-current efficiency over 50% and photocurrent densities for solar water reduction at 4 mA cm^{-2} under standard testing conditions.[4]

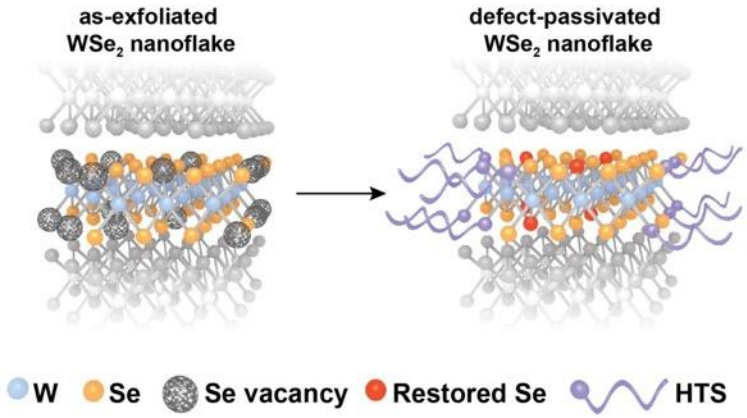

Fig. 1. Schematic of the WSe_2 defect passivation. As-exfoliated WSe_2 contains Se vacancies both at the exposed flake edges and internally in the few-layer flakes. Pre-annealed bulk powder is shown to reduce internal Se vacancies, and treatment with hexyl-trichlorosilane (HTS) surfactant fills exposed edge vacancies to give the final defect-passivated WSe_2.

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PLENARY

Graphene – the development pipeline

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Graphene is an extraordinary material with a combination of properties that include good electrical conductivity, exceptional strength and biocompatibility.

Careful control of all steps from sourcing the graphite, to exfoliation and chemical modification of graphene sheets, is important in rendering the dispersions obtained amenable to subsequent fabrication strategies such as spray coating, printing or fiber spinning.

Recent advances in our laboratories have involved the development of chemistries that retain the inherent properties of graphene while rendering it processable in aqueous or organic solvents.

Chemistries developed here have also enabled effective formation of graphene containing composites that are amenable to fabrication. This includes composites with engineering polymers and biopolymers.

Success in these areas has led to the application of graphene and structures containing it, for energy storage (batteries/capacitors) and conversion (including electrode platforms for reduction of CO_2 to useful fuels). Graphene containing structures have also found use in biomedical areas including neuronal recording and stimulation electrodes, as well as scaffolds for bone regeneration.

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PLENARY

Spin and charge transport in 2D materials

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Low dimensional materials constitute an exciting and unusually tunable platform for investigation of integer and fractional quantum Hall states. Here I will present our results on transport measurements of high quality few-layer graphene and black phosphorus devices. In Bernal-stack trilayer grapehne, we observe tunable integer and fractional quantum Hall states[1], substrate-induced band structure modification, and quantum parity effect at the charge neutrality point. In tetralayer graphene, we have observed a large intrinsic gap at half filling, up to 80 meV, that arises from electronic interactions in rhombohedral stacking[2], and multiple Lifshitz transitions in Bernal stacking[3]. Lastly, I will discuss our recent observation of robust long distance spin transport through the antiferromagnetic state in graphene[4].

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CONCURRENT SYMPOSIA 3 – PHYSICS

Vandium sulphide compounds at the 2D limit

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Vanadium disulphide (VS2) is challenging to prepare stoichiometrically in the bulk, and the single layer has not been successfully isolated until now [1]. As a result, VS2 has been understudied in comparison with many other transition metal dichalcogenides, despite the expectation that VS2 should possess fascinating properties in the bulk, including charge density waves and magnetism [2,3]. Here, we report the first realization of single-layer VS2, which we have grown epitaxially with high quality on the (111) face of Au in the octahedral (1T) structure. We find that we can controllably deplete the single layer of sulphur by annealing in vacuum so as to create an entirely new compound with no bulk analogue. The transition is reversible by annealing in a sulphur-rich gas atmosphere. We also identify an additional, intermediate sulphur-deficient phase that forms during the transition between the two others. Using a combination of scanning tunnelling microscopy, angle-resolved photoemission spectroscopy, and density functional theory, we have made a detailed investigation of both the structural and electronic properties of all three VS2 single layer compounds.

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Real-space mapping of polaritons in 2D materials

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The performance of the next-generation electronic devices based on graphene and other 2D materials is strongly influenced by the structure-function relationship. Scattering-type scanning near-field optical microscopy (s-SNOM) is the ideal technology to investigate such material systems at the nanoscale. s-SNOM combines the best of two worlds: (i) the high spatial resolution of Atomic Force Microscopy (AFM) and (ii) the analytical power of optical microscopy and spectroscopy. Achieving an unmatched spatial resolution below 10 nanometer this technology opens a new era for modern nano-analytical applications such as chemical identification, free-carrier profiling and plasmonic near-field mapping. Recent research highlights on graphene and other 2D materials include contact-free access to the local conductivity [1], the electron mobility, and the intrinsic electron doping by resolving propagating phonon- plasmon-, and exciton-polariton directly in space and time (Fig.1) [2].

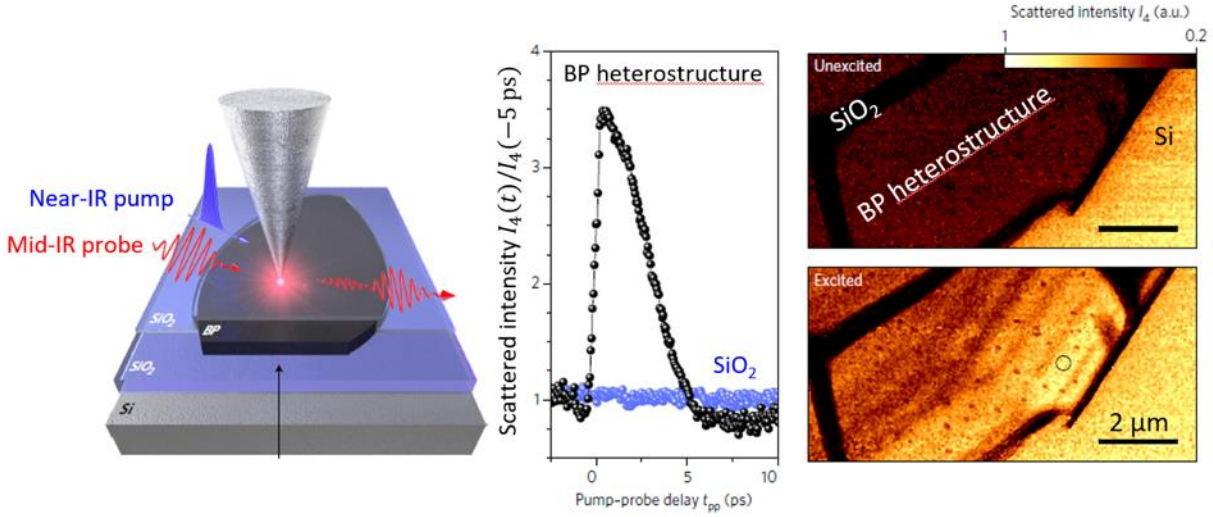

Fig. 1. Femtosecond photo-switching of interface polaritons in black phosphorus

In this presentation we will introduce the basic principles of near-field microscopy for imaging and spectroscopy with 10 nanometer spatial resolution and address their impact and key applications in the field of 2D materials.

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Doping effect on light polarization dependent photocurrent of a 2D semiconductor

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Elliptically polarized light (EPL) can lead to several photocurrent (PC) contributions in semiconductors. An elliptically polarized light can have circularly polarized state or linearly polarized state based on angle of photon polarization. If there is no light momentum transfer to the material, for the linearly polarized light absorption, based on particular directions of optical field and the point group symmetry of the material, this PC can be due to the linear photogalvanic effect (LPGE). If there is light momentum transfer, the PC will be only due to linear photon drag effect (LPDE). For the circularly polarized light absorption, this PC can be mainly due to the circular photogalvanic effect (CPGE). There are three major measurement configurations which can lead to three different PC behavior; two of these three configurations are two-probe, the other is the Hall bar configuration. In the first of the two two-probe configurations, optical field is parallel to the probes and EPL dependent PCs can be due to the LPDE and LPGE. For the configuration of the two-probe which is perpendicular to the optical field, the major PC will be due to the CPGE. For the Hall bar configuration the optical field is perpendicular to the sample plane and light induced Hall PC can be observed by both linearly and circularly polarized excitations. The CPGE has been studied in detail for III-V and II-VI semiconductor quantum wells and diluted magnetic semiconductors (DMS), also recently in the model 2D material, graphene [1]. In a monolayer semiconductor, MoS_2, which has a direct band gap in the visible range in K valley, broken inversion symmetry and strong spin orbit coupling, CPGE current was expected as a result of giant spin-valley coupling [2] which can be controlled by circularly polarized light and global back-gating. A large CPGE current polarization was observed for excitation on–resonance with exciton, which is negligible for off–resonance excitation [3]. Also a large on-off ratio of CPGE current as a function of carrier density was reported [4]. In Hall bar geometry, valley Hall effect was measured [5]. We discuss the modulation of the CPGE current, as well as the unusual magnetic field dependence of the valley Hall effect, in doped monolayer MoS_2.

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Electronic band structure study of exfoliated millimeter-sized mono-layer $MoTe_2$ using angle-resolved photoemission spectroscopy

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The transition metal dichalcogenide (TMDC) semiconductors MX_2 (M = Mo, W; X = S, Se, Te) exhibit intriguing properties in the mono- or few-layer forms. The monolayer MX_2 crystals of TMDC not only provide a unique platform for novel physical properties and functionalities not existing in their bulk counterparts, but also show great potential in the next-generation electronics, optoelectronics and spintronics. Of particular interest is the monolayer $MoTe_2$ which has the smaller direct band gap of 1.1 eV (quite close to that of Si) and stronger spin-orbit coupling. It indicates that monolayer $MoTe_2$ is a highly attractive material for use in electronic devices. In addition, the easy reversible switching between 2H phase and 1T'phase makes it a promising 2D material for phase-change memory device. Among all MX_2 monolayers, Te-based 2D crystals have remained virtually little explored. To our knowledge, no work on band structure measurement of monolayer $MoTe_2$ has been reported. We will present electronic structure study on pristine and alkali metal-doped $MoTe_2$ monolayer by high resolution angle-resolved photoemission spectroscopy (ARPES). By utilizing an improved exfoliation method, we have prepared milimeter-sized mono-layer $MoTe_2$ with the superior quality. We found experimental evidence of the direct gap transition in it as predicted by density functional theory. The observed direct gap and spin splitting of the upper valence band at K point is ~0.92 eV and ~215 meV, respectively. We also found some additional and interesting electronic state features which are to be discussed within the frameworks of quantum well state and monolayer $MoTe_2$-substrate interaction. Our study may pave a way for engineering band structure and tuning electronic properties as well as making high-performance nanoelectronic and optoelectronic device in mono-layer $MoTe_2$ semiconductor.

Configuring the structures of 2D materials and perovskites and their applications

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The optical and electronic structures of two-dimensional (2D) materials and perovskites often show very strong layer-dependent properties[1]. The properties can also be tuned by stacking configuration, which allows us to build electro and optical devices with the same material and the same thickness. Detailed understanding of the inter-layer interaction will help greatly in tailoring the properties of 2D materials for applications, e.g. in pn junction, transistors, solar cells and LEDs.
Raman/Photoluminescence (PL) spectroscopy and imaging have been extensively used in the study of nano-materials and nano-devices. They provide critical information for the characterization of the materials such as electronic structure, optical property, phonon structure, defects, doping and stacking sequence[2]. In this talk, we use Raman and PL techniques and electric measurements, as well as simulation to study 2- and 3-layer 2D samples and Perovskite materials. The Raman and PL spectra also show clear correlation with layer-thickness and stacking sequence. Electrical experiments and ab initio calculations reveal that difference in the electronic structures mainly arises from competition between spin-orbit coupling and interlayer coupling in different structural configurations[3].

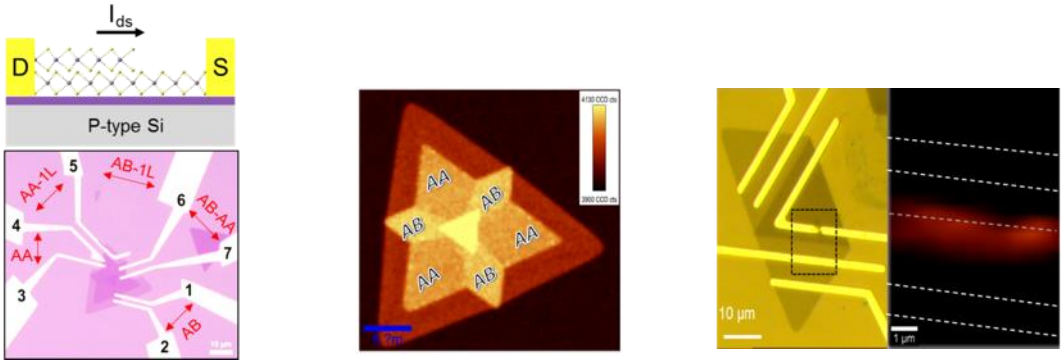

Fig. 1. Left: optical image of device used for electric measurement. Middle: details of the stacking order of the MoS_2 sample revealed by Raman imaging. Right: details of the device and photon response mapping showing the strongest photocurrent is in the AA/AB interface region between.

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Multifractal superconductivity in single-layer $NbSe_2$

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Single layers of transition metal dichalcogenides are ideal systems for exploring the interplay between 2D superconductivity and localization effects. Here we present a comprehensive characterization of the superconducting state of single-layer $NbSe_2$ (TC = 2 K [1]) in the vicinity of the critical point of the superconducting-insulator (SIT) transition by means of low-temperature (1.1 K) scanning tunnelling microscopy and spectroscopy (STM/STS). Our STS measurements show that even the weak intrinsic disorder present in the 2D material triggers strong spatial fluctuations in the width, depth and coherence peak heights of the SC gap. Spatially resolved mapping of these observables reveal that such fluctuations display in all cases patterns with well-defined wavelength of ~7 Å, nearly coincident with that of the quasiparticle oscillations visible near EF [2]. Statistical analysis of the local SC widths and the coherence peak heights reveal log-normal distributions, and for the former a two-point correlation function that decays as a power-law, both signatures of the multifractal character of the superconducting eigenstates [3]. This superconducting state offers a novel platform to tune and control superconductivity in quasi two-dimensional quantum materials.

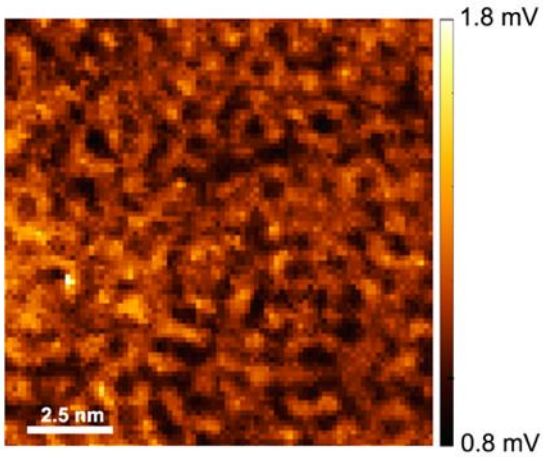

Fig. 1. Spatially resolved fluctuations of the local order parameter (SC width) in single-layer $NbSe_2$ at 1 K.

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CONCURRENT SYMPOSIA 3 – DEVICES

Van der Waals integration beyond 2D materials

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The heterogeneous integration of dissimilar materials is a long pursuit of material science community and has defined the material foundation for modern electronics and optoelectronics. The current material integration strategy such as chemical epitaxial growth usually involves strong chemical bonds and is typically limited to materials with strict structure match and processing compatibility. Materials with substantially different lattice structures cannot be epitaxially grown together without generating too much interfacial defects that seriously alter/degrade their intrinsic properties. Alternatively, *van der Waals* integration, in which pre-formed building blocks are physically assembled together through weak *van der Waals* interactions, offers a bond-free material integration approach. The flexible "physical assembly" process used in *van der Waals* integration is not limited to materials that have similar lattice structures or require similar synthetic conditions. It can thus open up vast possibilities for damage-free integration of highly distinct materials beyond the traditional limits posed by lattice matching or process compatibility requirements, as exemplified by the recent blossom in the *van der Waals* integration of a broad range of 2D heterostructures [1-4]. Here I will discuss *van der Waals* integration as a general material integration approach for creating diverse heterostructures with minimum integration-induced damage and interface states, enabling high-performing devices (including high speed transistors, diodes, flexible electronics) difficult to achieve with conventional "chemical integration" approach [4-12]. Recent highlights include the formation of *van der Waals* metal/semiconductor contacts free of Fermi level pinning to enable the first experimental validation of the Schottky-Mott rule since the initial prediction in 1930s [11]; and the development of *van der Waals* thin films for high performance large area electronics [12]; and the creation of a new class of van der Waals 2D-moecular superlattices with radically different layers yet atomic precision in each layer [9].

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Programmable doping of atomically thin van der Waals semiconductors with light probes

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We report new device architectures of two-dimensional (2D) integrated circuits (ICs), where atomically thin circuit components are seamlessly integrated within the single atomic-planes. The first type was achieved by coplanar heteroepitaxy of 2D transition-metal dichalcogenide (TMDC) polymorphs, [1-3] where the distinct metallic and semiconducting atomic layer crystals were stitched by a sequential chemical vapor deposition. It was verified that these coplanar metal-semiconductor contacts are atomically coherent, showing the lowest contact barrier height ever-reported, which immediately contributed to the substantial outperformance of the coplanar field-effect transistors (FETs) over conventional top-contact 2D TMDC FETs. The second one was realized by exploiting a novel concept of light-induced doping of a TMDC semiconductor film with a scanning light probe, [4-6] with which both n- and p-doped channels were self-assembled to form lateral p-n junctions [7]. Therein, we provide direct evidence of a microscopic doping mechanism by atomic scale imaging and spectroscopy. This real-time writing process is precisely controllable within a minute, in that diffusive doping profiles can be controlled at the sub-micrometer scale, and doping concentrations are tunable to vary the channel sheet resistance over five orders of magnitudes. As such, we assembled both n- and p-doped channels within the same atomic planes to fabricate 2D device arrays of n-p-n (p-n-p) bipolar junction transistor amplifiers and radial p-n photovoltaic cells in high performances. This doping method can be potentially used to fabricate designer 2D circuits based on atomically thin semiconductors in arbitrary shapes.

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Band alignment modulation of ZnO nanorods/monolayer MoS_2 mixed-dimensional heterosructure via strain engineering

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A growing number of two-dimensional (2D) materials has inspired worldwide efforts to integrate distinct 2D materials with any other dangling-bond-free materials to form van der Waals heterostructures [1, 2]. Due to ultrastrength of 2D materials, strain offers a new band-engineering strategy for tailoring properties of heterosturctures [3, 4]. However, this approach requires a stable method to apply strain and an understanding of strain effects on heterostructures. Here, we construct ZnO nanorods/ monolayer MoS_2 mixed-dimensional heterostructure and realize controlled strain engineering of MoS_2 during transfer process. We find that strain can efficiently tune the band gap of MoS_2 and enhance photoluminescence quenching effects. By theory calculations, we demonstrate that strain can modify the band alignment of ZnO/MoS_2, respectively (Fig. 1). Our results present an important advance toward controlling the band alignment and optoelectronic properties of mixed dimensional heterostructure via strain engineering, with important implications for designing novel devices.

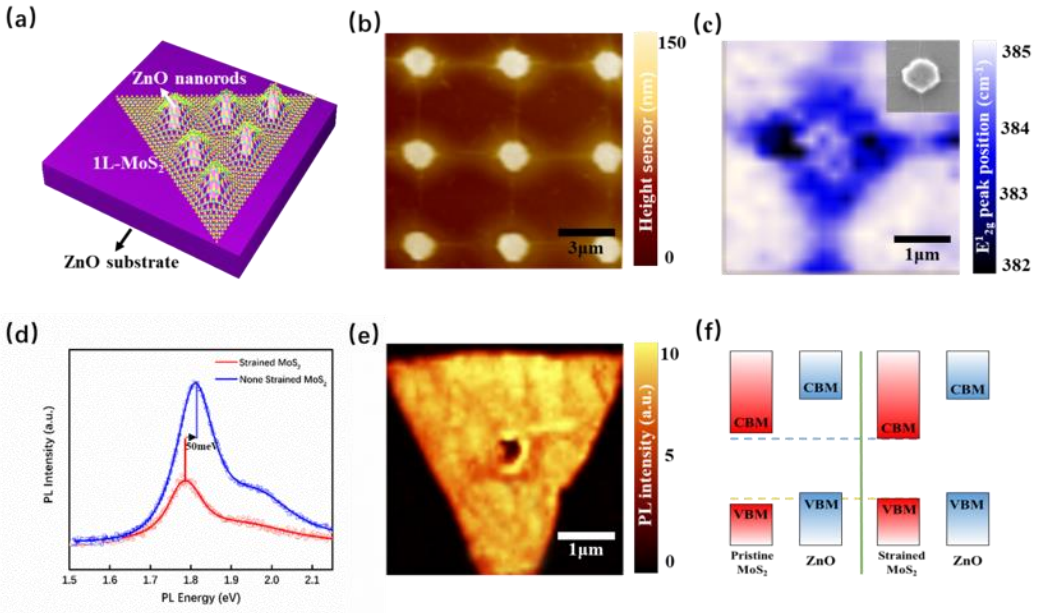

Fig. 1. (a) Schematic illustration of the ZnO nanorods/monolayer(1L) MoS_2 heterostructure; (b) AFM topography of the hybrid structure; (c) Scanning Raman spectroscopic maps plotting E^1_{2g} peak frequency (d) Photoluminescence(PL) spectra of strained-MoS_2 and none strained-MoS_2; (e) PL peak intensity mapping of MoS_2 on ZnO nanorods; (f) Biaxial strain effects on band structure of MoS_2 to modify the band alignment of ZnO/MoS_2 according to the theory calculation.

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One-dimensional edge contacts to monolayer MoS_2

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Electrical contacts play a critical role in realizing high performance 2D material devices. While formation of Ohmic contacts to graphene has been successfully achieved by 1D edge contacts [1], a similar approach for TMDCs has met with limited success so far [2-4]. We have realized reliable edge contact formation in hBN - 1L MoS_2 - hBN heterostructures for the first time by a combination of reactive ion etching, in-situ Ar^+ sputtering and annealing. In addition to hBN being an atomically smooth, nearly trap-free gate dielectric, encapsulation in hBN also preserves the intrinsic MoS_2 channel quality during processing, leading to low subthreshold swing (~100 mV/dec), very high on-currents (> 50 µA/µm), high mobility (upto 30 cm^2/Vs) and negligible hysteresis. In this talk, I'll present the fabrication process flow we have developed and show our recent experimental results together with quantum transport simulations. The performance of our edge contacts are comparable to the best-reported top contacts on MoS_2 with a similarly low L_{Ch} = 1 µm contact resistance but with enhanced long-term stability in ambient.
Moreover, our fabrication strategy also allows us to preserve p-type doping in MoS_2 enabling observation of hole transport in Nb-doped monolayer MoS_2 for the first time. The recipe we provide is valuable for electrical contacting TMDCs layers buried inside van der Waals heterostructures, especially those unstable in air.

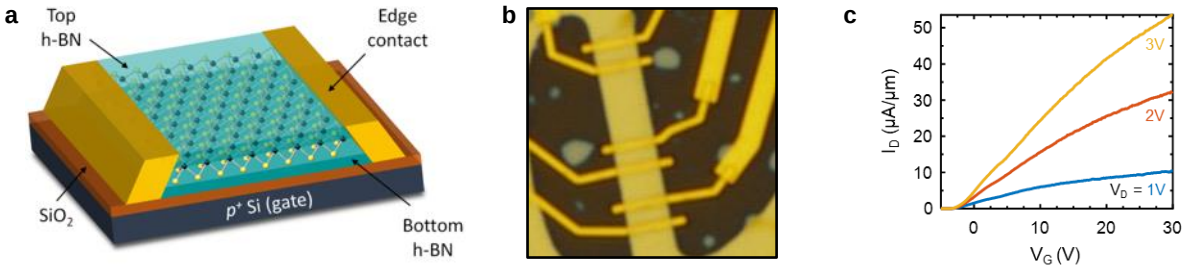

Fig. 1. (a) 3D illustration of an hBN-MoS_2-hBN heterostructure depicting the edge contact geometry. (b) Optical microscope image of an hBN encapsulated 1L-MoS_2 flake with Ti-Au edge contacts. (c) Room temperature I_D-V_G characteristics of edge contacted 1L-MoS_2 FETs showing high ON-currents.

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Universal conductance fluctuations as a direct probe to detect crossover of symmetry classes in topological insulators

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The non-trivial properties of topological insulators, which make it a good candidate for studying fundamental physics as well as achieving extraordinary applications, are subject to protection by time reversal symmetry. Upon lifting time reversal symmetry, topological insulator (TI) goes through a topological phase transition to a trivial insulator. In the framework of random matrix theory, this is described as a transition from symplectic to unitary symmetry of the Hamiltonian. In this work, we have directly probed this transition for the first time by measuring the mesoscopic conductance fluctuations in the TI $Bi_{1.6}Sb_{0.4}Te_2Se$, which shows an exact factor of 2 reduction on application of a magnetic field. The reduction provides an unambiguous proof that the fluctuations arise from the universal conductance fluctuations (UCFs), due to quantum interference, and persists from $T \sim 22$ mK to 4.2 K. We have also compared the phase breaking length l_ϕ extracted from both magnetoconductance and UCFs which agree well within a factor of 2 in the entire temperature and gate voltage range. Our experiment confirms UCF as the major source of fluctuations in mesoscopic disordered topological insulators, and the intrinsic preservation of time-reversal symmetry in these systems. [1].

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Defect engineering for modulating the trap states in 2D photoconductor

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The crystalline structures of 2D materials are enriched by a variety of intrinsic defects, including vacancies, adatoms, grain boundaries, and substitutional impurities, which would strongly influence their properties. [1]. Defect induced trap states are essential in determining the performance of semiconductor photodetectors. The de-trap time of carriers from a deep trap could be prolonged by several orders of magnitude as compared to shallow trap, resulting in additional decay/response time of the device. Here, we demonstrate that the trap states in two-dimensional ReS2 could be efficiently modulated by defect engineering through molecule decoration. The deep traps that greatly prolong the response time could be mostly filled by Protoporphyrin (H2PP) molecules. At the same time, carrier recombination and shallow traps would in-turn play dominant roles in determining the decay time of the device, which can be several orders of magnitude faster than the as-prepared device (Fig.1). Moreover, the specific detectivity of the device is enhanced (as high as ~1.89×10^13 Jones) due to the significant reduction of dark current through charge transfer between ReS2 and molecules. Defect engineering of trap states therefore provides a solution to achieve photodetectors with both high responsivity and fast response [2].

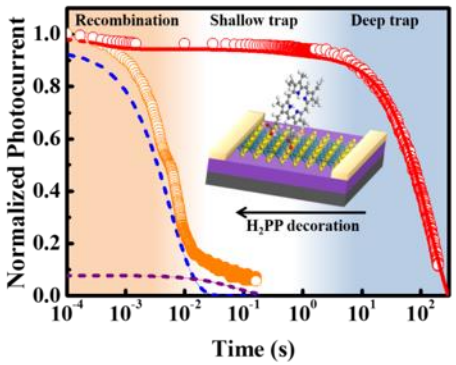

Fig. 1. Transient response of as-prepared and H2PP decorated ReS_2.

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SYMPOSIA 3 – DEVICES

Nanostructured graphene for ultra-broadband photodetectors

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Graphene is a broadband light absorber, due to the absence of an electronic bandgap. Since the photoexcited electrons do not have efficient cooling channels, they thermalize at a temperature higher than the lattice temperature, making graphene an ideal material for highly sensitive hot-electron bolometers that work in a very broad spectral range. Our recent work shows that nanostructured quantum-dot constrictions in epitaxial graphene grown on SiC yield detectors with extraordinarily high intrinsic responsivity, higher than 10^9 V W^{-1} at 3K and independent of wavelength from terahertz through telecom to ultraviolet radiation. These graphene quantum dot bolometers and their applications will be discussed.

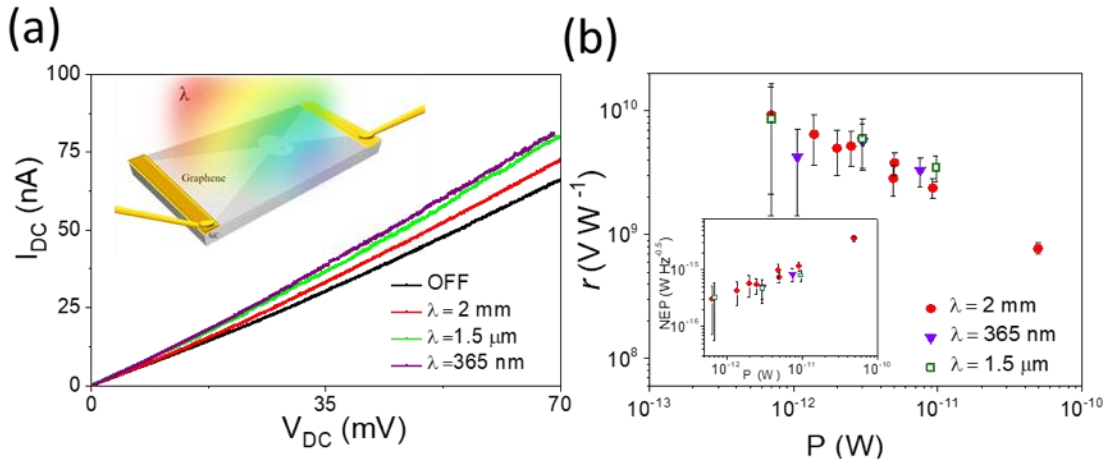

Fig. 1. (a) IV characteristic of a 200-nm dot without radiation (OFF, black) and with radiation at 2 mm (red), 1.543 mm (green), and 365 nm (purple) wavelength, having absorbed power of 0.4, 1.0, and 1.4 nW, respectively. (b) Responsivity of a 100-nm dot as a function of absorbed power at different wavelengths. Inset: calculated electrical NEP vs. absorbed power at different wavelengths, at 3K.

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This work was supported by the U.S. Office of Naval Research (awards N00014-13-1-0865 and N00014-16-1-2674) and the NSF (ECCS 1610953).

Infrared photodetectors based on 2D materials: progress, challenges, and opportunities

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Infrared photodetectors based on traditional thin-film semiconductors such as InGaAs, InSb, and HgCdTe as well as novel type-II superlattice exhibit highly sensitive detection capability. However these devices always need to work at low temperature, resulting in an additional large and expensive cooling system. Recently, 2D materials have attracted tremendous attention owing to their bandgap tunability and potential optoelectric applications[1]. Nevertheless, as a photoconductive detector, the signal-to-noise ratio could be very low without the suppression of dark current. Meanwhile, the performance of 2D photodetectors is strongly affected by surface states resulting in the restricted electron-hole separation efficiency, and intrinsic ultrathin absorption thickness of 2D photodetectors suffers the low quantum efficiency. In this talk, we will review the progress on infrared photodetectors based on 2D materials in my group. We fully exploit the detection ability of 2D materials by introducing localized-field, including ferroelectric filed, photo-induced field, Interlayer built-in field and so forth. With a strong induced localized-field, high performance photodetectors based on Graphene, TMDs, Black phosphorus, Black arsenic-phosphorus etc. in infrared wave band may lead to a disruptive revolution in prospective low dimensional optoelectronic devices[1-4]. Finally, we deliver an outlook, discuss the challenges and future directions, and give general advice for designing and realizing novel high-performance infrared photodetectors to provide a guideline for the future development of this fast-developing field.

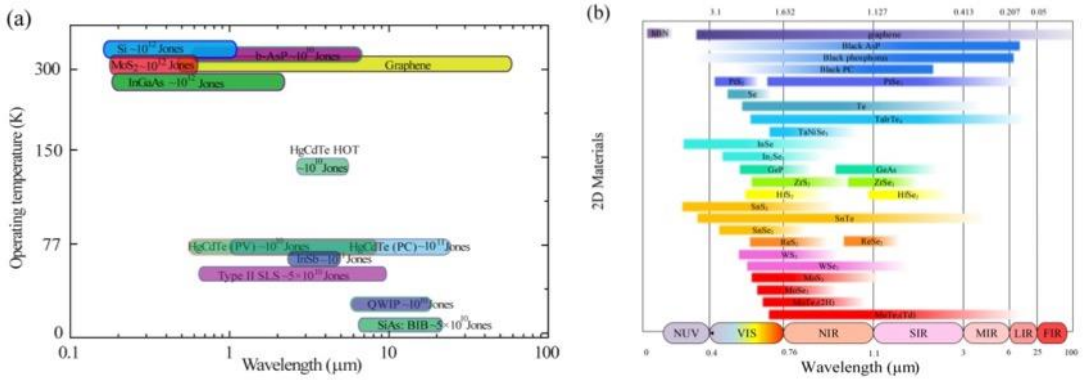

Fig. 1. (a) Operating temperature and spectral range of 2D photodetectors compared with that of commercial traditional photodetectors. (b) Band gap of 2D materials and corresponding detection range[1].

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Resistive memories and UV sensors based on layered MoO(3–x)

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The discovery of graphene in 2004 [1], has drawn the interests of both industries and the scientific community on 2D materials. Although the enhanced carrier mobility observed in graphene is highly desirable for electronic applications, the lack of intrinsic bandgap leads to the exploration of alternative 2D materials with semiconducting properties. α-MoO3 is one of the transition metal oxides that has a relative dielectric constant of ~500 (where as MoS_2 ~ 5) and can be exfoliated to minimum resolvable atomically thin 2D layers. But stoichiometric MoO3 has a wide bandgap (>3 eV) which is not viable for transistor applications [2]. However the bandgap of MoO3 can be easily manipulated to desirable values by several techniques such as hydrogen ion (H+) intercalation, UV irradiation, electron beam bombardment etc. [2,3] Such techniques produce partially reduced, sub-stoichiometric MoO(3-x), which possesses an increased carrier concentration and a high dielectric value, thus favoring an enhancement in charge carrier mobility [2]. Here we present the large area synthesis of layered MoO(3-x), via low pressure chemical vapour deposition. Cross-planar resistive memories based on the as-grown material show high cyclic endurance (~6000) while maintaining a switching ratio of 103. Planar photodetectors fabricated from the as grown material show high selectivity towards UV (365 nm) excitation. These devices exhibit significantly low response times (200 µs) at low bias voltages of 100 mV.

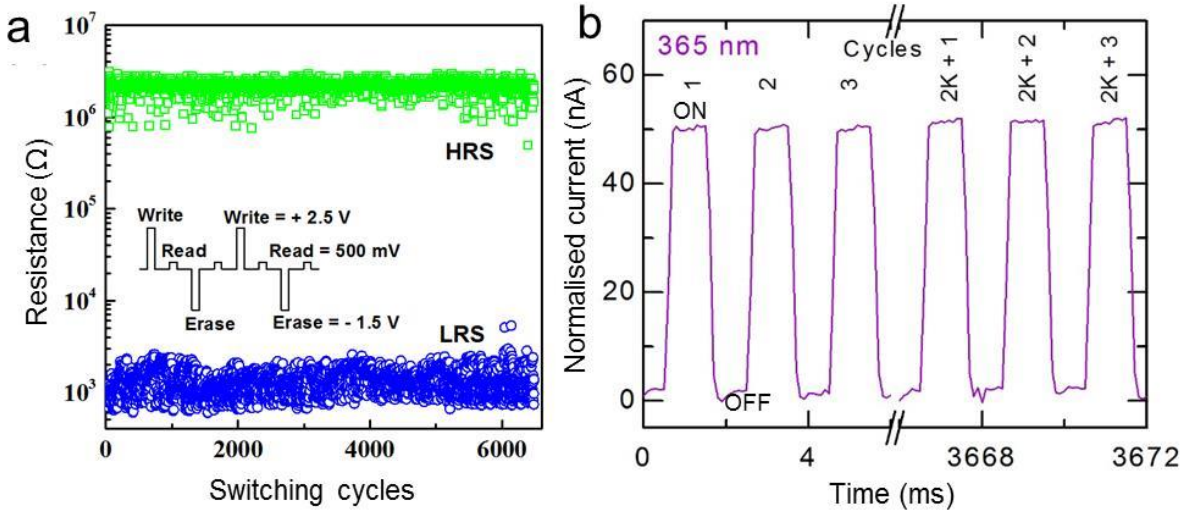

Fig. 1. (a) Cyclic switching endurance of the resistive memory devices. (b) Normalized photocurrent observed in the sensors, when subjected to pulsed UV (365 nm) illumination, at a 100 mV bias.

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Polarization-sensitive photodetectors based on 2D layered semiconductors

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Two dimensional (2D) materials have been attracting wide interest due to their peculiar structural properties and fascinating applications in the areas of electronics, optics, biology, and catalysis. As the promising substitutes for the gapless graphene, transition metal dichalcogenides (TMDCs, such as MoS_2, WS_2, etc.) which also have layered crystalline structure with strong in-plane bonding but weak interlayer action (van der Waals force) show natural band gaps. In our group, several 2D semiconductors and related alloys or heterostructures were successfully fabricated, and their optical properties and utilization in multifunctional optoelectronics were systematically investigated subsequently [1-5]. Photodetectors with high polarization sensitivity are in great demand in advanced optical communication. Here, we demonstrate that photodetectors based on 2D layered germanium selenide (GeSe) and titanium trisulfide (TiS_3) are extremely sensitive to polarized light (from visible to the infrared), due to its reduced in-plane structural symmetry. Both GeSe and TiS_3 showed the best device performance at 808 nm short-wave near-infrared band [2,5].

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Narrow-gap 2D semiconductors for IR and THz optoelectronics

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Narrow-gap semiconductors like Ⅲ-Ⅴ / Ⅱ-Ⅵ materials and their superlattices boost the infared (IR) and terahertz (THz) technologies and play a critical role in the fields of security inspection, bio-medical imaging, free-space communication, gas detection, and so on. Nowadays, conventional IR and THz devices encounter great challenges referring to the complex structures and expensive epitaxy growth, incompatible with silicon chips, etc. The rising of two-dimensional (2D) materials, with the advantages of atomic thickness, van der Waals integration and fantastic physical characteristics, paves the way for the evolution of advanced optoelectronics. For this end, we have paid our continuous effort on the growth and band engineering of novel narrow-gap 2D semiconductors and their applications in IR & THz devices, especially for lasers and photodetectors. Our recent progress focus on the following aspects:
(1) Exploration of novel 2D narrow-gap semiconductor materials: controllable growth, doping, and optoelectronic characteristics. [1-4]
(2) Application in IR & THz photodetectors: improving response performance and developing derived functionalities. [5-8]
(3) Application in IR & THz lasers: mode-lock and surface-emitting lasers. [9-10]

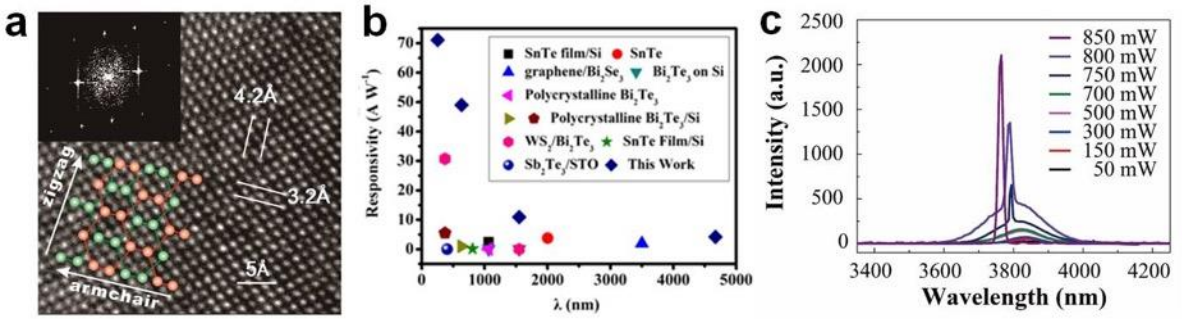

Fig. 1. Growth of Narrow-gap 2D semiconductors and their applications in IR & THz lasers and photodetectors. (a) HRTEM image of the as-grown high-quality black phosphorus film. (b) SnTe based ultra-broadband photodtector with room-temperature responsivity of 4.17 AW-1 at 4.65 μm. (c) MIR black phosphorus surface-emitting Laser operating at 3.76 μm.

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2D transition metal dichalcogenides: from field effect transistors to wafer-scale circuits

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Extensively investigated TMDs materials, such as MoS_2 and WSe_2 that are accessible by large-scale synthetic methods, are remarkably stable and allow superior gate control due to their 2D nature and favorable electronic transport properties, suggesting a bright future for digital and RF electronics. Here I will first discuss the large scale controlled synthesis of MoS_2, $MoTe_2$ and $PtSe_2$ by various approaches, together with major obstacles that have to overcome to achieve wafer-scale, uniform and high quality continuous film for practical electronic application. Then I will focus on the compatible device fabrication process for wafer-scale TMD films, mainly about the formation of electrical contact and dielectric layer for field effect transistors. Simple circuits will also be discussed for exploration of potential applications.

SYMPOSIA 3 – SYNTHESIS

Controlling growth of graphene and its electronic properties

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Graphene is a kind of two-dimensional □-conjugate material, which is a sheet of carbon atoms bound together with double electron bonds (called a sp^2 bond) in a thin film only one atom thick. At present, controllable and massive preparation of high quality graphene, property modulation (e.g. open up the energy gap), etc. still remain the bottleneck problems in terms of its practical applications. In this regard, we carried out comprehensive and deepening research, and a few representative results are as follows. We proposed a new concept for the growth of graphene by using liquid Cu as a catalyst in chemical vapor deposition (CVD) approach[1]. Uniform single-layered, self-aligned, large-sized, single-crystal HGFs and continuous monolayer films were prepared. We synthesized the N-doped graphene by a CVD method using NH_3 as N source, that was the first experimental example of the substitutionally doped graphene. Electrical measurements show that the N-doped graphene exhibits an *n*-type behavior, indicating substitutional doping can effectively modulate the electrical properties of graphene[2,3]. We developed an oxygen-aided CVD process for synthesizing high-quality polycrystalline graphene on a large scale. Graphene can be directly synthesized on dielectric substrates, which can be directly incorporated into field-effect transistor fabrication[4□6]. By using single-crystal graphene growth on a Cu surface as a model system, we demonstrate that trace amount of H_2O and O_2 impurity gases in reaction chamber is a key for the large fluctuation of graphene growth[7].

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Detecting valley splitting and valley-contrasting spin splitting at single-electron level around atomic defects of graphene

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Main text: Detecting broken-symmetry states around individual atomic defects (including single carbon vacancy and adatoms) of graphene requires nanometer-scale spatial resolution, which has so far eluded direct observation. Here, we realize the measurement of the subtle broken-symmetry states at the single-electron level around atomic defects of graphene by using edge-free graphene quantum dots, which are generated by combining the electric field of a scanning tunneling microscopy tip with perpendicular magnetic fields. Our experiments detect the largest valley splitting, ~ 43 meV, reported so far around the atomic defects of graphene. More importantly, we are able to measure different spin splitting in the two valleys of graphene for the first time. Large valley-contrasting spin splitting induced by spin-orbit coupling is observed near the defects, revealing unexplored exotic electronic states in graphene induced by the atomic defects.

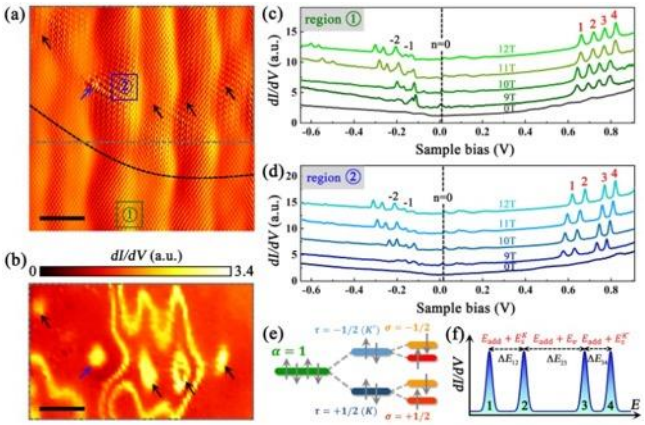

Fig. 1. A 15 nm × 15 nm STM image (V_{sample} = 200 mV and I = 0.4 nA) of graphene monolayer with atomic defects. Scale bar: 3 nm. The black dashed line roughly separates the lower regions without intervalley scattering (region 1) and the upper region with intervalley scattering (region 2). **B.** STS (*dI/dV*) map recorded in the region marked by grey dashed frame in panel A at the fixed sample bias 617 mV (I = 0.4 nA). Scale bar: 3 nm. The arrows mark the positions of the atomic defects. **C, D.** STS spectra taken from the region 1 and region 2 in the graphene monolayer, respectively. The curves are offset on the Y axis for clarity and the LL indices are labeled by black numbers. Red numbers 1-4 mark the first four charging peaks. **E.** Schematic confined energy levels in the edge-free GQD. The orbital level $\alpha = 1$ exhibits the valley splitting $E_v = E_{\alpha,\tau=-1/2,\sigma} - E_{\alpha,\tau=+1/2,\sigma}$ and the spin splitting $E_s^k = E_{\alpha,\tau=+1/2,\sigma=-1/2} - E_{\alpha,\tau=+1/2,\sigma=+1/2}$, $E_s^{k'} = E_{\alpha,\tau=-1/2,\sigma=-1/2} - E_{\alpha,\tau=-1/2,\sigma=+1/2}$ in K valley and K' valley respectively. **F.** Schematic for the first four charging peaks in *dI/dV* spectrum when there are valley splitting and valley-contrasting spin splitting. The energy spacings of the four charging peaks are marked as ΔE_{12}, ΔE_{23}, ΔE_{34} respectively.

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Ubiquitous interlayer coupling in two-dimensional materials and its effects on materials properties

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Two-dimensional (2D) layered materials have attracted increasing intense interest because of their unique mechanical, electronic and optical attributes. Interlayer coupling is a ubiquitous phenomenon residing among the atomically thin 2D layers. For different 2D materials, it may be dominated by the weak van der Waals interaction or by the long-range electrostatic Coulomb interaction. The interlayer coupling controls monolayer exfoliation process and assembly of 2D heterostructures, and behaves as a unique degree of freedom for engineering 2D materials properties (see Fig. 1). In this paper, we present based on van der Waals corrected density functional theory calculations several results related to the interlayer coupling effect. These include: (i) We demonstrate that the band gap and band-edge states evolution from multiple layers to monolayer in MoS_2 and InSe cannot be solely attributed to the assumed quantum confinement; the effect of interlayer coupling plays important role as well. (ii) We calculate the thermodynamic peeling energies of a series of 2D materials; the obtained insightful understanding could help design and optimize the exfoliation process, identify compounds with weak interaction and provide a desirable design strategy for nano-device base on assembled two-dimensional materials. (iii) We show how the interlayer coupling accompanying with the modulated periodic potential in a 2D Moiré superlattice of one wide-gap semiconductor can offer wide-range tenability of optical band gap. (iv) We will also show our recent results by collaboration with experiments on the coupling between other functional biomaterials, layered semiconductors and 2D material substrates.

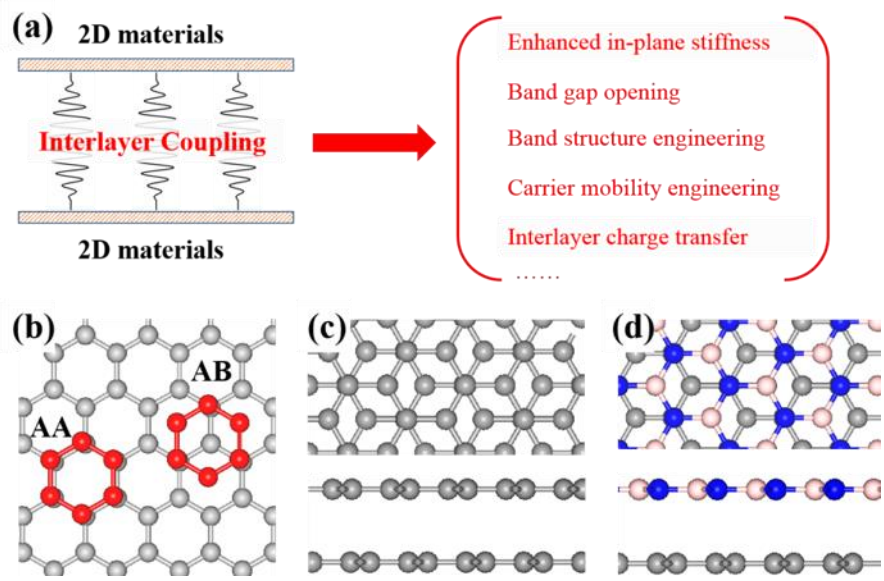

Fig. 1. The schematic diagram of the existing interlayer coupling and its potential effects on the 2D materials properties in the homogeneous and heterogeneous stacked layered materials.

Single layer tranverse flow carbon nanotube membrane for desalination

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By stacking carbon nanotubes (CNT) one on top of another, single layer CNT arrays can perform water-salt separation with ultra-high permeability and selectivity. Such outer-wall CNT slit membrane is named as the transverse flow CNT membrane [1].

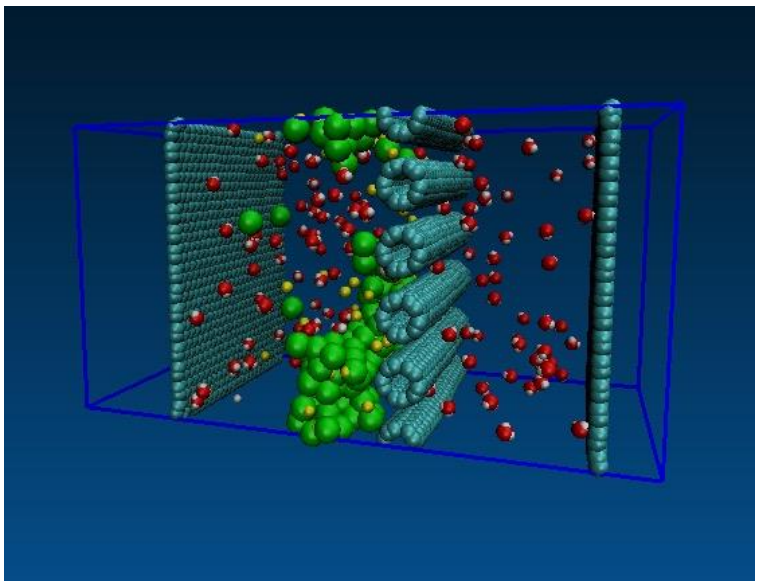

Fig. 1. An illustration of the transverse flow carbon nanotube membrane. Carbon atoms are represented by cyan spheres, oxygen as red spheres, hydrogen as white spheres, sodium ions as yellow spheres and chlorine ions as green spheres. Molecular dynamics simulation of the membrane shows that it can effectively sieve out monovalent sodium and chlorine ions, while allowing water to flow through at high permeability.

By adjusting the slit size between neighboring CNTs, the membrane can be configured to sieve out different solutes, right down to the separation of monovalent salt ions from water. Molecular dynamics (MD) simulation results show that the permeability of transverse flow CNT membrane is more than two times that of conventional axial-flow CNT membranes, and orders of magnitude higher than current reverse osmosis membrane. In addition, by carrying out MD simulations with different CNT size, it was observed that varying CNT size only has a minuet effect on the membrane's desalination performance [2]. This insensitivity of the transverse flow CNT membrane's performance to CNT size is a distinct advantage over axial flow CNT membrane designs. Not only does the membrane operate well under constant pressure desalination operation, but MD simulations further indicate that oscillatory operation can further enhance the membrane's desalination performance, making it suitable for operation such as electrodialysis reversal [3]. While there are still challenges that needs to be overcome, particularly on the physical fabrication of such membrane, it is hope that this versatile membrane design can bring the idea of using low dimensional structures for desalination closer to reality.

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Desired two-dimensional materials' properties by designed growth

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The emerging of two-dimensional transition metal dichalcogenides attracts tremendous research interests, due to their numerous exotic physical properties. Through the designed growth, it is possible to further realize the desired materials' properties and addition functionalities. As example, I will talk large scale self-assembly of 1T'-2H $MoTe_2$ homojunctions via solid-solid phase transformation. Thanks to the understood phase transformation mechanism (Fig. 1a-d), we are able to synthesize millimeter-scale few-layer single-crystal 2H-$MoTe_2$ and centimeter-scale continuous 2H-$MoTe_2$ thin film with large grain sides (Fig. 1e). By the designed two-step growth, patterned 1T'-2H MoTe2 homojunctions were achieved in a large scale (Fig. 1f-h). Their contact and electrical properties were studied.

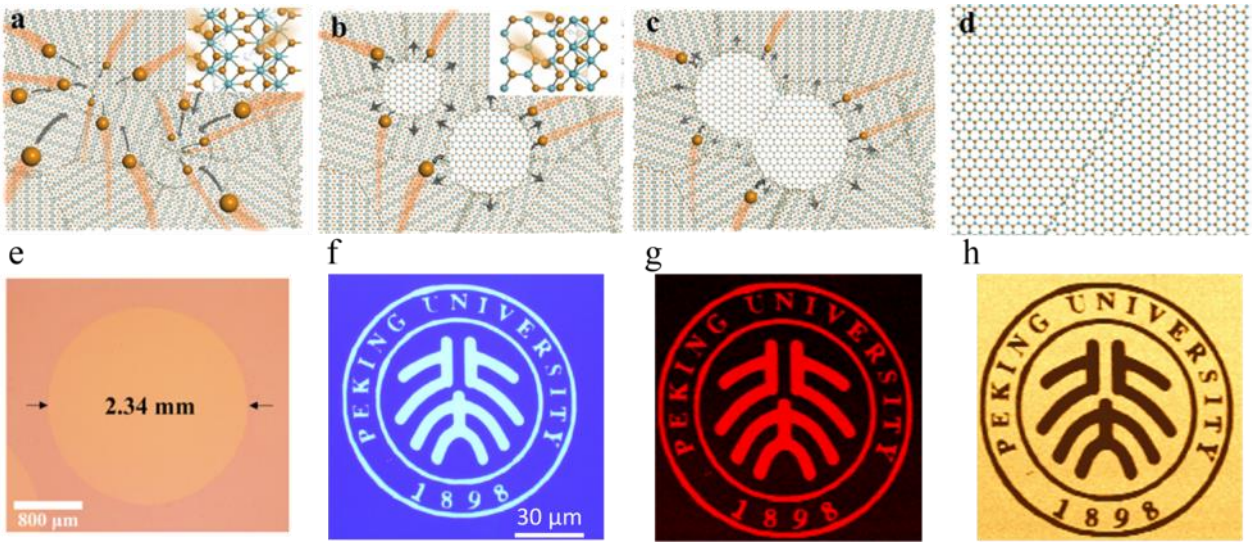

Fig. 1. (a-d) Schematic diagrams of the solid-solid phase transformation synthesis from 1T' to 2H phase $MoTe_2$ film. (e) Optical image of a single-crystalline 2H $MoTe_2$ domain with diameter of 2.34 mm. (f) Optical image of the patterned growth of the Peking University logo of 1T'-2H $MoTe_2$ homojunction. (g) Raman mapping of the 2H peak. (h) Raman mapping of the 1T' peak.

Computer simulation and design of 2D crystals with tunabel band gap and magnetic properties

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Exploring potential atomic-thickness 2D crystals with novel electronic and magnetic properties is of particular interest to develop electronics, optoelectronics, and spintronics in the nanoscale. In this talk, I present a number of new structures of 2D elementary materials or alloys, theoretically reported by using first-principles calculation combined with global structure search and molecular design. The interesting properties, such as structural and thermal stability, tunable band gap, intrinsic and room-temperature magnetic half metallicity, and photocatalytic properties, are observed. Some 2D materials have been confirmed by experiments, such as borophene and conjugated microporous polymer. In addition, the extended superstructures based on the predicted 2D crystals are demonstrated for the application of optoelectronics and photocatalytic water splitting. The new discovery of structures enriches the family of 2D materials, and often leads interests from experimental

SYMPOSIA 4 – PHYSICS

Quantum valley hall effect and valleytronics in bilayer graphene

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Conventional CMOS field effect transistors control current transmission by controlling the charge of carriers. The advent of two-dimensional materials with hexagonal crystal symmetry offers a new electronic degree of freedom, namely valley, the manipulation of which could potentially be exploited to develop new paradigms of electronic applications dubbed "Valleytronics". I will discuss our work on realizing a valley valve and tunable electron beam splitter in bilayer graphene[1][2]. In high-quality bilayer graphene, the application of a perpendicular electric field opens a tunable band gap, the sign of which can be reversed by reversing the polarity of the applied E-field. Theory predicts the existence of valley-momentum locked one-dimensional conducting channels at the artificial domain wall of two oppositely gapped bilayer graphene regions[3]. Known as the "kink states", they are hallmarks of the quantum valley valley Hall effect. The helicity of the kink states can be controlled by the polarity of the applied E-field. This unique attribute allows the design of a novel valve and electron beam splitter, where electrically controlled transmission and guiding of the kink states at a four-way intersection have been proposed [4]. In this talk I will show our experiments realizing the kink states in bilayer graphene and the operations of electrically controlled waveguide, valley valve and beam splitter. The kink states have mean free path of a few micronmeters. The on/off ratio of the valley valve is about 800% at T=1.5 K. Remarkably its operation does not require valley polarized current. The control of the Fermi level in a magnetic field enables a chirality-based beam splitting mechanism. We demonstrate a continuous tuning of the splitting ratio from 0 to close to 100%. The high quality, versatile controls and scalability of the system open the door to many exciting possibilities in valleytronics and in pursuing fundamental physics of helical 1D systems.

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Interacting electrons in bilayer graphene and bilayer graphene/hBN Moiré superlattices

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Bilayer graphene's electronic spectrum consists of chiral massive fermions [1] and has exhibited a number of spin- or valley-ordered many body phases and fractional quantum Hall states. Recent work by a number of groups has shown that Landau level (LL) crossings can be induced in bilayer graphene and used to study these states by applying a perpendicular electric displacement field *D*, which tunes the interlayer potential difference, e.g. [2], and the LL energies, e.g. [3]. These crossing LLs originate from symmetry-broken states belonging to the same quasi-degenerate multiplets. We will present our magnetotransport measurements of graphene bilayers at large perpendicular electric displacement fields, up to ~1.5 V/nm, where we observe crossings between Landau levels with different orbital quantum numbers with energies split by the cyclotron gap $\hbar\omega$, where ω is the cyclotron frequency and $\hbar$ is Planck's reduced constant. The displacement fields at the crossings for Landau level filling factors $\nu \leq -8$ are primarily determined by the layer polarizability of the Landau levels. Despite diminishing Landau level spacing with energy, successive crossings occur at larger displacement fields, resulting from decreasing Landau level polarizability with orbital quantum number. For particular crossings at large displacement fields, we observe resistivity hysteresis, indicating the presence of first-order transitions between states exhibiting easy-axis quantum Hall ferromagnetism. Moreover, we study dual-gated graphene bilayer/hBN moiré superlattices. Under zero magnetic field, we observe additional resistance peaks as the charge density varies. The peaks' resistivities vary approximately quadratically with an applied perpendicular displacement field *D*. Data fits to a continuum model yield a bilayer/hBN interaction energy scale ~30±10 meV. Under a perpendicular magnetic field, we observe Hofstadter butterfly spectra as well as symmetry-broken- and fractional Chern insulator states characterized by their Chern number *t* and miniband index *s* [4]. Their topology and lattice symmetry breaking is *D*-tunable, enabling the realization of new topological states in this system.

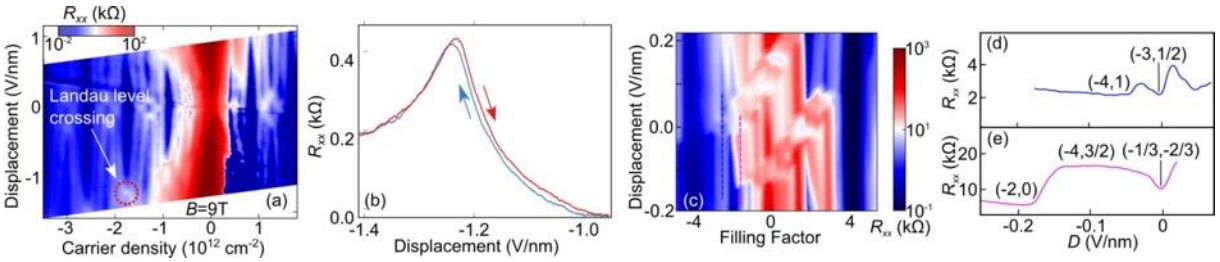

Fig. 1. (a) R_{xx} color plot vs. carrier density and perpendicular displacement field showing LL crossings. (b) Hysteresis observed at circled Landau level crossing in part a. (c) Color plot of R_{xx} vs. filling factor ν and *D* at 18 T and 300 mK for a bilayer graphene/hBN moiré superlattice device.(d) *D*-dependent state transitions are shown, corresponding to the blue dashed line and magenta dashed line in part c, along with the (*t*, *s*) indices.

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Effect of spin-charge disorder correlations on the AHE in 2D dirac fermions

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The anomalous Hall effect is a result of time reversal symmetry breaking,and coupling of (pseudo-)spin and orbital degrees of freedom. A minimal model that captures this effect is the 2D massive Dirac fermion, for which the disorder effects become important when the Fermi level rises above the gap. Although, the effects of scalar disorder and arbitrary disorder in all parameters in the gapped and critical regimes are studied in the literature, the interplay of charge disorder with 'mass' disorder due to magnetic impurities is not well understood when the Fermi level is tuned above the gap. Given that magnetic impurities tend to order ferromagnetically, we assume correlations between spin and charge impurity sectors and express the conductivity tensor in terms of strengths and correlation coefficients of such disorder potentials. We find interesting effects including a sign change in the AHE and relative enhancement due to such correlations.

Metallic carrier transport and superconductivity in novel transition-metal dinitrides; ReN_2 crystal

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Rhenium nitride (ReN_2) is a newly synthesized transition-metal dinitrides crystal from a metathesis reaction between $ReCl_5$ and LiN_3 under high pressure [1]. The structure of ReN_2 crystal is isostructural with MoS_2 (*$P6_3/mmc$*), confirmed by XRD profiles. Under optical microscope, the crystal shows a metallic luster like graphite or MoS_2 with reflected light. However, with transmitted light, it shows a unique red translucent color. Although the structure and mechanical strength of ReN_2 have been analyzed, its band structure and other electrical properties remain completely unknown.

In this work, we reveal the transport properties of ReN_2. First, we exfoliated ReN_2 crystal using Scotch tape onto Si/SiO_2 wafer with 290 nm oxide layer. The thickness of flakes obtained by AFM is about 60-80 nm. The flakes were confirmed as ReN_2 by Raman spectroscopy. We put electrode with Au 40 nm / Cr 40 nm by metal evaporation method.

The resistivity value of the sample measured by 4 probe method at room temperature was 4.2 Ω, and it decreased as the temperature became lower. The temperature dependence of longitudinal resistivity of the sample showed similar tendency with that of metal. Observed linear current-voltage characteristic also suggests that ReN_2 is a metal. These results are in agreement with the band structure calculated in the density-functional theory (DFT) framework. Weak antilocalization was observed under perpendicular magnetic field at low temperature, which indicated that the flake has 2 dimensional structure. ReN_2 can be utilized as 2D metal that has strong spin-orbit coupling, extending the possibility of van der Waals heterostructures.

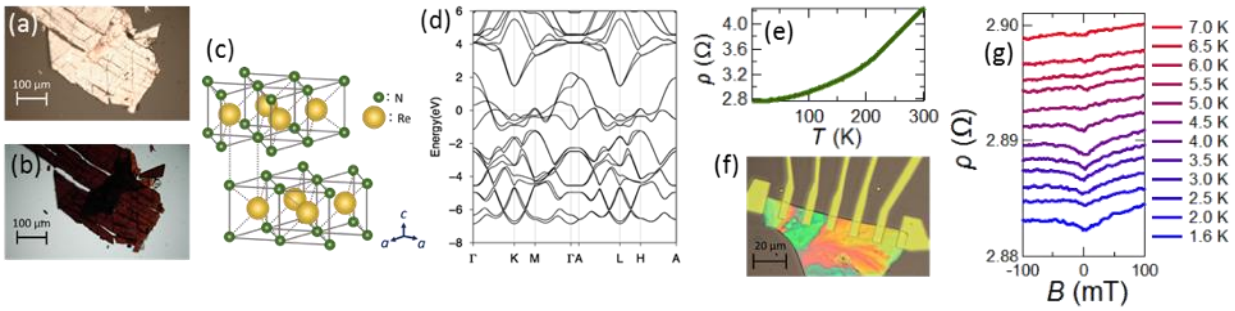

Fig. 1. (a),(b) Optical micrograph of ReN_2 crystal with reflected light (a) and transmitted light (b). **(c)** Schematic image of crystal structure. **(d)** Band structure calculated in the DFT framework. **(e)**Temperature dependence of resistivity. **(f)** Optical micrograph of ReN_2 sample on SiO_2 substrate. **(g)** Magnetic field dependence of resistivity. The curves are offset for clarity.

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Strong exciton effect in graphene nanoribbons

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Owing to their massless nature, charge carriers in graphene possess extremely high electron mobility. Yet, its gapless, semi-metallic nature can present a drawback for applications such as electronic transistors and photovoltaics. It has been a long-standing pursuit to open up and control the bandgap in graphene, by tailoring graphene into its nanoribbons with atomic precision. Recent advances in bottom-up synthesis allow atomic control of graphene nanoribbons (GNRs) with well-defined bandgap and optical properties. (References) A chemical synthesis approach has recently been introduced that enables making bulk quantities of well-defined, narrow graphene nanoribbons (GNRs) with widths as small as ~1 nm. (references) In these structures, carrier confinement in the lateral dimension induces a bandgap corresponding to visible wavelengths. Owing to the strongly reduced charge screening effect in these atomically flat nanoribbons, strong exciton effects are expected and exciton binding energies in excess of ~ 1 eV have been predicted. (References) We will present some our recent optical ultrafast conductivity studies on atomically precise GNRs using THz spectroscopy, which demonstrates and confirms the strong exciton and charged exciton effects. Time-dependent photoconductivity measurements shed light on the sub- picosecond dynamics of the different quasi-particles.

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SYMPOSIA 4 – DEVICES

Two-dimensional electrode materials for metal-ion batteries

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Energy storage is an important problem to realize low carbon society and there have been many challenges. Metal-ion batteries have attracted remarkable attention recently due to the high energy storage demands. The requirement of feasible electrode materials with high capacity and good cycling stability has promoted the exploration of various electrode materials for metal ion batteries. Materials engineering plays a key role in the field of battery research. In particular, engineering materials at the nanoscale offers unique properties resulting in high performance electrodes in various energy storage devices. Consequently, considerable efforts have been made in recent years to fulfil the future requirements of electrochemical energy storage devices. Various multi-functional 2 dimensional materials are currently being studied to improve energy and power densities of next generation batteries (Figure 1). In this talk, I will present some of our recent progress in the synthesis of different types of 2D nanomaterials to enhance the electrochemical energy storage properties of metal-ion battery [1-3].

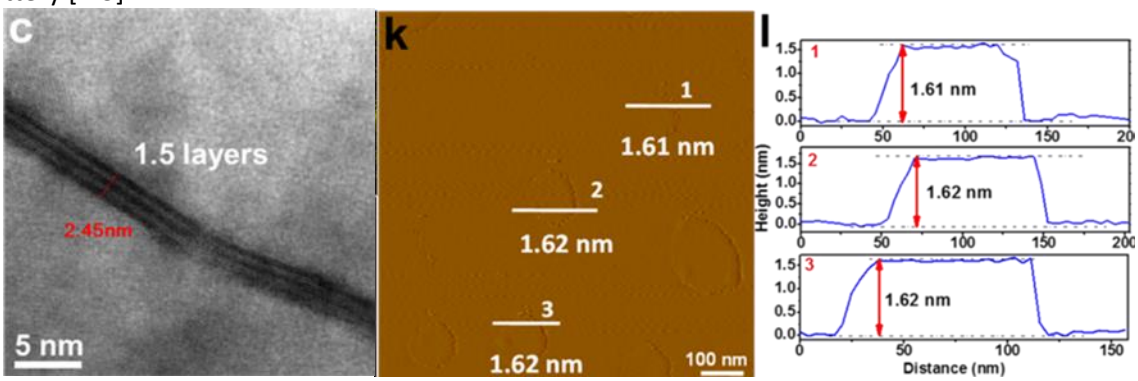

Fig. 1. High resolution TEM image, Atomic force microscope (AFM) image, and corresponding height profiles of ultrathin Bi_2MoO_6 nanosheets.

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Recent STM studies of gate-tunable 2D material devices

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2D materials with reduced dimensionality exhibit unprecedented tunability in both their electronic and optical, chemical properties due to the high susceptibility to the doping and the change of many-electron effects. Here we demonstrate a tunable band gap modulation in back-gated 2D material devices. Using low-temperature scanning tunnelling microscopy (LT-STM), we probed the quasiparticle electronic bandgap of recently-emerged 2D materials such as black phosphorus (BP) and 2D TMDs as a function of electrostatic gating. The demonstration of an electrical field tunable bandgap in 2D material devices paves the way to designing electro-optic modulators and photodetector devices that can be operated in a wider electromagnetic spectral range. I will also discuss our recent STM studies of atomic defects in 2D materials with an aim to correlate these defect physics to the device characteristics. Our findings may open up the new avenue for the investigation into charge transport through single defect and dopants in nanodevices.

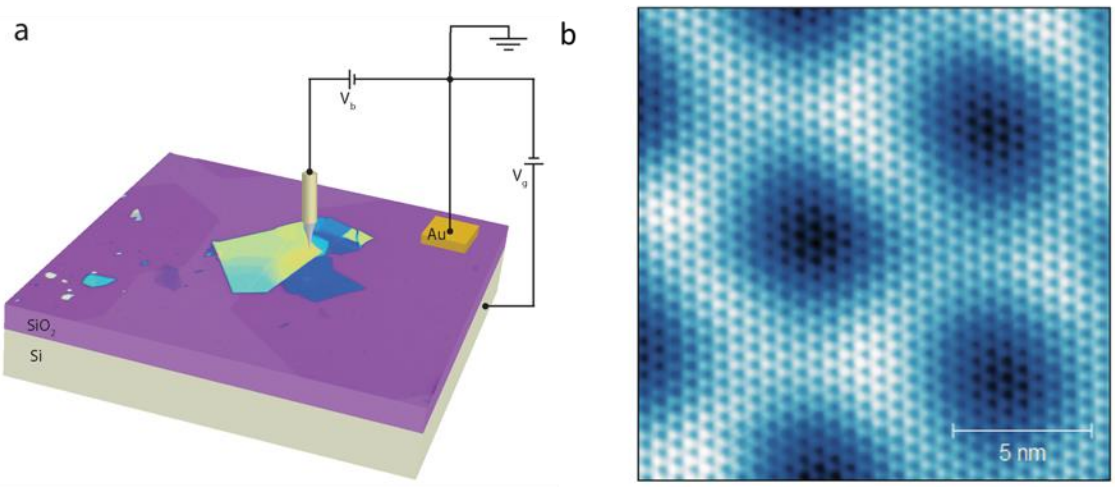

Fig. 1. (a) Schematic illustration of a back-gated 2D material device (b) Atomically-resolved STM imaging of gated 2D material devices.

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Novel all-solid-state supercapacitors based on snowflake-like Ni_3Si_2/ NiOOH /graphene hybrid nanostructures

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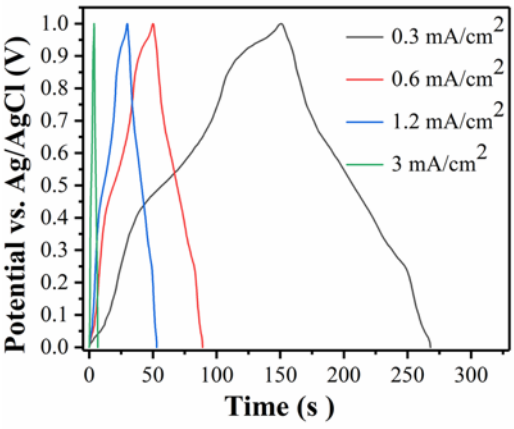
Main text: The recent development of synthesis processes in three-dimensional (3D) graphene-based structures, has tended to focus on continuous improvement of porous nanostructures, doping modification thin-film manufacture, and mechanisms for building 3D architectures. Here, we synthesized novel snowflake-like Ni_3Si_2/ graphene nanostructures on three-dimensional (3D) graphene/Ni foam by one-step low-pressure chemical vapor deposition (CVD). Through systematic micromorphological characterization, it was determined that the formation mechanism of the nanostructures involved the melting of the Ni foam surface and the subsequent condensation of the resulting vapor, the 3D growth of graphene through catalysis in the presence of Ni, and finally the nucleation of the Ni_3Si_2 nanostructure in the carbon-rich atmosphere. Electrochemical measurements indicated that the snowflake-like nanostructures showed excellent performance as a material for energy storage. The Ni_3Si_2 / NiOOH / graphene composites achieve a specific capacitance of 1080 mF/cm^2 at a scan rate of 1 mV/s. When integrated as all-solid-state symmetric supercapacitors, they offer a full cell specific capacitance as high as 80.4 F/cm^2 at a scan rate of 0.3mA/cm^2. Further, even after 6000 sequential cycles, the electrode retained 90.7% of its capacitance.



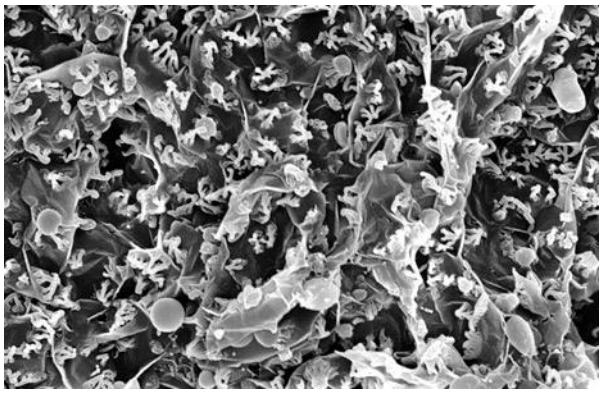


Fig. 1. All-Solid-State Supercapacitors Based on snowflake-like Ni_3Si_2/ NiOOH /graphene Hybrid nanostructures

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Physisorptive two dimensional tin sulphide nanoflackes with extraordinary sensitivity and selectivity to NO_2 at room temperature

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Nitrogen dioxide (NO_2) is a gas species that plays a vital role in certain industrial, farming, and healthcare sectors. However, there are still significant challenges for NO_2 sensing at low detection limits, especially in the presence of other interfering gases. The NO_2 selectivity of current gas-sensing technologies is significantly traded-off with their sensitivity and reversibility as well as fabrication and operating costs [1-5]. In this work, we present an important progress for selective and reversible NO_2 sensing by demonstrating an economical sensing platform based on the charge transfer between physisorbed NO_2 gas molecules and two-dimensional (2D) tin sulfide (SnS) flakes at room temperature. An extraordinary response factor of ~36 is demonstrated to ultralow 150 parts per billion (ppb) NO_2 at room temperature, within the physisorption temperature bands for SnS. The device shows high sensitivity and superior selectivity to NO_2 at operating temperatures of less than 140^o C, which are well below those of chemisorptive and ion conductive NO_2 sensors with much poorer selectivity [5-8]. The demonstrated 2D SnS based sensing device holds the greatest potential for producing future commercial low-cost, sensitive and selective NO_2 gas sensors.

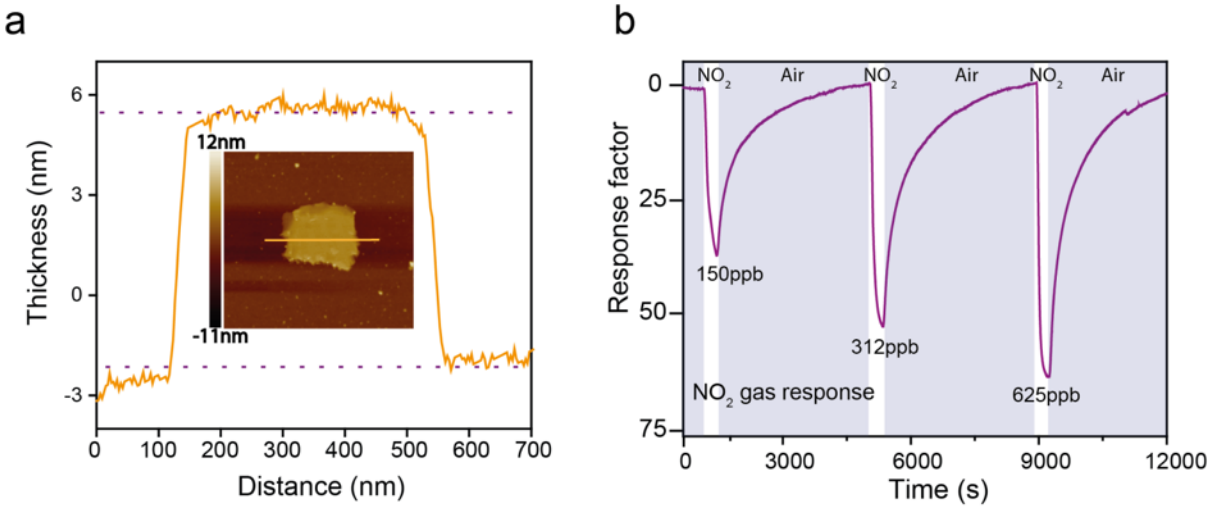

Fig. 1. (a) Height profile of a typical 2D SnS flake along the orange line in the AFM image inset. (b) Dynamic sensing performance of 2D SnS flakes toward NO_2 gas at concentrations ranging from 150 to 625 ppb under the operation temperature of 60^{o}C.

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Single nanostructure band gap engineering and heterostructures of atomic layered semiconductors

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Band gaps are one of the most important parameters of semiconductor materials for their optoelectronic applications since they determine the spectral features of absorptions and emission processes. Due to the limited band gaps of natural semiconductors, alloying of semiconductors with different band gaps have long been the standard methods of achieving semiconductors with new band gaps.[1-4] Band gap engineering on single semiconductor nanostructures is particularly important to construct semiconductor heterostructures with new optoelectronic functions for integrated device applications.[1,3,5,6] In this talk, firstly I will report our recent progress on the band gap engineering of two-dimensional (2D) atomically thin layered materials to realize composition and band gap continuously modulated 2D semiconductors through alloying of two semiconductor compounds with different band gaps. Secondly, the band gap and interface engineering within single 2D layered nanostructures will be reported, to achieve spatial composition graded and interfacially sharped lateral heterostructures. The band gap and interface engineering can be extended to construct vertically stacked 2D heterostructures with tunable interface band alignments and band structure types. Some interesting optical and optoelectronic properties and device applications will also be exhibited based on these novel 2D nanostructures.

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SYMPOSIA 4 – CHEMISTRY

Two-dimensional semiconducting materials: candidates for extending moore's law

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Internet of things and artificial intelligence demand further transistor performance improvements and device size scaling. In a conventional planar silicon field-effect transistor (FET), the gate controllability becomes weaker when its lateral dimension scales. Hence the transistor body thickness needs to be reduced to ensure efficient electrostatic control from the gate. When the silicon thickness reduces to a few nanometers, the fast mobility decay owing to the scatterings from imperfect silicon surfaces retards the further scaling. New materials with perfect surfaces are therefore needed and 2D semiconducting materials offer a great chance to continue the scaling. Silicon transistor evolution (road map) shall be discussed first. Many challenges are ahead for adopting 2D semiconductors as FET channel materials, including (1) selection of 2D materials, (2) reduction of contact resistance, (3) growth of wafer-scale and single-crystalline 2D materials, and (4) Integration of 2D materials to existing microelectronic fabrication processes. In this presentation, we will share our perspectives on these challenges and possible approaches.

Hot carrier optoelectronic devices based on van der Waals heterostructures

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Two-dimensional (2D) van der Waals semiconductors such as monolayer MoS_2 and WSe_2 are an attractive building block for novel photonic devices due to their strongly excitonic character. Monolayer transition metal dichalcogenides exhibit strong excitonic absorption due to band nesting [1] and allow exploration of hybrid quasi-particle states such as plexcitons [2] through strong dipole-dipole coupling [3]. The first part of this talk will focus on our approaches to realizing electrical generation, manipulation, and detection of excitons and their complexes based on various van der Waal heterostructures. Specifically, I will discuss how MIS-type heterostructures allow electrically tunable excitonic electroluminescence [4] and electro-optic upconversion in linear optics regime. We demonstrate that hexagonal boron nitride can serve as a unipolar tunnel barrier that allows hot carrier injection and energy harvesting. Our results reveal that interlayer charge transfer dynamics is tunable with electrical bias and competes with thermalization of hot photocarriers leading to distinct optoelectronic response at high photon energy excitation. The second part will discuss our recent discovery of a novel monolayer MoS_2 growth mechanism based on vapor-liquid-solid conversion [5]. We show that alkali metal plays a key role in reducing the melting point of the precursors and triggering the vapor-liquid-solid mode, yielding expitaxial growth of monolayer nanoribbons.

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Natural rubber/St-LDH/MWCNT hybrid bio nanocomposites as flexible EMI shield

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Recently the researchers have concentrated on developing flexible ecofriendly and portable advanced nanocomposites with high EMI SE value for EMI shielding by absorption mechanism to protect the humanities as well as highly sensitive precision electronic equipment from the harmful effects of electromagnetic radiations owing to the fabulous growth of telecommunications and electronic devices in the modern society. For this purpose Natural rubber/St-LDH/MWCNT Hybrid Bio-Nanocomposites were prepared by two roll mill mixing and compression moulding. The novelty of the work is that 1D MWCNT was used to exfoliate 2D St-LDH into the rubber matrix and 2DSt-LDH was used to disperse maximum1D MWCNTs into the rubber matrix without agglomeration so as to make the composite with sufficient conductivity and with high dielectric properties by lending hand to each other to satisfy the criteria for acting as EMI shield. In addition to that LDH sheets acts as compatibilizer for both MWCNT and natural rubber. The presence of LDH sheets helped to lower the conductivity and enhance the EMI SE value simultaneously than that expected due to the introduction of MWCNT into the rubber matrix so that it can be used as cover for mobile phones without fearing about lightning. Modification of LDH was carried out by memory effect and confirmed by XRD, FTIR and TEM. The morphological characterization of the composites was characterized by TEM, XRD and XPS and the strong interaction between the fillers and the matrix was confirmed by DMA. The EMI SE value of hybrid nanocomposites with different filler loading were carried out by two port vector network analyzer and dielectric measurements were conducted by impedance analyzer .It was observed that EMI SE value increases with increase in filler content for a given frequency and reached maximum value of -38dB which has not ever been reported for natural rubber nanocomposites because of agglomeration of conductive nanofillers which had been overwhelmed here and another advantage of this system is that it shields EMI mainly by absorption whereas in most of the reported ones the main mechanism of EMI shielding is reflection which again develop harmful effects on human beings.

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2D crystal heterostructures for water-oxidation

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2D layered materials, including transition metal dichalcogenides, are of great interest for opto-electronic devices due to their layer dependant electronic properties. Recent theoretical work has shown that both MoS_2 and WS_2 at mono-layer can function as a photoanode for water oxidation[1]. Experimentally, we have recently realized this in the form of thin films of chemically exfoliated MoS_2/WS_2 heterojunctions for water oxidation, which demonstrate a synergistic effect beyond either individual components performance. This effect arises from efficient charge transfer between the two van der Waals stacked components leading to electron-hole separation and increased reaction time at the surface[2]. Here, we present high crystal quality MoS_2/WS_2 vertical heterostructures grown in a single-step via chemical vapour deposition[3]. These heterostructures demonstrate photocurrents densities up to 0.8 mA/cm^2 (at 1-sun, +0.7V vs Ag/AgCl) and IPCE peaking at 1.6% in 3.5% NaCl (Figure 1). This performance is superior to both liquid phase processed heterostructures for water oxidation and WSe_2 for photo catalytic hydrogen evolution. These heterostructures can be grown over a cm^2 area with a high electrochemically active surface area (100 m^2/g). These results pave the way for the use of 2D crystal heterostructures in water splitting devices and provide a viable option for the energetically challenging water oxidation reaction.

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Tunable Photoluminescence in Organic Semiconductor/Two-Dimensional Transition Metal Dichalcogenides van der Waals heterojunction

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In recent years, two-dimensional (2D) monolayer transition metal dichalcogenides (TMDs) are attracting extensive attentions due to the direct band gap and strong light-matter interaction, rendering them the potential candidates for next-generation optoelectronic devices. TMD/TMD heterojunctions have attracted enormous attention due to extraordinary optoelectronic properties [1]. However, the stacking of different TMD monolayers on top of one another to form heterojunctions is a very tough work, normally done by mechanically transferring one layer onto the other under optical microscope. On the other hand, TMD materials combined with organic semiconductors have been gaining great interest [2] owning to the advantages of organic semiconductors, such as easy processing, synthetic tunability, and mechanical flexibility. We report the photoluminescence (PL) characteristics of van der Waals (vdW) heterojunction constructed by simply depositing organic semiconductor of 3, 4, 9, 10-perylene tetracarboxylic dianhydride (PTCDA) onto two-dimensional MoS_2 monolayer. The crystallinity of PTCDA on MoS_2 is significantly improved due to vdW epitaxial growth. We observe an enhanced PL intensity and PL peak shift of the MoS_2/PTCDA heterojunction as compared with the individual MoS_2 and PTCDA layer. The synergistic PL characteristics are believed to be originated from the hybridization interaction between the MoS_2 and the PTCDA as evidenced by the density functional theory calculations and Raman measurements [3]. The hybridization interfacial interaction is found to be greatly influenced by crystalline ordering of the PTCDA film on the 2D MoS_2.

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SYMPOSIA 4 – PHYSICS

Light-matter interactions in 2D materials

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Two-dimensional (2D) materials, such as graphene and monolayer transitional-metal-dichalcogenides (TMDs), have aroused great attention due to the underlying fundamental physics and the promising atomically-thin optoelectronic applications. Optical properties of these 2D materials are fundamentally interesting such as magneto-phonon resonance in graphene and strong excitonic emission in monolayer WS2. Meanwhile, development of practical optoelectronics based on 2D materials is very promising, which opens many opportunities for the next-generation light-emitting applications such as valley light-emitting diodes and on-chip vertical-cavity surface-emitting lasers (VCSELs). Here, we report observations of magneto-phonon coupling effects in graphene layers, wealthy excitonic emission states of monolayer WS2, and 2D semiconductor lasing from monolayer WS2 embedded VCSELs. Overall, our studies provide many new understandings on fundamental light-matter interactions in atomically thin materials and pave ways to develop industrially attractive light-emitting applications based on 2D semiconductors.

Visualizing quantum Hall liquids and their boundary modes

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In a series of experiment on 2D electron gas at the surface of Bi, we have been able to probe a number of novel features of quantum Hall liquids for the first time. First, we have been able to use the scanning tunneling microscope (STM) to directly visualize Landau orbits in real space. This new technique has been used to show that the electronic states associated with the valley state on the surface of Bi form nematic quantum Hall liquids. [1] By tuning the magnetic field, we have been able to stabilize different type nematic fluids, and have been able uncover a ferroelectric quantum Hall liquid that forms when only one of the valley get occupied. [2] We are able to demonstrate that the formation of these quantum Hall phases are driven by electron-electron interaction. Finally, in the most recent experiment, we have been able to uncover domain walls between different nematic quantum Hall states and to direct image the 1D Luttinger liquids that form at such interfaces. This new type of Luttinger liquids can become metallic or insulating depending on the number of valley-textured edge modes. [3]

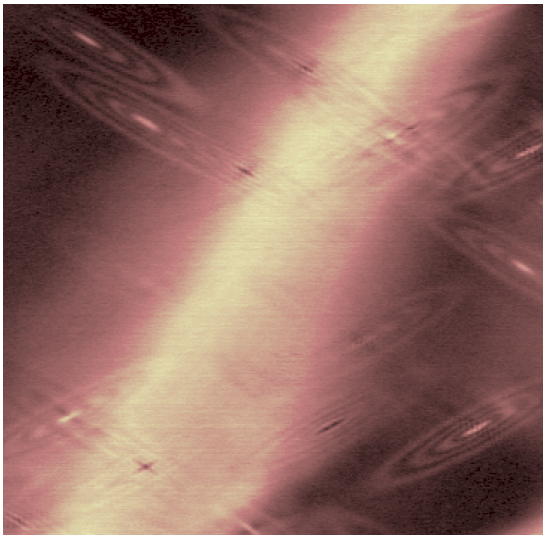

Fig. 1. STM conductance maps can be used to image individual Landau orbit in quantum Hall nematic phase and visualize the domain walls and associated boundary modes [3].

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An atomic-scale on/off switching of magnetism at point defects in graphene

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Pristine graphene is strongly diamagnetic. However, graphene with single carbon atom defects could exhibit paramagnetism. Here, we report direct experimental evidence of π magnetism by using a scanning tunneling microscope. We demonstrate that, in the vicinity of single carbon vacancies with a planar configuration, the localized state splits into two spin-polarized DOS peaks with energy separations of several tens of meV [1]. Moreover, this magnetism can be quenched when the unpaired C atom in defect performs an out-of-plane displacement, which can be controllably realized via the van der Waals attraction between STM tip and the unpaired C atom of defects. Hence, the on/off switching of magnetism can be realized reliably in the atomic scale [2]. Our research provides a comprehensive picture of the origin and manipulation of the magnetism induced by the point defects on graphene layers, suggestive a new insight of the atomic on/off switching of magnetism on graphene-based device.

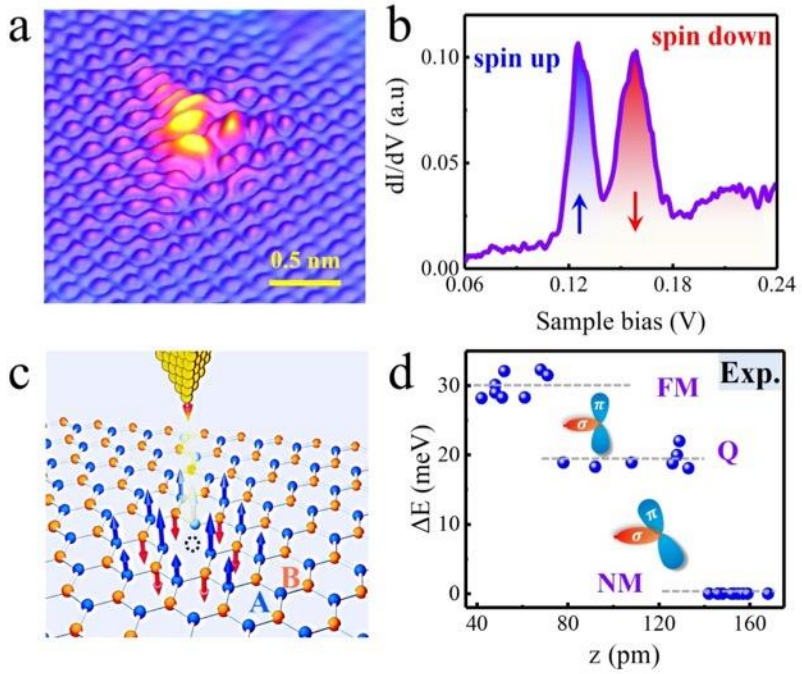

Fig. 1. (a) Atomic resolution STM topography of a single carbon vacancy in graphene. (b) STS spectra recorded at the single carbon vacancy. The two peaks reflect the DOS with opposite spin polarizations. (c) Schematic of the tip-induced atomic-scale on/off switching of magnetism at the defect. (d) Quantum phase transition of FM, Q, and NM states.

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Properties and applications of atomically thin boron nitride

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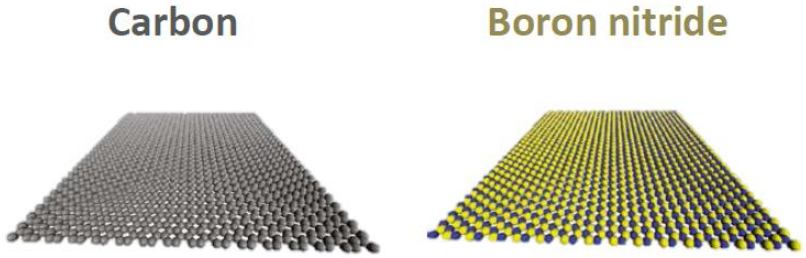
Atomically thin hexagonal boron nitride (BN), also called “white graphene” due to its analogous structure to graphene but white appearance, is a novel two-dimensional (2D) nanomaterials. They possess some characters similar to graphene but also many unique properties unavailable to its carbon counterpart. For example, graphene is a semi-metal; while atomically thin BN has a stable wide bandgap of ~6eV insensitive to thickness reduction. In contrast to the intensive studies and wide publicity of graphene, many fundamental properties and potential applications of atomically thin BN are obscure to academics and industries. Atomically thin BN has been one of the focuses of my research. We invented the first large-scale synthesis route of BN sheets.[1,2] The fundamental physical properties of the material have been systematically studied. It is revealed that monolayer BN nanosheets can sustain up to 850°C in air, while graphene starts to oxidize at 300°C.[3,4] We find that high-quality single-crystalline mono- and few-layer BN nanosheets are one of the mechanically strongest and thermally conductive electrically insulating materials.[5,6] We use both experiment and simulation to reveal the intrinsic dielectric screening, phonon dispersion, and Raman signature of atomically thin BN of different thicknesses.[7,8,9] It is also found that atomically thin BN as an adsorbent experiences conformational changes upon surface adsorption of molecules, increasing adsorption energy and efficiency.[10] The deep ultraviolet light emission from BN sheets is also investigated.[11,12] Thanks to the exciting properties of atomically thin BN, the material has strong potential to solve challenges in different fields, such as corrosion protection[13], ultra-sensitive sensing,[14-16], lubrication,[2,17] and thermal management.[6] The unique properties and applications of BN nanosheets will be reviewed in this talk.



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Visualizing the electronic structure of thin layers of $Bi_2Sr_2CaCu_2O_{8+delta}$

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The role of dimensionality in high Tc superconductivity is an interesting issue: Many of the high Tc superconductor have layered atomic structures, and yet the link between the high Tc superconductivity and the two-dimensional nature of the crystal structure remains elusive. We fabricated atomically thin $Bi_2Sr_2CaCu_2O_{8+delta}$ (Bi-2212) samples, and used scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS) to investigate their electronic structure. In this talk, I will discuss our recent results on the superconducting gap, pseudogap and charge order in Bi-2212 in the 2D limit.

SYMPOSIA 5 – PHYSICS

Topological nanostructures: bismuth and related materials

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Recently topological insulators have emerged as a new class of matter in which surface and / or edge states are protected from backscattering by a combination of spin orbit interactions and time reversal symmetry. Simple deposition techniques that exploit diffusion and aggregation turn out to be ideal for the growth of topological nanostructures, and allow the study of a range of outstanding fundamental issues. Of particular importance is the question of whether or not topological states found in bulk or 2D structures survive in nanoscale structures. Bulk $Bi_{1-x}Sb_x$ alloys were the first 3D topological insulators (in the critical alloy concentration range of x~0.07-0.22) and so nanostructures of these alloys are an obvious target. Here we present an overview of recent experiments that include detailed STM studies of the structure and electronic properties of both $Bi_{1-x}Sb_x$ alloy and pure Bi nanostructures, which are grown in a black phosphorous like structure. We have also studied sequentially deposited (layered) van der Waals heterostructures which allow the observation of additional topologically interesting allotropes of both Bi and Sb. We will also present ARPES data from single topological nanostructures of pure Bi and compare them with DFT calculations that reveal the presence of unusual Dirac cones in the bandstructure. Finally we present the first images / movies of the growth of these nanostructures via LEEM, revealing a major surprise: large islands comprising more than 100,000 atoms are observed to be mobile and undergo a unique shuttling motion - they jump back and forth over distances of hundreds of nanometers.

Realisation of flat band with possible non-trivial topology in electronic Kagome lattice

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The energy dispersion of fermions or bosons vanishes in momentum space if destructive quantum interference occurs in a frustrated Kagome lattice with only nearest-neighbor hopping. A discrete flat band (FB) without any dispersion is consequently formed, promising the emergence of fractional quantum Hall states at high temperatures. Here, we report the experimental realization of an FB with possible nontrivial topology in an electronic Kagome lattice on twisted multilayer silicene. Because of the unique low-buckled two-dimensional structure of silicene, a robust electronic Kagome lattice has been successfully induced by moiré patterns after twisting the silicene multilayers. The electrons are localized in the Kagome lattice because of quantum destructive interference, and thus, their kinetic energy is quenched, which gives rise to an FB peak in the density of states. A robust and pronounced one-dimensional edge state has been revealed at the Kagome edge, which resides at higher energy than the FB. Our observations of the FB and the exotic edge state in electronic Kagome lattice open up the possibility that fractional Chern insulators could be realized in two-dimensional materials.

Moiré phonons in twisted bilayer MoS_2

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The material choice, layer thickness, and twist angle widely enrich the family of van der Waals heterostructures (vdWHs), providing multiple degrees of freedom to engineer their optical and electronic properties. The moiré patterns in vdWHs create a periodic potential for electrons and excitons to yield many interesting phenomena, such as Hofstadter butterfly spectrum and moiré excitons. Here, in the as-grown/transferred twisted bilayer MoS_2 (tBLMs), one of the simplest prototypes of vdWHs, we show that the periodic potentials of moiré patterns also modify the properties of phonons of its monolayer MoS_2 constituent to generate Raman modes related to moiré phonons. The moiré phonons originate from the phonons in monolayer constituents with the basic vectors of moiré reciprocal lattices, which are folded onto the zone center due to the modulation of the periodic moiré potentials. However, the folded phonons related to crystallographic superlattices are not observed in the Raman spectra. Due to the weak vdW interlayer coupling between two monolayers, the phonon dispersion of monolayer MoS_2 (1LM) has been mapped by the θ-dependent frequency of moiré phonons in tBLMs, which are in line with the theoretical results by DFT calculations. The lattice dynamics of the moiré phonons are modulated by the patterned interlayer coupling resulting from periodic potential of moiré patterns, as confirmed by density functional theory calculations. The Raman modes of moiré phonons in the tBLMs are significantly enhanced when Eex matches to the C exciton energy. This study can be extended to other twisted bilayer two-dimensional materials and various vdWHs to deeply understand their Raman spectra, moiré phonons, lattice dynamics, excitonic effects, and interlayer coupling.

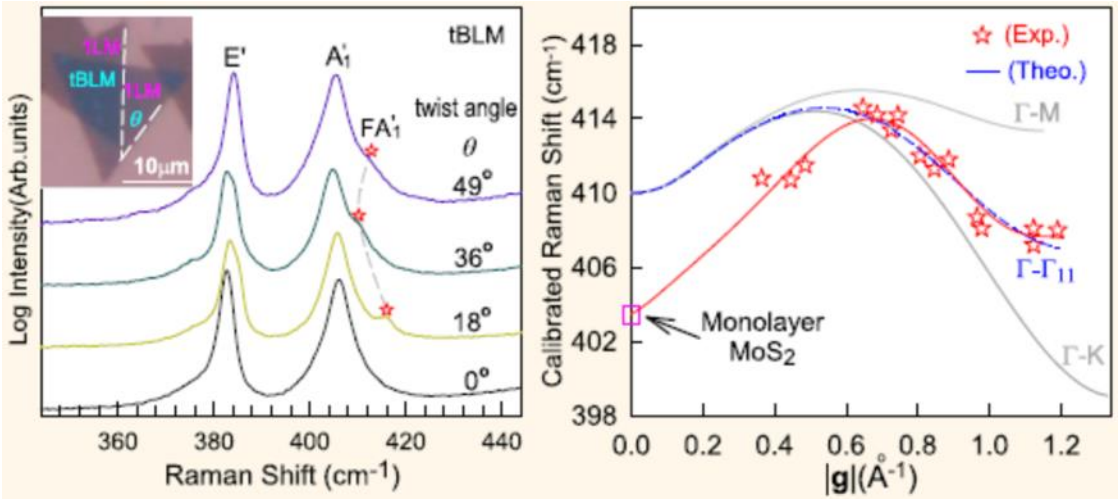

Fig. 1. Twist angle dependent FA'$_1$ modes and the derived phonon dispersion of the A'$_1$-related phonon branch.

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Functional design of MoS_2 via nanoscale ferroelectric control

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The nonvolatile, nanoscale controllable polarization of a ferroelectric gate offers unique opportunities to induce local potential variation and impose designed functionalities in two-dimensional van der Waals materials. In this talk, I will discuss how we utilize the ferroelectric field effect combined with nanoscale domain patterning to achieve programmable electronic states in 2D transition metal dichalcogenides MoS_2. By controlling the domain structures in an ultrathin ferroelectric polymer top-gate using scanning probe microscopy (Fig. 1a-b), we have achieved nonvolatile modulation of the channel conduction in monolayer MoS_2, which can be reconfigured between the transistor and homo-junction states (Fig. 1c), with the junction barrier height tunable by a back-gate [1]. We have also employed this approach to engineer the contact potential for metal-MoS_2 heterojunctions [2]. Our work points to a new route to designing programmable circuit elements in a single material platform for nanoelectronic and optoelectronic applications, and provides critical information on the performance limiting factors in the ferroelectric-2D hybrid material systems.

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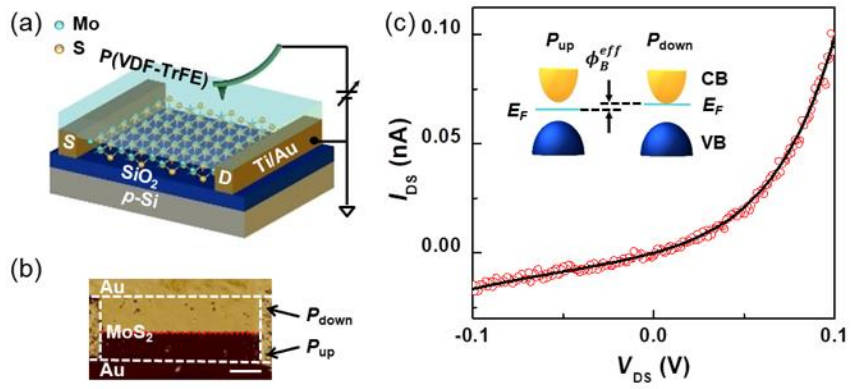

Fig. 1. (a) Schematic view of a MoS_2 transistor sandwiched between a ferroelectric polymer top-gate and a SiO2 back-gate. (b) Piezoresponse force microscopy image of a monolayer MoS_2 with the ferroelectric top-layer patterned into the half *P*down-half *P*up state. (c) Rectified source drain *I-V* characteristic of MoS_2 in the presence of the domain structure. Inset: schematic band alignment of the resulting homo-junction. Adapted from Ref. [1].

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Excited state biexcitons in atomically thin $MoSe_2$

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The highly enhanced Coulomb interactions in the atomically thin layered 2D materials, arising from the reduced dimensionality and weak dielectric screening, allows the formation of tightly bound excitons [1], trions [2,3], and biexcitons [4-6]. Biexcitons have been of keen interest for both fundamental studies of the remarkable many-body interactions and investigations of novel device applications, such as quantum logic gates, biexciton lasing devices, entangled photon sources, etc. [7] Recently, tightly bound biexcitons have been observed in monolayer TMDs, such as WSe_2, MoS_2 and WS_2. These biexcitons in monolayer TMDs show an ultra-large binding energy in the range of 50−70 meV, which is more than 1 order of magnitude higher than the values found in III−V quasi-2D quantum wells [8]. This strong binding necessitates the complete understanding of the structures of these biexcitons and their dynamics in 2D materials as well as characterization of their properties and full investigation of their potential functionalities. Hence, it is necessary to demonstrate a system that exhibits these biexcitons with high binding energy to make their study possible. Here we have successfully used PL spectroscopy to study biexcitons in free standing monolayer $MoSe_2$. We observed tightly bound biexcitons with a binding energy of ~60 meV in atomically thin $MoSe_2$ [9].

The measured binding energy matches well with the theoretically predicted value of the excited state biexcitons in $MoSe_2$. We further probed the formation dynamics of these biexcitons and found that the density of biexcitons increases with increasing density of negative trions and decreases with increasing density of excitons. This finding suggests that the biexcitons observed here are excited state biexcitons instead of ground state biexcitons. More importantly, we successfully triggered the emission of excited state biexcitons at room temperature in a freestanding bilayer $MoSe_2$ by modulating three independent parameters: (1) dielectric screening, (2) density of trions, and (3) excitation power. The implications of the tightly bound biexcitons at room temperature in 2D materials are far reaching. It provides a room-temperature 2D platform to explore fundamental many-body interactions, which provides a route for quantum logical devices and entangled photon sources operating at room temperature.

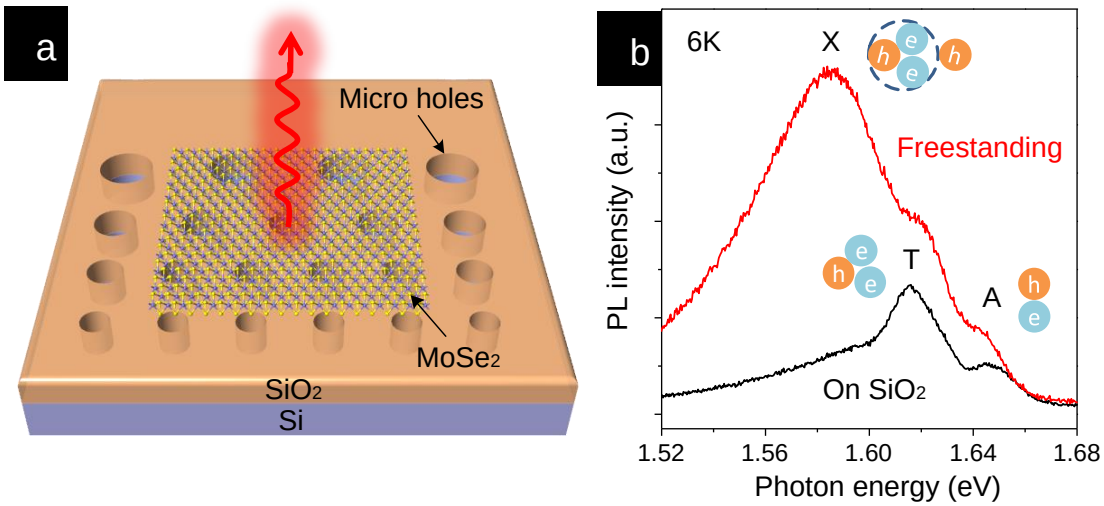

Fig. 1. a, Schematic diagram showing the 1L $MoSe_2$ deposited over micro hole containing substrate, showing the biexciton emission from suspended monolayer. **b**, Measured PL spectra from freestanding (red line) and SiO_2-supported (black line) 2L $MoSe_2$ at 6 K. The labels “A,” “T” and “X” represent the emissions from excitons, trions and a new emission peak, respectively with corresponding schematics.

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SYMPOSIA 5 – DEVICES

Redefining the "things" in the IoT: graphene-enabled internet of materials for large area sensing

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Imagine has developed sensing technology based on graphene and the IoT that allows data to be extracted from surfaces, such as in smart buildings, roads and infrastructure. We are redefining what the "things" and "devices" are in the IoT. Graphene has unique properties that allow it to function in many different applications, however, graphene is not a product, it is a raw material that is used in other products. The challenges of introducing a new raw material into any supply chain are many-fold and complex, ranging from customer demand to cost to safety to standards to supply. Understanding the whole supply chain allows the critical points where value can be captured now and where it can be captured as the supply chain matures. In the case of large-area sensing, graphene offers both a cost and functional advantage over existing solutions. As a nascent industry, the challenges for graphene are accentuated by a lack of established manufacturing base, access to capital and in Australia especially, by the lack of market size and distance from larger markets. Imagine has developed a strategy where we have developed an advantage over incumbent technologies and leveraged this into new applications of the technology, entering adjacent and complimentary market verticals. Beginning with an Australian strength, mining, Imagine has developed smart materials for large-scale mining applications into a novel large-scale sensing technology based on the enabling properties of graphene and the cost advantage that graphene offers.

Large-area two-dimensional organic single crystals

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The two-dimensional organic single crystals (2DOSCs) are thin layers of periodically arranged organic molecules held together by weak interactions in the 2D plane. They show high-performance due to the elimination grain boundaries and are compatible with modern thin-film processing technology, making them promising candidates for flexible and large-area electronics. Their large-area production requires both low nuclei density and 2D crystal growth mode. As an emerging type of material, their large-area production remains a case-by-case practice. We present a general, efficient strategy for large-area 2DOSCs. The method grows crystals on water surface to minimize the density of nuclei. By controlling the interfacial tension of the water/solution system with a phase transfer surfactant, the spreading area of the solvent increases tens of times, leading to the space confined 2D growth of molecular crystals. As-grown subcentimeter-sized 2DOSCs floating on the water surface can be easily transferred to arbitrary substrates for device applications.

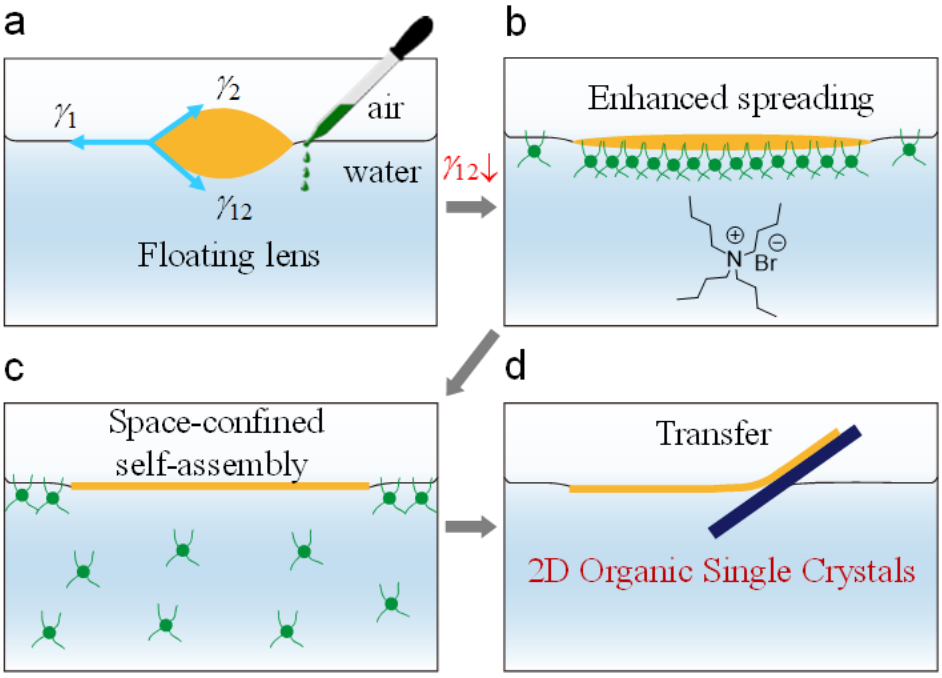

Fig. 1. Procedures of the space confined strategy toward large-area two-dimensional organic single crystals

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Graphene bolometers for sensitive detection of nitrogen-vacancy spin states in diamond

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A pair of electrons in nitrogen-vacancy (NV) centers in diamond form two particle spin singlet or triplet state, where two of ground triplet states can be regarded as a qubit. Since the discovery of spin dependent fluorescence and related optically detected magnetic resonance (ODMR), NV centers in diamond have shown remarkable coherence at room temperature, and attracted much attention for constructing quantum information platform. Moreover, NV electron spins interacts with nearby nuclear spin states through hyperfine interaction, providing a route to manipulate and measure multiple spins in diamond. The photon-counting method reads out spin states of NV centers by measuring fluorescent light. This, however, is inherently inefficient and requires long signal integration time due to significant photon loss in conventional confocal microscope-based photo-detection scheme, posing a significant limit on high throughput quantum measurement of this spin system. Here we propose graphene bolometer devices for fast electronic measurement of NV centers. We present two types of design; Type I: graphene Josephson junction, and Type 2 : graphene noise thermometric devices. In both designs, utilizing graphene's unique property for sensitive bolometer combined with bandgap engineering, highly efficient energy non-radiative transfer, weak electron-phonon interaction, and high electron mobility, we show that the proposed platform can enable fast and precise electronic read-out of the spin states. We also report experimental progress to realize the proposed scheme and discuss application of the devices for high fidelity quantum states.

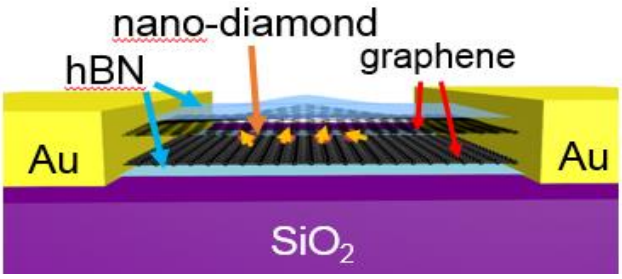

Fig. 1. A cross-sectional diagram of the proposed graphene bolometer device with nano-diamonds between the two monolayer graphenes.

Enhancing electronic fingerprints of physisorbed molecules of graphene

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Graphene has been well regarded as a promising platform for rapid and sensitive molecular sensing owing to its unique electronic properties [1, 2]. In recent years, we have seen a growing interest of using graphene-based nanodevices in the field of electrochemical sensing and biosensing [3-5]. However, the success of these prototypes is overshadowed by a lack of understanding of the nature of graphene-molecule interactions. Addressing this fundamental problem could allow us to further modify the nanodevice setup and improve their performance. Here we have systematically studied the evolution of electronic structure of graphene-molecule systems under the influence of functional groups, adsorption concentration adsorption geometry and molecular dipoles as well as their response to an external electric field using density functional theory calculations with van der Waals corrections.

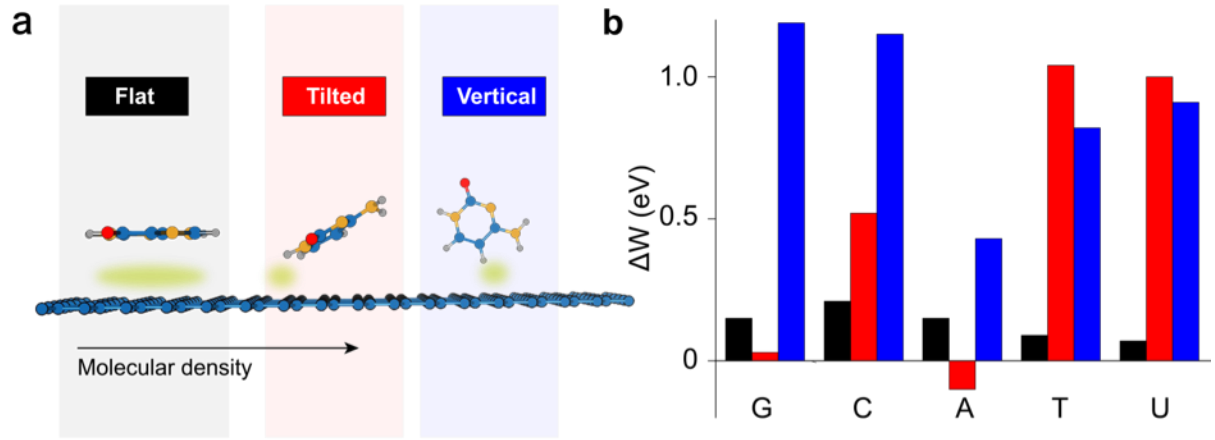

Fig. 1. Electronic structure modification of graphene-nucleobase system. (a) Three scenarios considered in the study: flat, tilted and vertically-aligned adsorption. (b) Corresponding work function changes for nucleobase molecules at each scenario.

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2D material devices as lab-on-a-chips to explore novel states of matter

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2D material device is a lab-on-a-chip to explore novel states of matter that are inaccessible in its bulk counterpart, because of the small size of thin flakes. It has been recently revealed that the reduction in thickness or volume not only causes the significant change in electronic structure, but also results in the dramatic slowdown of the ordering kinetics, which provides opportunities to realize metastable states. For example, metastable superconductivity was discovered just by thinning a layered material 1T-$IrTe_2$, which is non-superconducting in its bulk crystal form (see Fig. 1) [1]. Also, the small system size allows very high electric fields and current densities to be generated, followed by the discovery of an unprecedented metastable CDW state in 1T-TaS_2 [2].

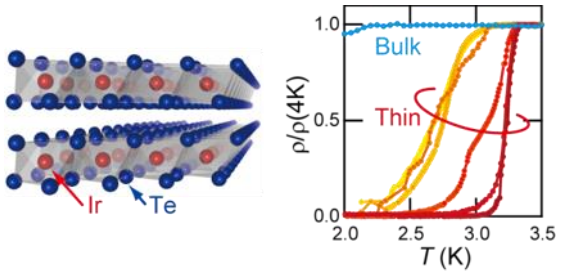

Fig. 1. Thinning-induced metastable superconductivity in 1T-$IrTe_2$ thin flake devices [1].

However, it is always difficult to characterize the newly discovered states in a 2D material device, because of its small volume. It is necessary to develop in situ microscopy technique to elucidate the novel states realized in the microscale device. For instance, the microbeam X-ray available at synchrotrons was found to be a useful tool to identify the crystal structures of thin flakes (see Fig. 2) [3].

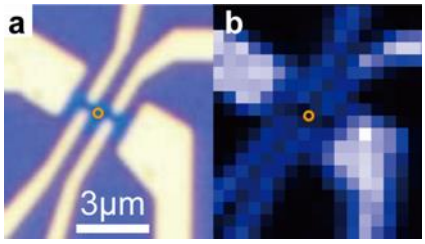

Fig. 2. Images of a thin flake device captured by (a) optical microscopy and (b) fluorescent X-rays from the gold electrodes. The orange circles represent the position at which the microbeam X-ray impinges [3].

In my talk, I will first introduce the unprecedented metastable states discovered in 2D material devices, and second present our on-going efforts to elucidate the microscopic structure of the novel phases by performing (quasi-) in situ microscopy measurements.

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SYMPOSIA 5 – CHEMISTRY

Strain-enhanced two-dimensional electrocatalysts for water splitting and beyond

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Our global energy consumption has reached 18 terawatts. Thus, any alternative energy resources for the future must be able to scale up to terawatt level. Hydrogen fuel is one of the most promising clean and renewable energy resources that can be scaled up to terawatts. Electrochemical water splitting driven by sustainable energy such as solar, wind and tide, is attracting ever-increasing attention for sustainable production of clean hydrogen fuel from water. Leveraging these advances requires efficient and earth-abundant nonprecious catalysts, which is abundant enough to scale up, to accelerate the kinetically sluggish hydrogen and oxygen evolution reactions (HER and OER). A large number of advanced water splitting nonprecious electrocatalysts have been developed through recent understanding of the electrochemical nature and diverse nanostructuring techniques. Specifically, strain engineering offers a novel route to promote the electrocatalytic HER/OER performance for efficient water splitting. In this talk, I will discuss about the recent progresses of applying strain to enhance heterogeneous two-dimensional electrocatalysts for water splitting, and then the future opportunities are discussed. I will begin with a brief introduction of the fundamentals of water splitting reactions, and the rationalization for utilizing mechanical strain to tune an electrocatalyst. Then, I will discuss about experimental approaches for creating and characterizing strain in two-dimensional materials. Afterward, I will discuss about the recent advances on strain-promoted HER using two-dimensional electrocatalysts, with special emphasis given to combined theoretical and experimental approaches for determining the optimum straining effect for catalysis. Finally, I will propose some two-dimensional electrocatalysts system and reaction cell structures that can utilize strained two-dimensional electrocatalysts for water splitting and beyond.

Superphenylphosphines: ligands that direct metal coordination and bulk assembly via "nanographene" substituents

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Phosphines are an important class of organophosphorus compounds in chemistry, and remain the most common supporting ligands in transition metal catalysts.[1] An attraction of tertiary phosphines as ligands for metal complexes is the ability to tune their electronic and steric properties. The incorporation of two phosphorus donor atoms gives a chelating ligand with the "bite angle" programmed into the ligand's covalent backbone. An alternative to conventional chelating ligands is the assembly of monodentate ligands though non-covalent interactions, an unexplored approach using π-stacking interactions due the weakness of these interactions for simple groups such as phenyl and naphthyl. Large polycyclic aromatic hydrocarbons (PAHs) have gained considerable interest because of their electronic and optical properties, as well-defined molecular models for "nanographenes" and for the strong π-interactions that direct their assembly into columnar stacks.[2] One such PAH is hexa-*peri*-hexabenzocoronene (HBC), consisting of 42 carbon atoms in 13 fused rings; the hexagonal geometry and stability comparable to benzene has led to HBC being described as 'superbenzene' (Fig. 1). As part of our research into well-defined PAH molecules and ligands, we have synthesized a series of 'superphenylphosphines'.[3] The coordination of these phosphines to metals has been investigated, along with the role the HBC fragment plays in influencing coordination geometry and driving assembly of the phosphines and their complexes in the bulk crystalline phase.

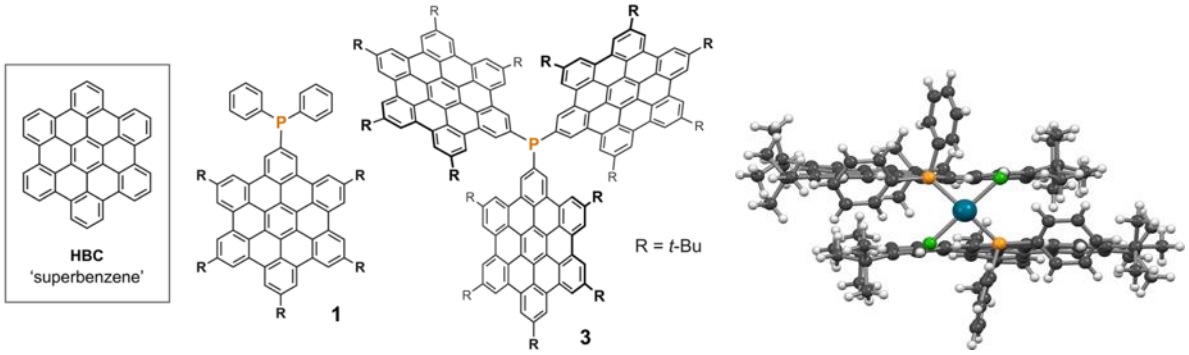

Fig. 1. Diagrams of superbenzene, superphenylphosphines **1** and **3**, and the crystallographically-determined structure of the complex $PdCl_2(\mathbf{1})_2$ showing intramolecular π-stacking.

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Ab initio design of carbon based hybrid electrocatalysts

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Renewable energy technologies, such as fuel cells, water electrolysis and metal-air batteries, are crucial for sustainable energy supply. Developing efficient and inexpensive catalysts for the pivotal electrochemical reactions in these energy devices is imperative for the large scale commercialization. Here we design a series of electrocatalysts by hybridizing heteroatom-doped graphitic carbon materials with transition metals, transition metal oxides and carbides, and MXenes for oxygen evolution reaction (OER), oxygen reduction reaction (ORR) and hydrogen evolution reaction (HER) [1, 2]. These carbon-based hybrid materials show synergistic effect and their catalytic activity can be correlated to the p-band center of the carbon sheets. Our theoretical results screen efficient novel catalysts and prescribe their design principles for renewable energy applications.

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Controlled growth and versatile applications of metallic transitional metal dichalcogenides

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Metallic transition metal dichalcogenides (MTMDCs) have manifested a wealth of intriguing properties in their bulk states, such as magnetism, charge density waves (CDW), and superconductivity. Very recently, nano-thick MTMDCs have been reported to be essential building blocks for constructing next-generation electronic and energy-storage applications, as well as for exploring unique physical issues associated with the dimensionality effect. However, batch production of such envisioned few-layer MTMDCs remains challenging based on the existing physical or chemical exfoliation methods. Our group reported the direct synthesis of high-quality semiconducting and metallic TMDCs materials on both on conducting Au foil substrates and insulating substrates towards different applications. Particularly, we designed a facile chemical vapor deposition route (CVD) for the direct production of VS_2 nanosheets with sub-10 nm thicknesses on SiO_2/Si substrates. The obtained nanosheets represented spontaneous superlattice periodicities and excellent electrical conductivities (~3×10^3 S cm^{-1}), enabling a variety of applications as contact electrodes for monolayer MoS_2 devices, and as supercapacitor electrodes in aqueous electrolytes. Subsequently, we also developed a van der Waals epitaxial strategy for the direct synthesis of thickness tunable metallic 1T-VSe_2 monocrystalline nanosheets on mica substrate via a similar CVD method. The few-layer 1T-VSe_2 nanosheets possess extremely high electrical conductivity up to 106 S m^{-1}, which is 1-4 orders of magnitude higher than that of state-of-the-art conductive 2D materials. We also realized the first achievement of thickness-tunable 2H-TaS_2 flakes and centimeter-size ultrathin films on an electrode material of Au foil via a CVD route. We also detected the transition from nearly commensurate to commensurate CDW phases with our ultrathin 2H-TaS_2 flakes. Remarkably, we obtained extra high hydrogen evolution reaction efficiency on as-grown 2H-TaS_2 flakes directly synthesized on Au foils with the efficiency even comparable to traditional Pt catalysts. All these work provides brand new insights into the direct synthesis and property investigations of nano-thick metallic 2D TMDs crystals.

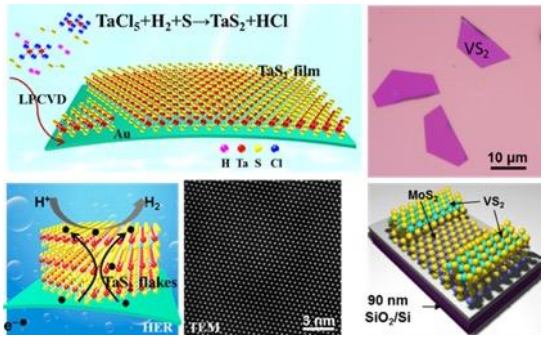

Fig. 1. Controlled growth and versatile applications of metallic transitional metal dichalcogenides

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Facile solution-phase synthetic strategy of 2D SnS nanosheets and its ethanol sensing characteristics

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With the discovery and preparation of grapheme [1], two-dimensional (2D) materials have attracted great interests of scientists and engineers. Subsequently, a series of graphene analogs, for example hexagonal boron nitride (h-BN) [2] and transition metal dichalcogenides (TMDs) [3], were also predicted and successfully synthesized. These thinnest 2D crystals exhibit excellent properties of electrical, optical and mechanics [4 - 6], and have been employed in various applications, such as catalysis [7, 8], light harvesting [9], batteries [10], solid lubricants [11], and sensors [12, 13]. 2D tin (II) sulfide nanosheets were prepared using $SnCl4•5H_2O$ and S powders as raw materials in the presence of H_2O by solution reaction. Our studies showed that the SnO_2 intermediate is the key process to the valence reduction of Sn (from IV to II). This is a high-yielding, environmentally friendly and simple synthesis approach. The SEM and TEM analyses indicated that the thickness of orthorhombic SnS nanosheets is about 100 nm and the lateral dimension is 2 ~ 10 μm. The sensors fabricated from SnS nanosheets exhibited the best sensing factor of 20 for 100 ppm of ethanol (EtOH) gas at 160°C. The response and recovery times are 25 s and 15 s, respectively. It is worth mentioning that this SnS material has low response to acetone and methanol gases, which are the most disturbing reducing organics for EtOH sensors.

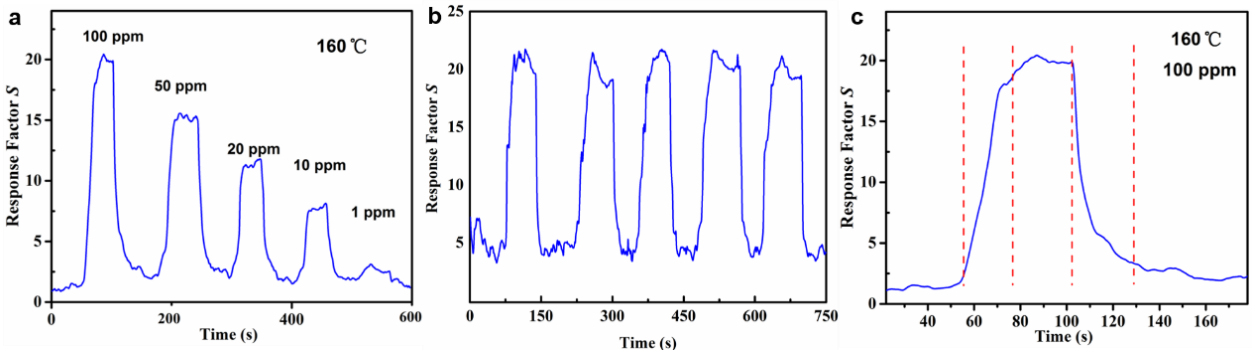

Fig. 1. Gas-sensing performance of SnS nanosheets. (a) Dynamic sensing

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SYMPOSIA 5 – SYNTHESIS

Advanced composite two–dimensional energy materials by simultaneous anodic and cathodic exfoliation

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Composite materials based on graphene and other two–dimensional (2D) materials are of considerable interest in the fields of catalysis, electronics and energy conversion and storage, because of the unique structural features and electronic properties of each component and the synergetic effects brought about by the compositing. Approaches to the mass production of 2D materials and their composites in a facile and affordable way are urgently needed to enable their implementation in commercial applications. Recently, we have developed a novel electrochemical exfoliation approach to prepare 2D composites, which combines simultaneous anodic exfoliation of graphite and cathodic exfoliation of other 2D materials (namely MoS_2, MnO_2, Sb and graphitic carbon nitride). The synthesis is carried out in a single–compartment electrochemical cell to *in situ* produce functional 2D composite materials. Applications of the as-prepared 2D composites are demonstrated as (i) effective hydrogen evolution catalysts; (ii) supercapacitor electrode materials and (iii) effective CO_2 reduction electrocatalyst. In particular, application of cathodic exfoliation turns antimony, an inactive material for carbon dioxide (CO_2) reduction in its bulk form, to an active 2D electrocatalyst for reduction of CO_2 to formate with high efficiency. The high activity is attributed to the exposure of a large number of catalytically active edge sites. Moreover, this cathodic exfoliation process can be coupled with the anodic exfoliation of graphite in a single compartment cell for *in situ* production of few–layer antimony nanosheets and graphene composite. The observed further increased activity of this composite is attributed to the strong electronic interaction between graphene and antimony. The method enables the compositing of semiconductive, or even nearly insulating, 2D materials with conductive graphene in an easy, cheap, ecofriendly, yet efficient way, liberating the intrinsic functions of 2D materials, which are usually hindered by their poor conductivity. The method is believed to be widely applicable to the family of 2D materials.

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Exploring the quantum states and quantum degrees of freedom in 2D van der Waals materials and topological insulators

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Recent advances in nanofabrication technology and the development of topological materials as well as two-dimensional (2D) crystals based on van der Waals (vdW) materials have enabled new possibilities to explore novel quantum states and to manipulate different quantum degrees of freedom (*e.g.*, spin, valley, symmetry, topology, etc.). We have developed scalable fabrication techniques to synthesize high-quality vdW materials by PECVD methods for graphene [1] and graphene nanostripes [2], and by CVD methods for insulating hexagonal boron nitride (h-BN) [3], semiconducting transition metal dichalcogenides (TMDCs), and their heterostructures. By nanoscale strain engineering [4] through placing nearly strain-free, PECVD-grown monolayer graphene and monolayer h-BN on top of arrays of lithographically fabricated nanostructures, we have been able to achieve giant pseudo-magnetic fields (up to 10^3 ~ 10^4 Tesla), strong valley polarization, and robust "topological channels" for protected valley-polarized propagation, as manifested by scanning tunneling spectroscopic (STS) studies and corroborated by tight-binding calculations and molecular dynamics simulations. We have also synthesized monolayer WS_2 single crystals with controlled hetero-phased domains that exhibit spontaneous valley polarization. We have further conducted STS and electrical transport studies under circularly polarized light (CPL) on magnetic topological insulators [5] and monolayer TMDCs in order to elucidate the effect of CPL on the valley and spin degrees of freedom in these strong spin-orbit coupled materials. Finally, the implication of our findings on applications to valleytronics, optoelectronics and spintronics will be discussed.

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New mechanical exfoliation technique for preparing large area 2D materials and special structures

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In the past ten years, mechanical exfoliation method has been widely used to study the intrinsic properties of 2D materials, many important phenomena were discovered on exfoliated samples. However, even though the exfoliated 2D materials show high quality, the size of monolayer samples is quite small (usually few micrometer) and yield ratio is also very low, which limited the investigation progress for 2D materials. In recently, we developed a new mechanical exfoliation technique for preparing large area and high quality 2D materials [1]. Many monolayer 2D materials with milimeter size were successfully exfoliated through this modified method, including graphene, MoS_2, WSe_2, WTe_2 et al. The core of this new mechanical exfoliation technique is to enhance the van der Waals interaction between layered materials and substrates, which can be realized by optimize the exfoliation process, such as substrate types, temperature and vacuum. We also used Raman, AFM, STM and ARPES et al. to test the quality of exfoliated 2D samples, and the results are all prove that the large area monolayer samples have high quality. Besides, some special structures (like bubble and wrinkle) can be prepared by using different parameters, therefore, many unique properties will be observed on these structures. For example, standing wave induced Raman osciallition was first discovered on the exfoliated graphene bubbles [2]. In the near future, the new mechanical tecnique will show great potential for exploring new properties of 2D materials.

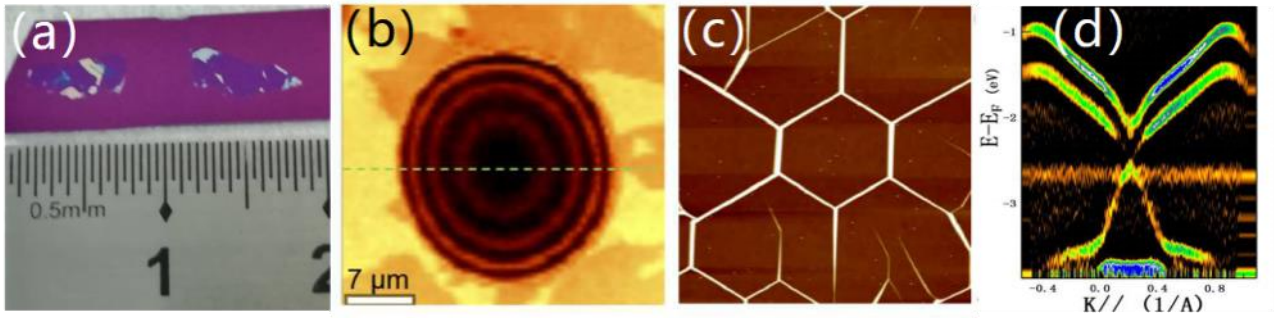

Fig. 1. (a) Optical image of exfoliated large area 2D material (MoS_2). (b) Raman oscillation image on graphene bubble. (c) AFM image of graphene wrinkle. (d) Band structure of large area monolayer WSe_2 measured by ARPES.

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Growth of environmentally stable transition metal selenide films

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Two-dimensional transition metal selenides possess fascinating physical properties. However, most as-prepared selenides are small in size and environmentally unstable, which greatly hinder their wide applications in high-performance electrical devices. Here we develop a general two-step vapour deposition method and successfully grow different selenide films with controllable thickness, wafer size and high crystalline quality. In stark contrast to the poor stability of most two-dimensional materials, these selenide films show superior environmental stability even after long time exposure or being heated in air, annealed in vacuum or immersed in aqueous solutions. The superconductivity of grown $NbSe_2$ film is comparable with sheets cleavaged from bulks, and can well maintain after a variety of harsh treatments. The unique properties of these selenide films can be ascribed to the absence of oxygen during the whole growth process. Such unprecedented environmental stability could greatly simplify devices assembling procedure, and should be of both fundamental and technological significance in developing TMS-based devices with extraordinary performances.

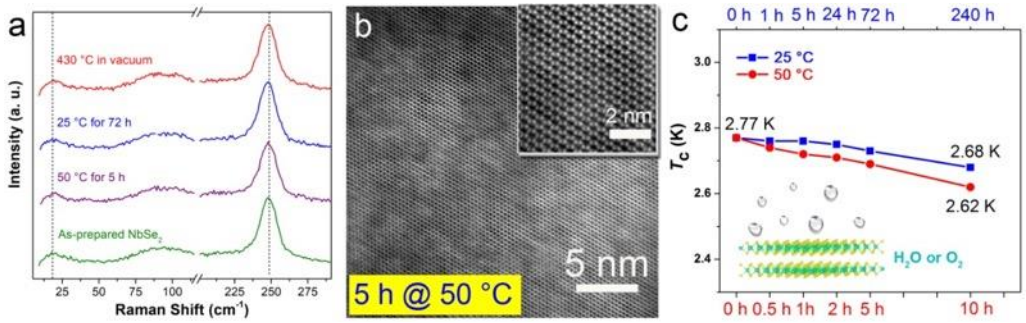

Fig. 1. Growth of environmental stable $NbSe_2$ films: a, Raman spectra with perpendicular polarization for the $NbSe_2$ films after different treatments. b, Different magnified atomic image of $NbSe_2$ film after heat treatment at 50 °C for 5 h in air, where no obvious atomic vacancy is observed. c, Time-dependent evolution of superconducting T_c in bilayer $NbSe_2$ films after exposure in air at different temperatures.

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In situ growth control and further physical and chemical engineering of CVD MoS_2

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MoS_2 flakes were grown in a homemade CVD system equipped with an in situ optical monitoring of the sample during the growth. The optical visibility due to interference effects on SiO_2/Si persisting at growth temperatures of 700-900 °C, introduced a level of growth control. Subsequent manipulation of monolayers by PDMS transfer method to different substrates enabled us to evaluate growth strain and sample quality at the atomic level [1]. In the context of use of CVD MoS_2 in nanomechanical devices we have investigated extended monolayers consisting of connected grains and grain boundaries, and characterized their optical absorption under controlled application of uniaxial tensile strain [2]. The optical properties of MoS_2 dramatically change with applied strain and our results indicated that the applied strain was fully transferred across grain boundaries of the CVD-grown monolayer. In fact, a strain-dependent shift of the A exciton peak was identical to mechanically exfoliated native MoS_2 monolayers and the same value was measured at investigated grain boundaries. Finally, we have investigated the effect of Li adsorption on MoS_2 by means of Raman and circularly polarized PL spectroscopies. We found that increased Li dosing resulted in new peaks in the Raman spectrum and at the same time the overall decrease in the intensity and degree of circular polarization in the PL spectrum, indicating electron-doping and disorder effects, both induced by Li adatoms.

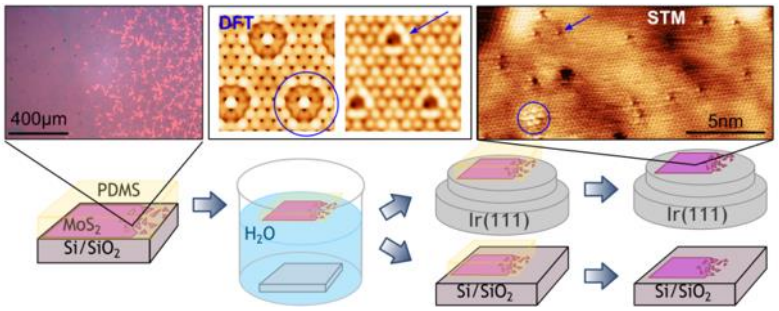

Fig. 1. Synthesis, transfer and atomic scale characterization of CVD grown MoS_2.

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Thursday 13 December

PLENARY

Graphene and 2D materials films and membranes: fabrication and applications

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Graphene, as a representative of 2D materials, has excellent properties, such as high mechanical strength and modulus, high thermal and electrical conductivities, very stable thermal and chemical stabilities, and unique electronic properties. Therefore, films and membranes of graphene and 2D materials are expected to be used in various applications.

Graphene and 2D material films and membranes can be synthesized by CVD and assembly from chemically exfoliated nanosheets. We developed an ambient pressure CVD to synthesize large-area monolayer graphene [1] and WS2 [2] films, large and small size single crystal graphene grains and their continuous films [3-5]. Moreover, we invented an electrochemical bubbling method to efficiently transfer these grains and films [3]. Large area and continuous graphene and 2D material transparent conductive films are produced by an integrated R2R process of CVD and bubbling transfer. Recently, we have developed a green electrochemical water oxidation exfoliation process of graphite to produce high-quality graphene oxide [6] and an intemediary-assisted physical exfoliation techniaue to produce h-BN nanosheets [7]in large quantity and high yield. More importantly, we have invented a continuous centrifugal casting process to rapidly produce high-quality graphene and 2D material membranes in large area and tunable thickness from chemically exfoliated 2D sheets [8]. These graphene and 2D material films and membranes may have wide applications in many fields, from electronics to optoelectronics, from sensors to wearable devices, and from separation to water treatment [9,10]. However, great efforts are highly needed for the research, development, commercialization, and market explorations of these films and membranes.

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Methods and Materials for Van der Waals Heterostructures

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Artificial *van der Waals heterostructures* of two-dimensional materials offer the possibility of creating layered structures with a wide variety of starting materials and control of composition at the single atomic layer limit. To create such structures, we developed a *van der Waals transfer* technique which largely eliminates interfacial contamination[1]. We have used this technique to encapsulate 2D materials within crystalline h-BN with nearly perfect interfaces, which allows for near-intrinsic behavior in materials such as graphene, transition metal dichalcogenide semiconductors[2], and 2D superconductors[3]. However, significant challenges toward functional heterostructures remain. This talk will detail our recent progress in the materials engineering for van der Waals heterostructures, including control over disorder, achieving robust electrical contacts[4], controlling interlayer rotation angle[5], and improving the quality of the constituent materials[5].

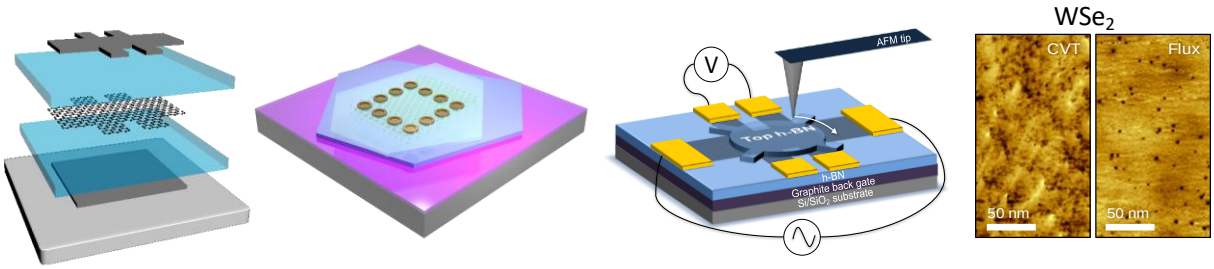

Fig. 1 (Left-Right): Assembly of van der Waals heterostructures; hBN-embedded 'via' contacts; rotatable heterostructures; flux synthesis of TMDC crystals with low defect density.

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SYMPOSIA 6 – PHYSICS

Point-like defects in transition metal dichalcogenides characterized by SPM simulations

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Defects are frequently present in 2D materials, and as such have been extensively studied on suspended samples. However, to describe realistically their electronic properties and their SPM characterization, simulations need to take into account the presence of the metallic substrates commonly employed during the growth and the characterization processes, which might substantially alter the electronic structure of the 2D material. The interaction between metallic substrates and pristine transition metal dichalcogenides (TMDs) can greatly vary depending on the metal [1]. In this work, we have studied the interaction of several point-like defects in TMDs monolayers with underneath Ir(111) and Au(111) substrates by means of DFT calculations and SPM simulations, revealing a notably different behavior depending on the metallic substrate considered. The hybridization of the S states with those of the Ir(111) substrate induces a shift of ~1 eV of the MoS_2 states towards the valence band and a large broadening of the defect states [2]. The interaction with a gold substrate is much weaker, as confirmed by experimental data [3], leading to sharper defect states (Fig.1), much more similar to those found for freestanding MoS_2.

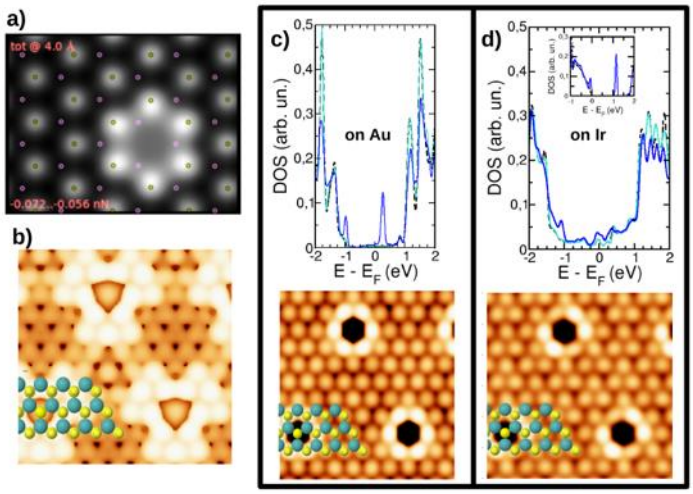

Fig. 1. Left panel: AFM (a) and STM at -0.1 V (b) images of a S vacancy at the top layer for freestanding MoS_2. Right panel: LDOS of top S atoms close (blue) and far (cyan) of the defect site and STM images at V = -0.1 V for a top S vacancy in epitaxial MoS_2/Au(111) (c) and MoS_2/Ir(111) (d). Inset in d): LDOS of a top S vacancy in freestanding MoS_2.

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Generation of localized, optically active defects in tunable 2D materials, using helium ion irradiation

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Atomically thin two-dimensional layered materials receive great interest because of their unique physical properties. Particularly, monolayers of semiconducting transition metal dichalcogenides (SC-TMDs), such as MoS_2, excel due to their strong light-matter interaction that is dominated by exciton phenomena [1-3]. Key to the integration of SC-TDM monolayers into circuitries is the possibility to tune and engineer their properties on demand and on-chip e.g. by defects, dielectric environment or doping [4-8]. We apply inelastic light scattering together with emission, absorption and transport measurements to study the manifold coupling mechanism in van der Waal hetero- and hybrid structures. I will introduce a methodology based on helium ion microscopy (HIM) to controllably realize single optically active emission centers in MoS_2, which show clear indications of quantum dot-like behaviour. Our results demonstrate the potential of HIM to deterministically engineer the optical properties of SC-TDMs at the nanometer scale [5,9]. I thank J. Klein, A. Kuc, F. Sigger, F. Merbeler, J. Wierzbowski, M. Altzschner, F. Kreupl, K. Müller, M. Kaniber, M. Florian, M. Lorke, M. Knap, R. Schmidt, J.J. Finley, and U. Wurstbauer for a fruitful collaboration and the DFG via excellence cluster NIM and project HO3324/9-1 for financial support.

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Single photon-phonon entanglement in WSe_2 quantum dots

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Recently discovered quantum dots (QDs) in 2D materials such as WSe_2 and hBN are a promising platform for combining valleytronics with quantum optics. Here, we unveil entanglement between photons emitted from a confined neutral exciton (X^0) and chiral phonons (CPs) of WSe_2. Fig. 1(a) shows X^0 emission from two QDs (D1a & D2a), exhibiting telltale fine-structure comprising of two orthogonal, linearly polarized peaks split by electron-hole exchange interaction. In addition, we also observe replicas (D1b & D2b), which are separated from their parent peaks, D1a & D2a respectively, by 23 meV. The replicas exhibit spectral wandering identical to their parent peaks. Furthermore, Raman spectroscopy confirms replicas to arise from 23 meV CP. Fig. 1(b), shows the polarization of phonon replica peaks, which unlike the parent peaks, is completely unpolarized, although no loss of polarization information occurs in a coherent scattering. We understand this puzzling behavior by realizing that the phonons involved are doubly degenerate CPs carrying angular momentum and couple to the two opposite helicities comprising the linearly polarized X^0 emission. In other words, due to two indistinguishable paths involved in the scattering process, the state of photon and phonon gets entangled (Fig 1(c)). In our experiment, we do not gain any information about the phonon part of the system and tracing it out gives a completely random state for the photon polarization. Finally, magnetic field is used to lift the degeneracy of the two circularly polarized states comprising each peak of X^0 doublet, which destroys the entanglement by distinguishing the paths and recovers the polarization of the replica peak.

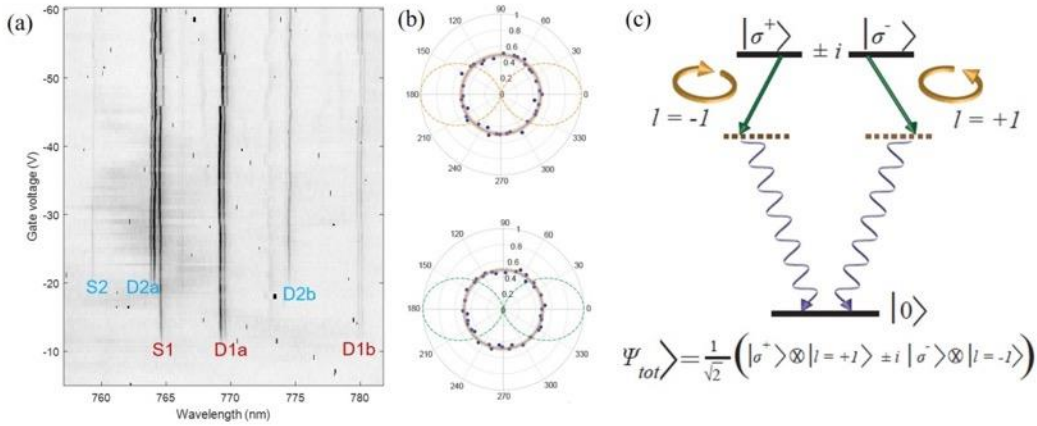

Fig. 1. WSe_2 QDs and their phonon replicas. (a) Gate-dependent PL intensity map of QDs. (b) Polarization of the red peak from a b-doublet in the linear and circular bases. (c) A cartoon explaining the entanglement scheme.

Twisted graphene bilayer around the first magic angle engineered by heterostrain

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Very recently, twisted graphene bilayer (TGB) around the first magic angle $\vartheta \approx 1.1°$ has attracted a plethora of attention for the realization of exotic quantum states, such as correlated insulator behavior [1] and unconventional superconductivity [2]. Here we elaborately studied a series of TGBs around the first magic angle engineered by heterostrain, where each layer is strained independently, by scanning tunneling microscopy/spectroscopy (STM/STS) measurements. Our experiment indicated that a moderate heterostrain enables the structural evolution from the small-angle TGB (ϑ ~ 1.5°) to the strained magic-angle TGB (ϑ ~ 1.1°), exhibiting the characteristic low-energy flat bands. Moreover, the heterostrain can even drive the system into highly strained tiny-angle TGBs (ϑ << 1.1°) with deformed tetragonal superlattices, where a unique network of topological helical edge states emerges [3,4]. Furthermore, the predicted domain wall modes, which result in hexagon-triangle-mixed frustrated lattice derived from Kagome lattice, are firstly observed in the strained tiny-angle TGBs. Our findings not only pave a new way to realize previously inaccessible twisted van der Waals heterostructures based on heterostrain engineering, but also provide an unprecedented platform to study the interplay between different nontrivial states, involving topological edge states and many-body states.

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Electric field-tuned topological phase transition in ultra-thin NA3BI

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Na_3Bi in bulk form represents a zero-bandgap topological Dirac semimetal (TDS), but when confined to few-layers is predicted to be a quantum spin Hall insulator with bulk bandgap of 300 meV.[1] Furthermore, application of an electric field to few-layer Na_3Bi has been predicted to induce a topological phase transition from conventional to topological insulator.[2] I will discuss our efforts to grow epitaxial few-layer Na_3Bi via molecular beam epitaxy, and probe its electronic structure and response to an electric field using scanning probe microscopy/spectroscopy and angle-resolved photoelectron spectroscopy. We are able to demonstrate that monolayer and bilayer Na_3Bi are quantum spin Hall insulators with bandgaps >300 meV. Furthermore, via application of an electric field the bandgap can be tuned to semi-metallic and then re-opened as a conventional insulator with bandgap ~100 meV.[3] The demonstration of an electric field tuned topological phase transition in ultra-thin Na_3Bi provides a viable platform for the creation of a topological transistor.

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SYMPOSIA 6 – DEVICES

Ultrafast laser interaction with 2D materials

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Two-dimensional (2D) materials and their derivatives have attracted unprecedented enthusiasm during the past decade due to their exceptional mechanical, thermal, optical, and electrical properties not available in conventional materials. This article explores the femtosecond laser pulse interaction with 2D materials and the functional optoelectronic 2D material devices enabled by the one-step mask-free direct laser printing (DLP) method [1]. Our results have demonstrated the great potentials of 2D material films as an emerging integratable platform for ultrathin, light-weight and flexible photonic and electronic devices towards all-optical communication, microscopic imaging and energy storage applications [2-6].

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Si-quantum-dots-based optoelectronic devices by employing doped-graphene transparent conductive electrodes

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To overcome small- and indirect-bandgap nature of Si, a lot of efforts have been made to employ Si quantum dots (SQDs) in optoelectronic devices based on quantum confinement effect. Graphene is currently being recognized as one of the candidates promising for its application in transparent conducting electrodes (TCEs). In this talk, I'll report our recent studies on the use of doped-graphene TCEs for SQDs-based optoelectronic devices.
I introduce first fabrication of graphene/SQDs-heterojunction tunneling diodes that work as photodetectors (PDs) showing high performances very sensitive to the variations in size of SQDs as well as in doping concentration of graphene. The photoresponse is remarkably enhanced in the near-ultraviolet range compared to commercially-available bulk-Si PDs. We also first employ graphene TCEs for SQDs-based solar cells, showing a maximum power conversion efficiency (PCE) of 16.61%, much larger than ever achieved in SQDs solar cells with metal TCEs as well as in bulk-Si solar cells with graphene TCEs. The graphene TCEs are doped with three kinds of impurities such as $AuCl_3$, Ag nanowires, Bis(trifluoromethanesulfonyl)-amide (TFSA) for efficient collection of the carriers photo-induced in SQDs. Especially, the TFSA is very effective for enhancing the stabilities of the devices. The encapsulation of the doped-graphene TCE with another graphene layer prevents the doping elements from being desorbed, thereby making the PCE higher, its doping dependence more evident, and the long-term performance more stable.

Large-area heterostructures from graphene and encapsulated colloidal quantum dots via the langmuir-blodgett method

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Heterostructures comprised of CQDs or colloidal nanosheets and graphene are a prime example of such a hybrid quantum system, with numerous studies carried out in the past few years. Energy- and charge-transfer dynamics between these two materials have been explored and exploited to fabricate optoelectronic devices. To the best of our knowledge, a hybrid system composed of graphene and silica (SiO_2)-encapsulated semiconducting CQDs has not yet been investigated. These encapsulated colloidal quantum dots (ECQDs) are attractive because of their increased functionality, solubility in polar solvents, and possible biological applications (because of their decreased toxicity). This work explores the assembly and characterization of heterostructures comprised of a two-to-three-monolayer ECQD film sandwiched between two graphene sheets, all supported on a SiO_2/silicon substrate. The bottom graphene sheet can operate as a graphene field-effect transistor (GFET), while the top graphene sheet serves as a top gate, with the two sheets separated by the dielectric ECQD film (see Figure 1). Solution processing methods, used to synthesize the ECQD dielectric film in the heterostructure, are inexpensive, easy to handle, and suited for mass production while allowing for many possible applications. Using transparent graphene as the top electrode allows optical access to the underlying layers. After completion of the heterostructure, PL and Raman spectroscopy measurements confirmed that the optical and structural properties of both materials were maintained [1]. The SiO_2 shells of the ECQD films electrically isolated the top and bottom graphene sheets, allowing the top sheet to be used as a gate for a GFET device. The successfully assembled heterostructures presented in this work pave the way for the development of new optoelectronic devices.

Optical modulation of THz radiation *via* 2D perovskite

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Research on THz radiation has attracted great attention recently in view of its attractive properties and important applications in imaging, sensing and spectroscopy. The recent development of metamaterials and plasmonics has facilitated new approaches for modulating THz radiations. The electromagnetic response of metamaterials structures and plasmonic arise from the combined contributions of the dielectric material properties and sub-wavelength metal structures. In this work, terahertz spectroscopy is employed to investigate the dielectric response and terahertz conductivity of (C4H9NH3)2PbBr4 perovskite. An efficient THz radiation modulator is realized based on (C4H9NH3)2PbBr4 decorated metastructure.

Nonlinear optics with 2D materials

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In this talk, I will discuss our recent results on nonlinear optics with 2D layered (e.g., graphene [1-2], transition metal dichalcogenides [2-4], and black phosphorus [5-6]) materials. These results show advantages of utilizing low-dimensional nanomaterials for various photonic and optoelectronic applications, such as high-purity quantum emitters [7], wavelength converters [1-4], and actively [8] and passively [1,5] mode-locked ultrafast lasers. Further, I will present our recent advances employing hybrid structures, such as two-dimensional heterostructures [1], plasmonic structures [9-10], and silicon/fibre waveguides integrated structures [9-10].

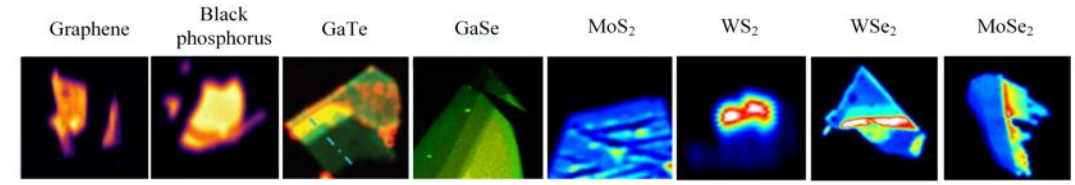

Fig. 1. Nonlinear optical images of different two-dimensional layered materials [10]

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SYMPOSIA 6 – CHEMISTRY

Two dimensional ferroelectric films

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Two-dimensional (2D) ferroelectrics has attracted interests recently for nonvolatile memory applications and can be used to construct ferroelectric schottky diode or ferroelectric tunneling diode, with promise of fast switching speed, high on-off ratio and non-destructive readout. 2D Indium selenide (In_2Se_3), which has modest band gap and robust ferroelectric properties stabilized by dipole-locking, has recently emerged as an excellent candidate for ferroresistive memory applications. To address the current bottleneck in large scale synthesis, we report the molecular beam epitaxy of large area monolayer α-In_2Se_3 on graphene and demonstrate its use in ferroelectric Schottky diode by employing gold as the top electrode. Polarization-modulated Schottky barriers across these interface exhibits giant electroresistance ratio of 3.9×10^6, with readout current density of >12 A/cm^2, which is more than 200% higher than the state-of-the-art. Our MBE growth method allows high quality ultrathin film of In_2Se_3 to be made readily, enabling the fabrication of novel 2D ferroelectric semiconductor memory junction for the advancement of information storage technologies. We have also studied another 2-D ferroelectric material SnS. STM studies reveal a spontaneous electric polarization along the in-plane armchair direction of orthorhombic SnS, and the horizontal depolarization field is mitigated by an out-of-plane buckling mechanism unique to 2D materials. In particular, ferroelectric switching is demonstrated in SnS-based lateral memory devices, and the atomically-thin nature of SnS crystals enables tuning of the hysteresis loops by a bottom-gate electrode. Our work reveals tunable in-plane ferroelectricity in ultrathin SnS films.

Graphene oxide thin film based in vivo device for continuous monitoring of interferon-γ in inflammatory mice

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Cytokine sensing is challenging due to their typically low abundances in physiological conditions. Nanomaterials fabricated interfaces demonstrated unique advantages in ultrasensitive sensing. Graphene oxide (GO), with its exceptional physical and chemical properties and biocompatibility, holds a tremendous potential for sensing applications. In this study, GO, acting both as the electron transfer bridge and the signal reporter, was attached on the interface to develop an amperometric sensing device based on structure-switching aptamers for long-term detection of cytokines in a living organism. The device incorporates a single layer of GO acting as a signal amplifier on glassy carbon electrodes. The hairpin aptamers specific to interferon-γ (IFN-γ), which were loaded with redox probes, are covalently attached to GO to serve as bio-recognition moieties. IFN-γ was able to trigger the configuration change of aptamers while releasing the trapped redox probes to introduce the electrochemical signal. This *in vivo* device was capable to quantitatively and dynamically detect IFN-γ down to 1.3 pg mL^{-1} secreted by immune cells in cell culture medium with no baseline drift even at high concentration of other nonspecific proteins. The biocompatible devices were also implanted into subcutaneous tissue of enteritis mice, where they performed precise detection of IFN-γ over 48 hours without using physical barriers or active drift correction algorithms. Moreover, the device could be reused even after multiple rounds of regeneration of the sensing interface.

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Preparation and application of 1T'-PHASE $ReS_{2x}Se_{2(1-x)}$ (x = 0 – 1) nanodots for hydrogen evolution reaction

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Layered transition metal dichalcogenides (TMDs) such as MoS_2 and WS_2 are well known for their ability to catalyze hydrogen evolution reaction in water splitting process. Many methods have been employed to control the structure of TMDs in order to enhance their electrocatalytic performance, most commonly by making bulk crystals into nanosheets or nanodots and simultaneously engineering the defects, strain and crystal phases of the resulting nanomaterials [1-3]. The crystal phase control and the formation of vacancies are among the most important factors responsible for the high activity of TMD nanomaterials toward HER [2]. However, most of the studies focused on TMDs with symmetrical structures including trigonal prismatic 2H and octahedral 1T phase. As a result, the mechanism of asymmetrical TMD catalysts toward HER remains inconclusive. In our work, we successfully prepared alloyed $ReS_{2x}Se_{2(1-x)}$ nanodots with native 1T' phase and investigated the influence of their distorted structure on HER performance [4]. The preparation of the nanodots was done successively by chemical vapor transport and Li-intercalation method. The chemical exfoliation process induced the formation of different types of anion vacancies on the ultrasmall nanodots, with the low-site S vacancies having the highest impact on the activity of the alloyed nanodots due to their free energy being close to 0.00 eV. The excellent HER performance of TMD nanomaterials was observed in our ReSSe (x=0.5) nanodots, with a low overpotential of 84 mV at the current density of 10 mA cm^{-2}, a Tafel slope of 50.1 mV dec^{-1} and a long-term stability.

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Strong interlayer coupling and new phases of two-dimensional optoelectronic semiconductor InSe

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Recently, few-layer InSe as a post-transition metal chalcogenide has been synthesized via physical and chemical methods, exhibits promising characteristics for optoelectronic applications. High tunability in the band gap with varying layer thickness, carrier mobility reaching 10^3 $cm^2V^{-1}s^{-1}$ at room temperature have been reported, which is the highest among TMDCs and superior to black phosphorus. This paper consists of two aspects of studies:
(i) Previous studies on 2D InSe have illustrated the evolution of electronic structure with thickness, which is generally attributed to quantum confinement effect. In this topic, by a fitting of one dimensional finite potential well model of band-edge heights, we find that the coupling effect in layered InSe is not as weak as generally believed. The existence of strong interlayer coupling (Fig. 1) also manifests itself in three aspects with increasing thickness: indirect-to-direct band gap transitions, fan-like phonon splitting of shear and breathing modes, and strong layer-dependent carrier mobilities.[1]
(ii) By using the global structure searching method and first-principles calculations, we have identified two new InSe phases (simply as T-InSe and R-InSe) that are certified as the thermodynamic-stable and kinetic-stable structures. They are formed by the centrosymmetric monolayer (Fig. 2d) under different stacking orders, also, they possess the broadband photoresponse, visible phonon frequency shifts, and excellent transport properties that are comparable to β-InSe and γ-InSe.[2]

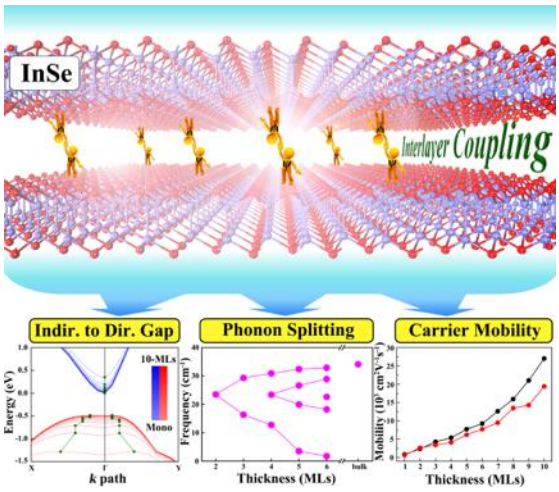

Fig. 1. Evolutions of the properties associated with the interlayer coupling (band-edge position, phonon frequency and carrier mobility) with varying thickness.

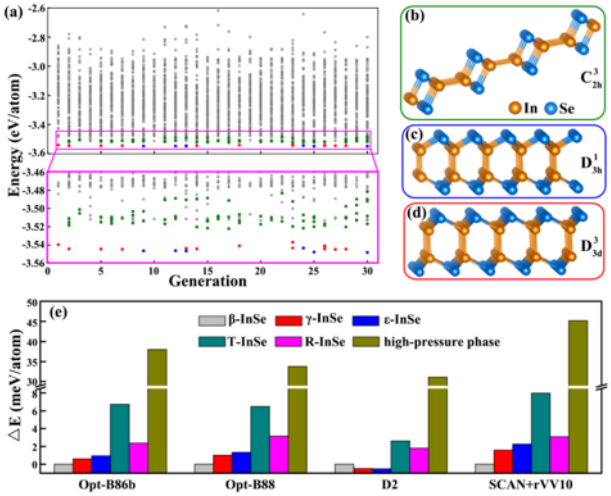

Fig. 2. Energy of explored structures as a function of generation for the structure search and the energy difference of InSe phases under different vdWs functionals of first-principles calculations.

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Heavy-metal-free 2D semiconductor nanoplatelets: synthesis, growth mechanism and applications

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Hybrid nanomaterials provide a freedom to achieve heterostructures with controlled functionalities and predictable linkages owing to their synergistic interactions. Here, we have developed a synthetic strategy that produced hexagonal shape nanoplatelets (NPLs) of Au-Fe_7S_8 with Au embedded inside them by means of a seeded growth method. By using thiol-capped Au nanoparticles (NPs) as a seed, chemoselective nucleation of iron precursor was facilitated, leading to the formation of two-dimensional (2-D) Au-Fe_7S_8 NPLs. The injection temperature and surface ligand of the seed (Au) were two critical factors that determined the structure and final morphology of the Au-Fe_7S_8 NPLs. This strategy was further expanded using Ag NPs as the seed to construct heterodimers, producing Ag_2S-Fe_7S_8 heterostructures. The as-synthesized 2-D Au-Fe_7S_8 NPLs were used as the catalyst in the hydrogen evolution reaction (HER), showing its potential as an electrocatalyst.

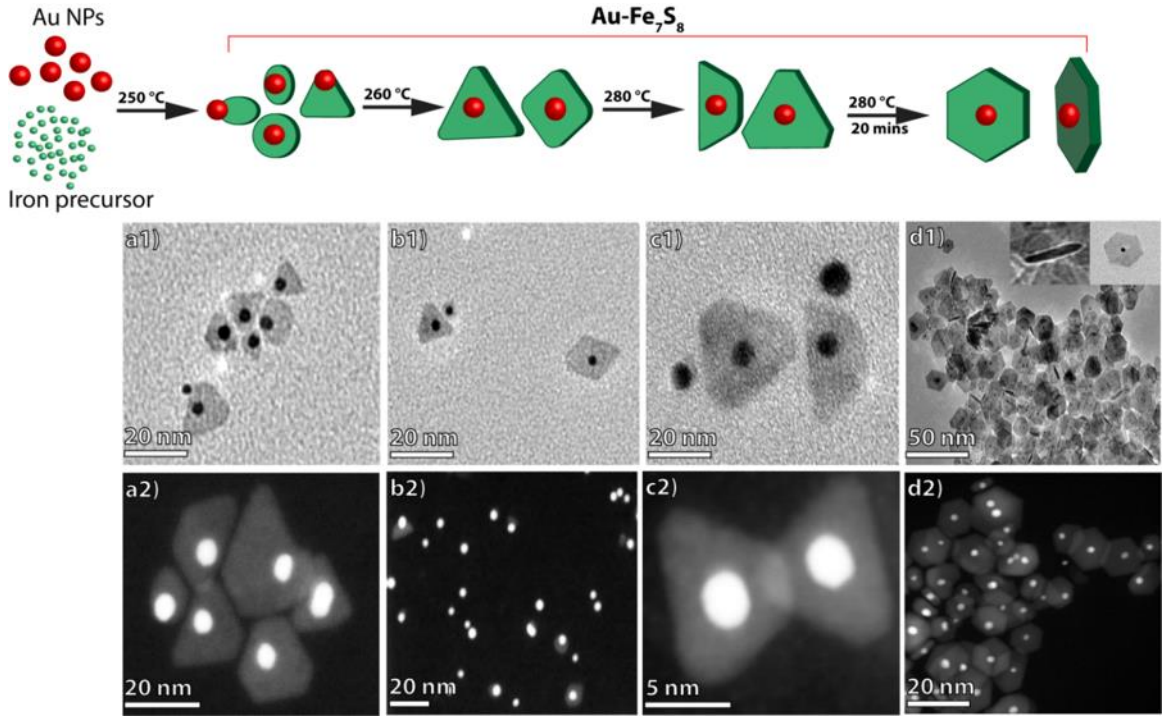

Fig. 1. Stepwise schematic representation of the formation of hybrid hexagonal shape heterodimers of Au-Fe_7S_8 along with the temperatures and reaction time. Representative TEM and HAADF-STEM images of the aliquots show Au-Fe7S8 at (a1,-a2) 250, (b1-,b2) 260, (c1-,c3) 280 and (d1-,d2) 280 °C after 20 mins.

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SYMPOSIA 6 – SYNTHESIS

Liquid metals from metallic core to two-dimensional skin

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Liquid metals and their alloys are extraordinary materials with rich physics and chemistries. Yet our knowledge about them is inadequate and their usage has largely remained limited to centuries-old conventional applications. This talk presents some of the novel concepts that liquid metals can offer and present some of the efforts for the unification the scattered works on liquid metals that have emerged in recent years. In addition to conventional applications, liquid metals have been explored as solvents for reintroducing their unique chemistry and their cores and skins have been investigated as reaction media to create new materials. Fundamental observations were pursued to harness the power of electron-rich liquid metallic environments. The findings were used for creating materials and systems of superior functional applications. The autors will present the progress of the work on liquid metals in their group to date that ranges from applications in microfluidics to incorporating liquid metals as reaction media for the synthesis of low dimensional metal compounds.

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Taking inspiration from biology to preserve photo-sensitive 2D materials against ambient oxidation

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Recent developments have seen a keen interest in 2D materials for a variety of applications [1]. However, the high reactivity of some of these materials in ultrathin morphologies has posed challenges in keeping them stable enough for deployment in practical devices. Few-layer black phosphorous (BP), commonly known as phosphorene, is one of such materials that face rapid ambient degradation. The most common strategies employed to protect BP have relied upon preventing its direct exposure to the environment which has practical challenges. Motivated by these observations, our work has attempted to understand the mechanisms of photo-oxidative damage to BP [2,3], and has tried to identify biological processes through which nature overcomes the issues of photooxidative insults. These insights have allowed us to develop a new approach that permits photosensitive 2D materials to remain stable without requiring their isolation from the ambient environment [4]. In particular, our work draws inspiration from the unique ability of the biological systems to avoid photo-oxidative damages caused by reactive oxygen species (ROS) by utilising antioxidant pathways. Since BP and other 2D materials undergo similar photo-oxidative degradation, we could employ imidazolium-based ionic liquids as quenchers of these damaging species on the BP surface (Fig. 1). This chemical sequestration strategy allowed BP to remain stable for over three months while retaining its key electronic characteristics. This study opens opportunities to practically implement BP and other environmentally-sensitive two-dimensional (2D) materials for next-generation nanophotonic and nanoelectronic applications.

Wafer scale synthesis of two dimensional $GAPO_4$ from liquid metal featuring a large out of plane piezoelectric response.

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Two dimensional (2D) piezotronics can significantly benefit from the emergence of temperature independent crystals featuring high piezoelectric coefficients. Gallium phosphate ($GaPO_4$) is an archetypal piezoelectric material with wide-ranging industrial applications. This material does not naturally crystallize in a stratified structure and hence cannot be exfoliated using conventional methods. Here we present a low temperature liquid metal 2D printing and synthesis strategy to achieve this goal. We exfoliate and surface-print the interfacial oxide layer of liquid gallium, followed by the vapor phase reaction between the gallium oxide sheet and phosphoric acid. The method offers access to large-area, uniform wide band gap 2D $GaPO_4$ nanosheets of unit cell thickness (~1.1 nm), while featuring lateral dimensions reaching centimeters. The unit cell thick nanosheet presents a large effective out-of-plane piezoelectric coefficient of 7.5 ± 0.8 pm/V. The developed liquid metal based process is also suitable for the synthesis of free-standing 2D $GaPO_4$ nanosheets over micron sized cavities. The low temperature process is compatible with a variety of electronic device fabrication procedures, providing a route for the development of 2D piezoelectric materials for sensing and energy harvesting.

Wet-chemical synthesis of ultrathin two-dimensional metallic nanosheets for (electro)catalytic applications

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Inspired by the success of traditional two-dimensional (2D) nanomaterials such as graphene, ultrathin 2D metallic nanosheets have attracted tremendous research interest. Featuring their high surface area-to-volume ratio and high density of exposed atoms on their surface, 2D metallic nanosheets have exhibited promising (electro)catalytic performances, compared to their bulk counterparts and nanostructures in other dimensionalities. Wet-chemical synthesis is a facile method to prepare 2D metallic nanosheets with control over their compositions, architectures, crystal phases, etc. As an example, ultrathin PdCu alloy nanosheets with various Cu/Pd atomic ratios and thickness of 2.8 ± 0.3 nm are prepared by the wet-chemical one-pot synthesis strategy under mild conditions. Impressively, post-treatment with ethylenediamine (EN) effectively removes the capping agent, oleic acid, to expose the catalytically active sites. The EN-treated PdCu alloy nanosheets show excellent electrocatalytic activity toward formic acid oxidation, compared to the previously reported Pd-based catalysts measured under similar conditions. [1] Besides alloy nanosheets, ultrathin Pd@Ru nanosheets with lateral size of 7.8 ± 0.7 nm and thickness of ~1.9 nm are prepared by the wet-chemical seed-mediated method. Strikingly, unlike the conventional core-shell structure with a complete coverage of shell over the core atoms, Pd@Ru nanosheets expose both core and shell atoms, i.e., Pd nanosheets are incompletely covered by the submonolayered Ru. Impressively, the Pd@Ru nanosheets exhibit excellent catalytic activity toward the reduction of 4-nitrophenol and the semihydrogenation of 1-octyne, compared to the pure Pd nanosheets and Ru nanosheets. [2] The aforementioned studies reveal the promising role of ultrathin 2D metallic nanosheets as (electro)catalysts. We believe the strategies presented here may shed light on the preparation of novel 2D metallic nanosheets with desired compositions, architectures and morphologies to better benefit the (electro)catalysis fields.

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Single-atom cobalt covalently bound to distorted 1T-MoS_2 for unprecedented hydrogen evolution catalysis

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The grand challenge in the development of atomically dispersed metallic catalysts is their low metal-atom loading density, uncontrollable localization and ambiguous interactions with supports, posing difficulty in maximizing their catalytic performances [1]. Herein, we achieve a conceptionally new interface catalyst consisting of single cobalt atoms covalently bound onto distorted 1T MoS_2 nanosheets (SA Co-D 1T MoS_2) through a new assembly/leaching strategy. We find that the phase transformation of MoS_2 from 2H to D-1T, induced by the strain from lattice mismatch, and the formation of Co-S covalent bond between Co and MoS_2 during the assembly of Co nanodisks on MoS_2 nanosheets, are the essential factors in forming the highly active single-atom catalyst. SA Co-D 1T MoS_2 achieves unprecedented Pt-like hydrogen evolution reaction (HER) catalysis with high long-term stability, which represents the best performance among the reported non-noble-metal catalyst for HER [2]. The combined data from an active-site blocking experiment together with density functional theory (DFT) calculations reveal that the single-atom Co in SA Co-D 1T MoS_2 is the principal catalytic centre for HER catalysis.

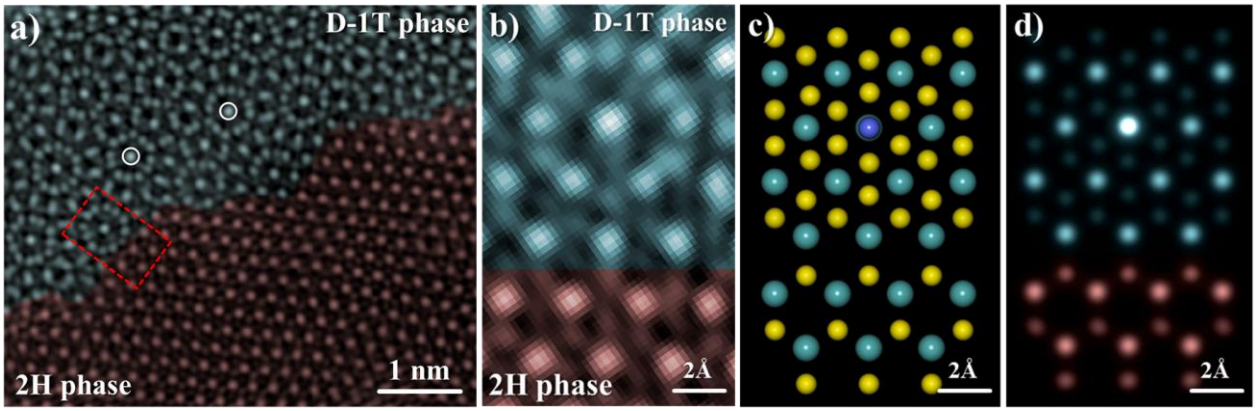

Fig. 1. a, Aberration-corrected HAADF-STEM image of SA Co-D 1T MoS_2, showing the obvious junction between SA Co-D 1T MoS_2 (dark cyan) and pristine 2H MoS_2 (wine). The *inset* shows the HRTEM and EELS spectrum of SA Co-D 1T MoS_2. b, Enlarged HAADF-STEM image in the red square area of a. c, Theoretical model and d, simulated STEM images using QSTEM simulation software**.**

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SYMPOSIA 7 – PHYSICS

Deformed graphene membranes: from electronic waveguides to valley filters

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As an atomically thin membrane, graphene is highly flexible and strain engineering can be used to control its electronic properties. Wrinkled or rippled graphene on various substrates as well as suspended samples, reveal inhomogeneous charge distributions whose origin can be traced back to the underlying strain fields affecting electron dynamics. Furthermore, scanning tunneling microscopy measurements on locally deformed samples demonstrated electron confinement with peculiar charge distributions that break sublattice symmetry [1]. The phenomena that differentiates continuous carbon atoms in each unit cell, results in local valley currents with important applications in the field of valleytronics, i.e. the manipulation of the valley degree of freedom for electronic purposes. Because valley filtering properties in these structures is, however, highly dependent on the type of deformation and setups considered, it is important to identify the relevant factors determining optimal operation and detection of valley currents. We present a comparison of two typical deformations commonly found in graphene samples: local centro-symmetric bubbles and extended wrinkles or folds. While both are predicted to produce regions with confined charge, the extended fold geometry serves as an electronic wave-guide [2] as revealed in recent transport measurements [3]. After reviewing these results, I present an analysis of the dependence of charge confinement and valley polarization on the geometrical parameters of these model deformations, and discuss their experimental realizations. Our study reveals that extended deformations act as better valley filters in broader energy ranges and present more robust features against variations of geometrical parameters and incident current directions [4].

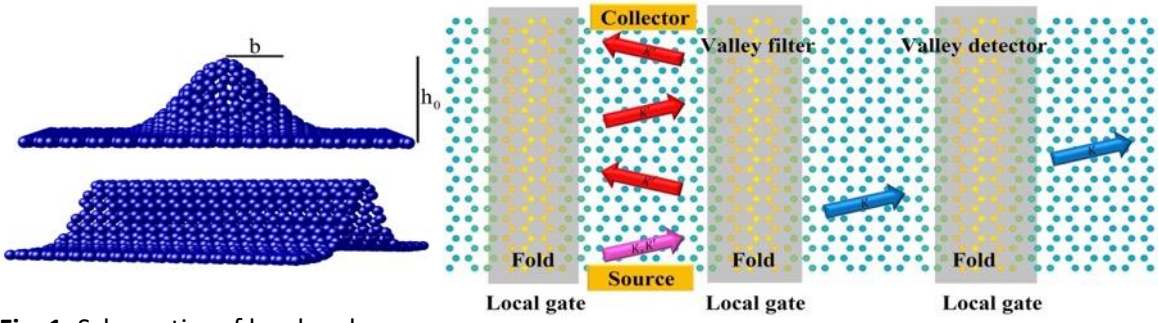

Fig. 1. Schematics of local and extended deformations. Right panel: Proposed setup for valley filtering and detection of polarized beams.

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Quantum capacitance and spin susceptibility of HGTE quantum wells

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The two-dimensional (2D) topological insulators (TI) realized in inverted semiconductor quantum wells exhibit unusual electric-transport properties [1] that have attracted great interest [2]. TI behavior is also found in other 2D and bulk materials [2,3]. The potential for interesting interplays between a TI's electronic and magnetic degrees of freedom has motivated our detailed theoretical study of electronic compressibil-ity [4] and spin response [5] for electrons in the mercury-telluride-based 2D TI. Our work reveals uncon-ventional properties that distinguish this paradigmatic TI material from all other currently known 2D elec-tronic systems. See Fig. 1. We thus provide alternative means for experimental identification of the topo-logical regime and extend current knowledge about the fundamentals of many-particle collective behav-iour in solids.

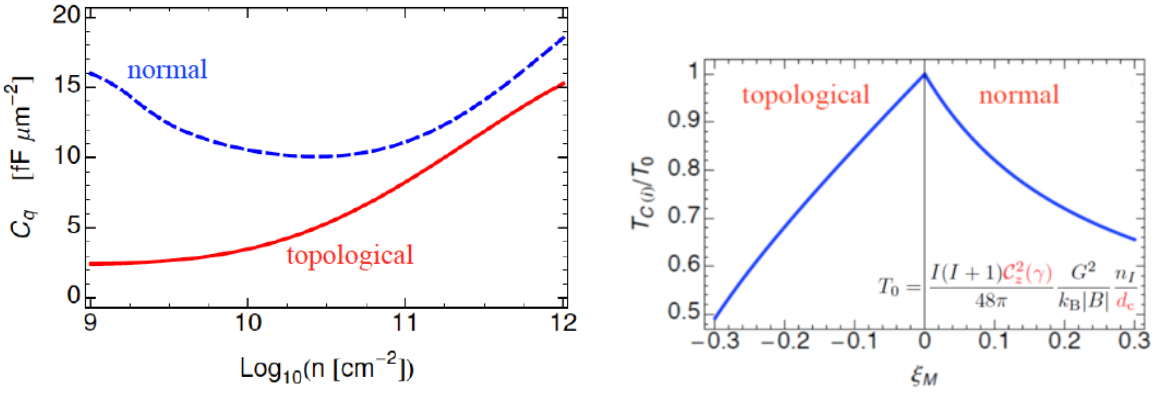

Fig. 1. Distinctive collective-electron properties characterize the topological and normal regimes of a HgTe quantum well. Left panel: Quantum capacitance C_q plotted as a function of the 2D-electron sheet density n. Notice the opposite trends exhibited at low density. Right panel: Transition temperature T_c for RKKY-mediated ferromagnetism of magnetic dopants in a HgTe quantum well, plotted as a function of the quantum-well gap parameter ξ_M M. Here M<(>)0 corresponds to the situation with (non-)inverted bands.

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Influence of C-rich domain in h-BN on carrier transport of graphene/h-BN van der Waals heterostructures

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Hexagonal boron nitride (h-BN) is the only insulating 2D material to construct van der Waals heterostructures, thus it has been widely used as an atomically-flat substrate for various 2D materials. Although h-BN crystal grown under high temperature and high pressure has very high crystal quality, carbon-impurity-rich domain has been found to be created in a central region of the crystal. The C-rich domain is unable to be distinguished with an optical microscope nor AFM, but can be recognized by measuring emission spectrums; The domain area emits light with a wavelength of 320 nm corresponding to carbon impurity, whereas h-BN exciton emission is observed at 210 nm. What is remarkable here is that these domains still exist even after exfoliation. It is thus very important to investigate the influence of the C-rich domain on carrier transport and optical properties of 2D materials above, particularly when van der Waals superlattices are fabricated using our automatic robotic assemble systems [1]. In this work, we study the effect of C-rich domain on transport properties of graphene by fabricating h-BN/graphene/h-BN van der Waals heterostructures with graphene across the border between domain and normal h-BN flake. First, we distinguished h-BN flakes with C-rich domain by the ultraviolet light photo luminescence (UV-PL), and placed graphene on the border of C-rich domain region. After capping the graphene with another h-BN layer, we put electrodes to be able to compare the transport properties of graphene inside/outside of the C-rich domain. The carrier mobility of graphene inside C-rich domain at 1.5 K was 50,000 cm^2/Vs, whereas the carrier mobility exceeded 100,000 cm^2/Vs in graphene outside of C-rich domain. Under high magnetic field, characteristic bending of Landau-fan diagram is observed in graphene/C-rich domain at the electron-doped side, suggesting that carbon atoms in h-BN generate an impurity level in the graphene.

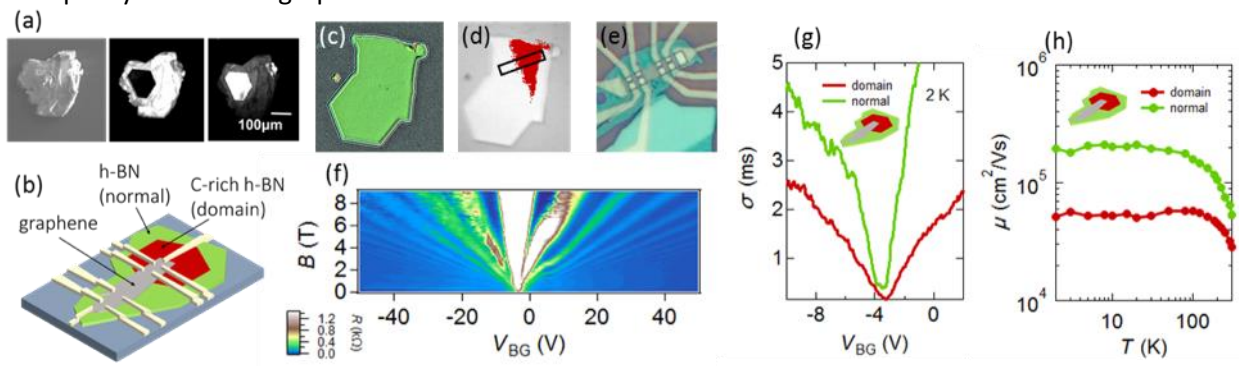

Fig. 1. (a) Impurity-rich domain in as-grown h-BN crystal recognized with CL images at 210 nm (center) and 320 nm (right). **(b)** Schematic image of sample structure. **(c)** Optical micrograph of the h-BN flake on SiO_2 substrate. **(d)** Domain region (red area) detected by UV-PL. **(e)** Graphene channel is located on the black square in (d). **(f)** Landau fan diagram of graphene on C-rich h-BN domain. **(g)** Conductance of graphene on normal and C-rich h-BN regions. **(h)** Carrier mobility of graphene on normal and C-rich h-BN regions.

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Quasiparticle interference study of topological semimetal ZrSiS due to surface defects at 4.5 K

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3D topological semimetals are emerging as a novel class of materials that host gapless linear dispersions within their bulk and feature novel quasiparticle responses and surface states. Different from the point nodes of Dirac or Weyl semimetals [1,2,3], Dirac nodal line semimetals (DNLSs) possess close loops in the Brillouin zone along which conduction band and valence band touch (the nodal line). ZrSiS, as an air-stable in its bulk form, easily-grown DNSL [4], has been experimentally studied extensively, showing exciting quasiparticle transport such as unusually large magnetoresistance and mobility [5], and enhanced electron correlations [6], as well as effective pseudospin scattering [7]. Here, we show quasi-particle scattering and interference (QPI) at various defects on the cleaved surface (001) of ZrSiS single crystals, studied by Fourier transform scanning tunneling spectroscopy (FT-STS) at 4.5 K. Our results are expected to aid to understand basic aspects that are specific to DNLSs, a research hotspot in condensed matter physics.

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Interaction-driven finite-temperature phase transitions in graphene multilayers

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Here, we investigate transport properties of ultraclean suspended graphene multilayers (Bernal-stacking) at zero magnetic field (*B=0*), and show that they exhibit strong effects of Coulomb interactions that lead to broken symmetry states at charge neutrality point [1,2]. More interestingly, by realizing that in such high-quality devices, the width of the resistance peak is sensitive enough to capture the change of density of states with temperature (Fig. 1) [3,4], we were able to find that the system undergoes phase transitions at finite temperature (T_c) which increases—systematically—with the layer thickness from 12 K for bilayers to ~90 K for 6-layers [3]. These findings represent the first unambiguous experimental proof of the finite-T_c phase transitions driven by Coulomb interactions at *B=0* in low-dimensional systems. We explain the phenomenon in terms of the minimal tight-binding model augmented with interaction-induced staggered layer potential which gaps only the bilayer-like bands not the monolayer's which is present only in odd-layers [1-3]. Furthermore, this method allows us to find—for the first time—the clear signature of the gapped bilayer-like band in Bernal-trilayer graphene which is expected from our model, even though the system remains conducting at low *T* due to ungapped monolayer band. We further discuss implications of our results in understanding various interactions effects in graphene layers as well as in other low-dimensional systems.

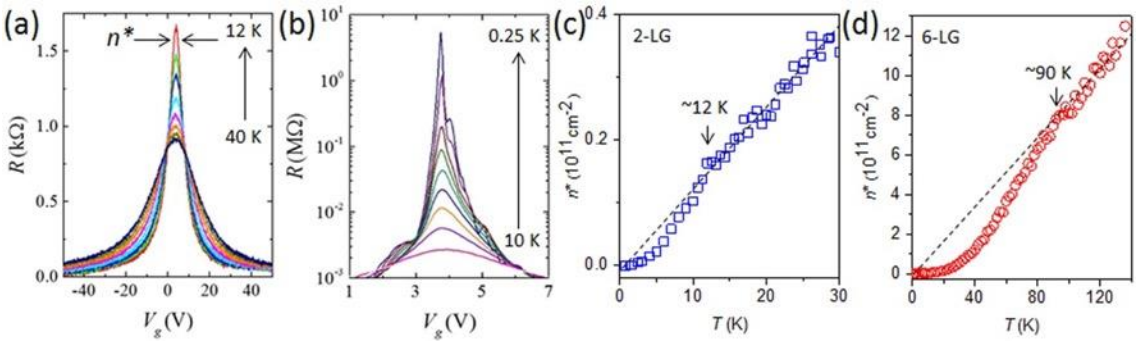

Fig. 1. Identifying T_c in 2- and 6-LG. (a,b) Gate-dependence of the resistance measured in suspended bilayer graphene above (a) and below 12 K (b), exhibiting a clear insulating behaviour at charge neutrality upon lowering *T* below 12 K. (c,d) Width of the resistance peak (*n**; see a panel (a)) as a function of *T* shows a suppression starting at $T_c \approx$ 12 K for bilayer (c) and ~90 K for 6-layer (d) below the density of thermally excited charge carriers expected for the ungapped system (linear dashed lines).

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SYMPOSIA 7 – DEVICES

Electrical control of spin-valley photocurrent in a monolayer semiconductor by circular photogalvanic effect

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In spintronic devices optical methods such as the circular photogalvanic effect (CPGE) can be utilized to drive spin currents using circularly polarized light, creating imbalanced spin populations of photo-excited carriers and spin photocurrent at room temperature. Monolayers of the group VI transition metal dichalcogenide (TMDC) provide a unique direct bandgap semiconductor platform to explore spintronics because of the intrinsic link between polarized optical transitions and the spin texture of free and bound carriers in the band structure. By exploiting valley-contrasting magnetic moment and berry curvature which have opposite signs between two degenerate valleys, valley-locked spin-polarized photocurrent by CPGE have been demonstrated in TMDC recently [1-3]. An interesting next step would be to electrically manipulate spin photocurrents in monolayer TMDC devices in which the requisite symmetry for CPGE generation is intrinsic to the material. Here, we report electric tuning of the magnitude and the polarization degree of spin photocurrent in monolayer MoS_2 devices at room temperature without any direct magnetic methods involved. We show that the magnitude and polarization degree of spin-polarized photocurrent can be modulated strongly by source-drain voltage and electrostatic gate tuning. Gate-controlled charging induces substantial screening for defects, which is confirmed by the quenching of defect emission in gate-dependent photoluminescence (PL) experiments. This screening effect reduces defect-associated intervalley scattering, which can enhance the generation of CPGE spin-valley photocurrent and thus spin photocurrent polarization. This capability for tuning and optimization could be useful for future spin-related devices made from large-area TMDC thin films and heterostructures.

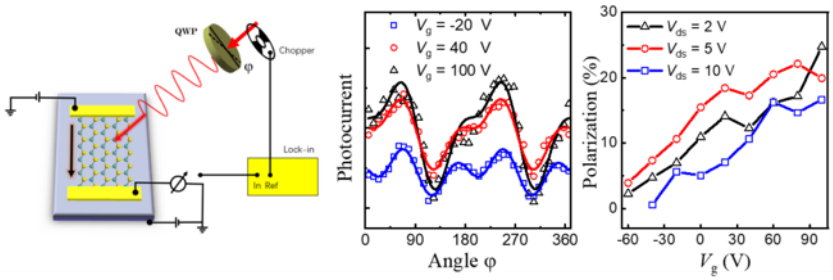

Fig. 1. (left panel) Schematic of the experimental set-up and device geometry. (middle panel) Gate-dependent CPGE spin photocurrent. (right panel) The modulation of the spin photocurrent polarization degree *P by* gate voltage.

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On-surface synthesis of organic 2D materials

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One of the goals of nanoscience is achieving precise control over the structure and function of nanoscale architectures at surfaces. Bottom-up approaches using molecular building blocks present a flexible and intuitive approach to this challenge (Fig. 1). Combining the Lego-like modularity of molecules with the epitaxial and reactive influences of surfaces creates a range of opportunities to build exciting new nanoarchitectures. On-surface synthesis can potentially allow for the fabrication of extended covalent nanostructures with enforced planarity and interesting properties. I will discuss our recent work in studying the reactions of halogenated [1] and carboxylated [2] molecules at metal surfaces. The polymeric product is sensitive to a range of parameters, and we have been focusing in particular on developing an understanding of how the coupling reaction and its by-products influence crystallinity.[3] We have variously employed scanning tunneling microscopy, photoelectron spectroscopy and near-edge x-ray absorption fine structure to gain a well-rounded insight into the process and products.

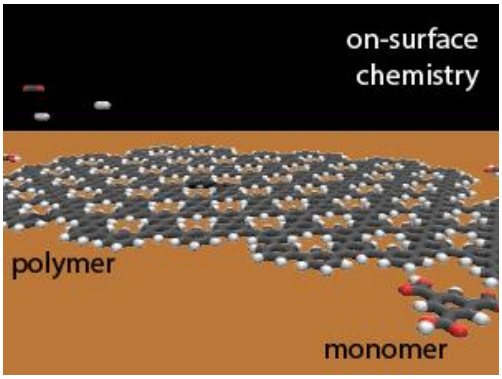

Fig. 1. Conceptual representation of on-surface synthesis of 2D organic materials. Molecular precursors are activated and coupled on the surface to form an extended low-dimensional network.

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High performance electronics and optoelectronics based on two dimensional layered films

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Two dimensional layered films such as graphene and layered inorganic materials are promising for future nanoscale electronics and optics. We also performance of dielectric layer and metal contacts on the performances of field effect tranisistors based on InSe. We discover that carrier scattering from chemical impurities of hydroxyl groups and absorbed water molecules at oxidized dielectric plays a central role in determining the mobilities of 2D layered semiconductors based FETs, and suppression of this carrier scatter can significantly enhance the performance of 2D layered semiconductor devices. Further, we demonstrate high performance multilayer InSe transistors on poly-(methyl methacrylate) **(**PMMA)/Al_2O_3 bilayer dielectric with a room-temperature mobility > 1000 $cm^2V^{-1}s^{-1}$, comparable to that of strained-silicon thin-film. The first GaS nanosheet-based photodetectors are demonstrated on both mechanically rigid and flexible substrates. Photocurrent measurements of InSe nanosheet phototransistors exhibit a photo-responsivity up to 10^4 $AW^{-1,}$ which exceeds that of graphene, MoS_2, or other 2D materials-based devices. Additionally, the linear dynamic range of the devices on SiO2/Si and PET substrates are 97.7dB and 78.73 dB, respectively. Both surpass that of currently-exploited InGaAs photodetectors (66 dB). Our research indicates that the two dimensional nanostructure of Indium selenide is a new promising material for high performance electronics and optoelectronics.

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Two dimensional indium sulfide with excellent optoelectronic properties

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Two dimensional (2D) post-transition metal chalcogenides is an emerging group of promising materials for high-performance electronic and optoelectronic devices [1-2]. However, the synthesis of this group of 2D materials with a lateral dimension of > 50 μm has been a challenge [3-4]. In this work we present a facile way to synthesis 2D indium sulfide (In_2S_3) from sulfurization of the surface oxide layer of a melted indium metal. 2D In_2S_3 is determined to feature p-type semiconducting behavior with a direct bandgap of ~2.9 eV, potentially offering the broad detection range from UV to visible blue light region. The 2D In_2S_3 based photodetector exhibits a very high photoresponsivity of 8364.4 AW^{-1} with an excellent external quantum efficiency of 3.7067×10^4% and a detectivity of 4.4205×10^{10} Jones. The synthesis technique is facile, scalable and holds promise for creating atomically thin semiconductors at wafer scale. Furthermore, the impressive optoelectronic properties of 2D In_2S_3 represent it a suitable candidate for future generation optical and electronic devices.

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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_2) and type-II Weyl semimetal (WSM) tungsten ditelluride (WTe_2). We observed interesting in-plane anisotropic transport and mechanical properties of ReS_2, together with its potential electronic and optoelectronic applications.[1] In thin tungsten ditelluride (WTe_2) 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/$MoS_{2-x}O_x$/graphene.[3] Our latest results on high-performance photodetectors based on atomically thin vdW heterostructures made of black arsenic phosphorus and transition metal dichalcogenides will also be presented.[4]

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SYMPOSIA 7 – CHEMISTRY

Fused aromatic organic networks form syntheses and applications

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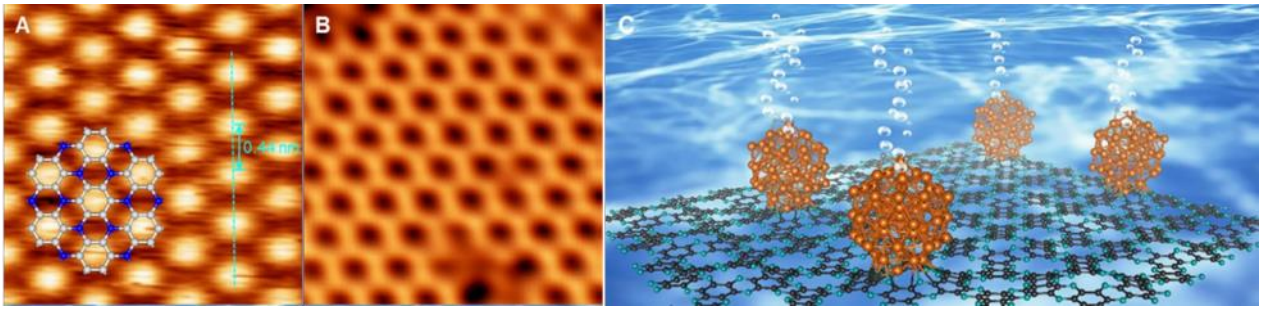
Since the discovery of graphene in 2004, 1 two-dimensional (2D) fused aromatic organic networks have attracted immense interest due to their unique electronic, optoelectronic, magnetic and electrocatalytic properties. In addition, their tunable structures and properties promise to offer more opportunities than graphene in various applications. However, even after years of intensive exploration of layered 2D materials in science and technology, facile and scalable methods capable of producing stable organic networks with uniformly decorated heteroatoms with/without holes remain limited. To overcome these issues, new fused aromatic organic networks have been designed and synthesized. They have uniformly distributed heteroatoms, 2 holes with heteroatoms 3 and transition metal nanoparticles in the holes. 4 The structures were confirmed by various techniques including scanning tunneling microscopy (STM) (Fig. 1A-1B). Based on the stoichiometry of structural units in their basal plane, they were, respectively, named as C3N, C2N and M@C2N (M = Co, Ni, Pd, Pt, Ru). Their electronic, electrical (Fig. 1C) and magnetic properties were evaluated by electrooptical, electrochemical and SQUID measurements, respectively, along with density-functional theory (DFT) calculations. Furthermore, robust three-dimensional (3D) cage- like organic networks have also been constructed and they show high sorption properties.5,6 The results suggest that these newly-developed 2D and 3D fused aromatic organic networks offer great opportunities, from wet-chemistry to device applications.



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MXene for wearable energy storage

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A recently discovered family of 2D materials called "MXene" has been used to prepare films, papers, and composites with electrical conductivity of up to ~10,000 S cm^{-1} and volumetric capacitance of up to ~1,500 F cm^{-3}. However, small sheet size (<2 µm), weak inter-sheet interactions, and lack of efficient processing have made it challenging to fabricate MXene-based fibers or yarns. Here, we present strategies to achieve fibers or yarns from the most prominent member of MXene family (Ti_3C_2). First, by coating MXene on carbon fibers, we achieve a yarn-shaped supercapacitor device with a high length capacitance of ~132 mF cm^{-1} which is higher than the literature reports (typically lower than 100 mF cm^{-1}). We then produce hybrid fibers with up to ~88 wt. % MXene using a wet-spinning technique which takes advantage of the templating role of liquid crystalline graphene oxide. The MXene hybrid fiber demonstrates excellent flexibility and a high volumetric capacitance of ~341 F cm^{-3}. By employing a biscrolling technique that traps MXene nanosheets within carbon nanotube yarn scrolls, we achieve yarns that are predominantly composed of MXene (containing up to ~98 wt. % MXene). This MXene-based yarn provides an areal capacitance of as high as ~3,188 mF cm^{-2} (volumetric capacitance ~1,083 mF cm^{-3}), which exceeds the previously recorded performance for any fiber or yarn supercapacitor electrode. The yarn supercapacitor device with the asymmetric electrode configuration reaches a maximum energy and power densities of ~61.6 mWh cm^{-3} and ~5428 mW cm^{-3} respectively. We show that the MXene-based fibers and yarns are useful for powering small electronic devices when knitted or woven into a textile. This work introduces new classes of fibers and yarns from an emerging family of 2D materials, which are excellent candidates for integration with textile-based electronics to meet the energy demands of future wearable devices.

Tunable photoluminescence in organic semiconductor/two-dimensional transition metal dichalcogenides van der Waals heterojunction

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In recent years, two-dimensional (2D) monolayer transition metal dichalcogenides (TMDs) are attracting extensive attentions due to the direct band gap and strong light-matter interaction, rendering them the potential candidates for next-generation optoelectronic devices. TMD/TMD heterojunctions have attracted enormous attention due to extraordinary optoelectronic properties [1]. However, the stacking of different TMD monolayers on top of one another to form heterojunctions is a very tough work, normally done by mechanically transferring one layer onto the other under optical microscope. On the other hand, TMD materials combined with organic semiconductors have been gaining great interest [2] owning to the advantages of organic semiconductors, such as easy processing, synthetic tunability, and mechanical flexibility. We report the photoluminescence (PL) characteristics of van der Waals (vdW) heterojunction constructed by simply depositing organic semiconductor of 3, 4, 9, 10-perylene tetracarboxylic dianhydride (PTCDA) onto two-dimensional MoS_2 monolayer. The crystallinity of PTCDA on MoS_2 is significantly improved due to vdW epitaxial growth. We observe an enhanced PL intensity and PL peak shift of the MoS_2/PTCDA heterojunction as compared with the individual MoS_2 and PTCDA layer. The synergistic PL characteristics are believed to be originated from the hybridization interaction between the MoS_2 and the PTCDA as evidenced by the density functional theory calculations and Raman measurements [3]. The hybridization interfacial interaction is found to be greatly influenced by crystalline ordering of the PTCDA film on the 2D MoS_2.

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PT/graphene foam biofilm for highly sensitive and selective in-situ adsorption and detection of superoxide anions released from living cells

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Various critical biological processes in live-cells are very important for biological science, medical diagnosis and treatment, but the investigations in particular in situ detection of the activity of small molecules with fast decay such as superoxide ($O_2^{\bullet -}$) are usually limited by disappointed performance of poor cell culture/non-sensitive detection platforms. Herein, a unique platform of Pt particles on graphene foam (Pt@GF) is developed with well-defined surface and interface properties to realize in-situ sensitive monitoring $O_2^{\bullet -}$ released from living cells. Results show the Pt particles-impregnated, cell-grown GF bioplatform renders rich and more positive steric-reaction sites for strong $O_2^{\bullet -}$ adsorption, while the negatively charged graphene surface can well trap, grow and retain cells for generating a superior biofilm. The human melanoma cells@Pt@GF bioplatform based $O_2^{\bullet -}$ biosensor can achieve a high sensitivity (1597.17 μA nM^{-1} cm^{-2}), low detection limit (10 nM), fast response (3.6 s) and good selectivity. In particular, this detection limit is the best over the reported studies with cells directly growing on biosensors. The biosensor can also successfully in-situ monitor $O_2^{\bullet -}$ released from living cells under drug stimulation. This work sheds a light for rationally designing graphene-based composite biosensors, while providing a sensitive platform to in-situ monitor $O_2^{\bullet -}$ released from living cells for biosciences research and medical diagnosis.

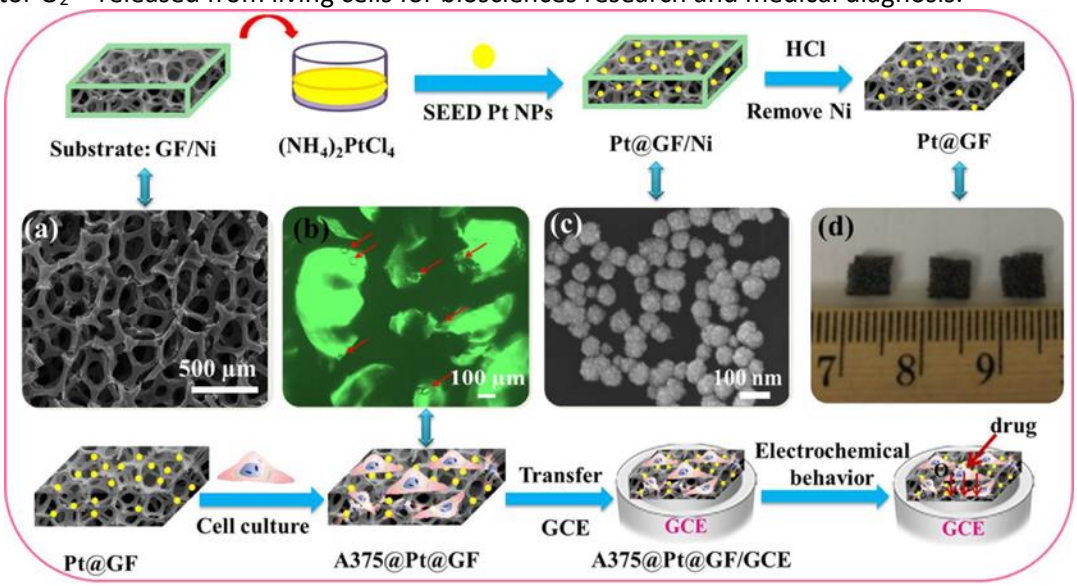

Fig. 1. Illustration of preparation of A375@Pt@GF/GCE live-cell biosensor.

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Organic photocatalysts for energy， environment and anti-tumor

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A new class of organic supramolecular photocatalysts with full visible spectrum response has been successfully developed. The texture structure, crystal structure, photoelectric physicochemical properties, organic electron energy band structure, photocatalytic oxidation and anticancer properties can be adjusted via molecular structure and stacking structure. The degradation ability, water splitting ability and anticancer came from the HOMO and LUMO level. The photocatalytic activity came from molecular dipole, ordered stacking and nanostructure. The full spectrum responsive supramolecular photocatalyst, SA-TCPP has been synthesized via an easy-conducted π-π stacking. The SA-TCPP can powerfully spilt water to hydrogen and oxygen at 40.8 and 36.1 μmol·g-1·h-1 without co-catalyst. The organic pollutants can be efficiently mineralized by the SA-TCPP under visible light irradiation. The degradation performances of SA-TCPP were over 10 times better than the inorganic photocatalysts. The single crystalline structure of π-π stacking promoted the transportation and separation of photogenerated carriers. Supramolecular photocatalyst SA-TCCP of bio-safe amount, targeted injection into the solid tumor inside, completely kill the tumor within 10 min under the deep penetration of red light (600-700 nm) irradiation. Photogenerated holes work as the most significant radical in the photocatalytic therapy process, which is abundant on the surface of photocatalyst in cytoplasm. The solid tumors was completely removed via photocatalysts injection and red-light irradiation.

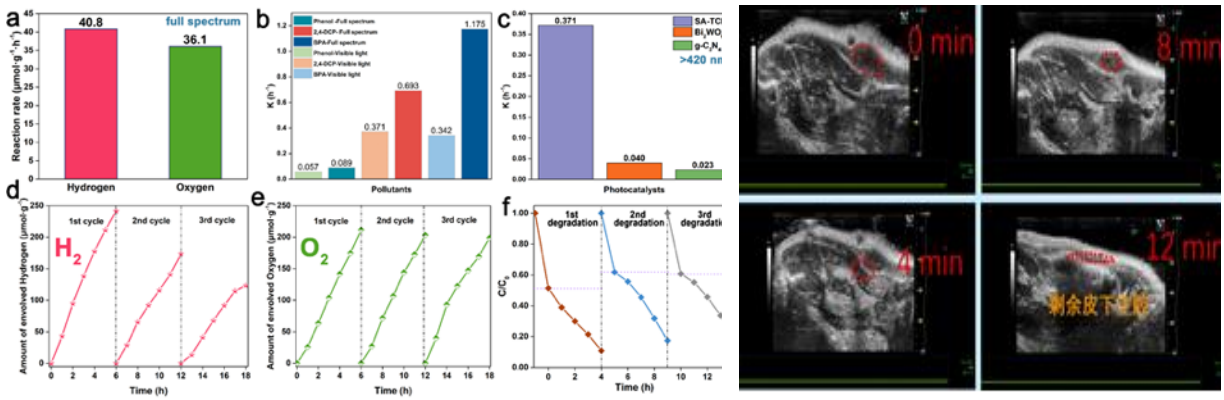

Fig. 1. The performances for degradation， production of H_2 and O_2 and anti-tumor via photocatalysis of superamolecular photocatalysts under visible light

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SYMPOSIA 7 – SYNTHESIS

Optical spectroscopic study of two-dimensional layered materials and their heterostructures

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Two-dimensional (2D) layered materials including graphene, transition metal dichalcogenides (TMDs), and other atomically thin layers, have aroused great attentions due to their rich physics and novel properties as well as great potential applications in nanoelectronics and optoelectronics. In this talk, I will present our recent works on optical spectroscopic study of two-dimensional layered materials and their heterostructures from the view of the interaction between light and phonon, electron, exciton. The results presented here are highly relevant to the application of 2D materials and their heterostructures in nanoelectronic and optoelectronic devices, and also help in developing a better understanding of the physical and electronic properties of those 2D materials.

Tunable room-temperature single-photon emission in atomically thin materials

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Quantum technologies require robust and photostable single photon emitters (SPEs) that can be reliably engineered. Hexagonal boron nitride (hBN) has recently emerged as a promising candidate host to bright and optically stable SPEs operating at room temperature.(1) However, the emission wavelength of the fluorescent defects in hBN has, to date, been shown to be uncontrolled.(2) The emitters usually display a large spread of zero phonon line (ZPL) energies spanning over a broad spectral range (hundreds of nanometers), which hinders the potential development of hBN-based devices and applications. We demonstrate bottom-up, chemical vapor deposition growth of large-area, few-layer hBN that hosts large quantities of SPEs: ~100 per 10 × 10 μm^2. Remarkably, more than 85% of the emitters have a ZPL at (580 ± 10) nm—a distribution which is over an order of magnitude narrower than previously reported.(3) . Exploiting the high density and uniformity of the emitters, we demonstrate electrical modulation and tuning of the ZPL emission wavelength by up to 15 nm.

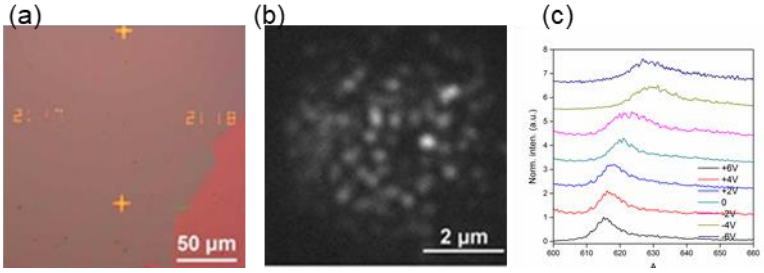

Fig. 1. a. An optical image shown CVD hBN film transferred to the Si substrate. **b**. a wide-field EMCCD image shows the density of the emitters from CVD-grown hBN. **c**. Modulation ZPL of a SPE which can be tuned by up to 15 nm using a polymer electrolyte in the range of ±6 V.

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Efficient and layer-dependent exciton pumping across atomically-thin organic-inorganic type-I heterostructures

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The fundamental light-matter interactions in monolayer transition metal dichalcogenides might be significantly engineered by hybridization with their organic counterparts, enabling intriguing optoelectronic applications. Here, we fabricated atomically thin organic-inorganic (O-I) heterostructures, comprising of monolayer $MoSe_2$ and mono-/few-layer single-crystal pentacene samples. These heterostructures show type-I band alignments, allowing the efficient and layer-dependent exciton pumping across the O-I interfaces.[1] The interfacial exciton pumping has much higher efficiency (>86 times) than the photoexcitation process in $MoSe_2$, although the pentacene layer has much lower optical absorption than $MoSe_2$. This highly enhanced pumping efficiency is attributed to the high quantum yield in pentacene and the ultra-fast energy transfer between the O-I interface. Furthermore, those organic counterparts significantly modulate the bindings of charged excitons in monolayer $MoSe_2$ via their precise dielectric environment engineering.[2,3] Our results open new avenues for exploring fundamental phenomena and novel optoelectronic applications using atomically thin O-I heterostructures.

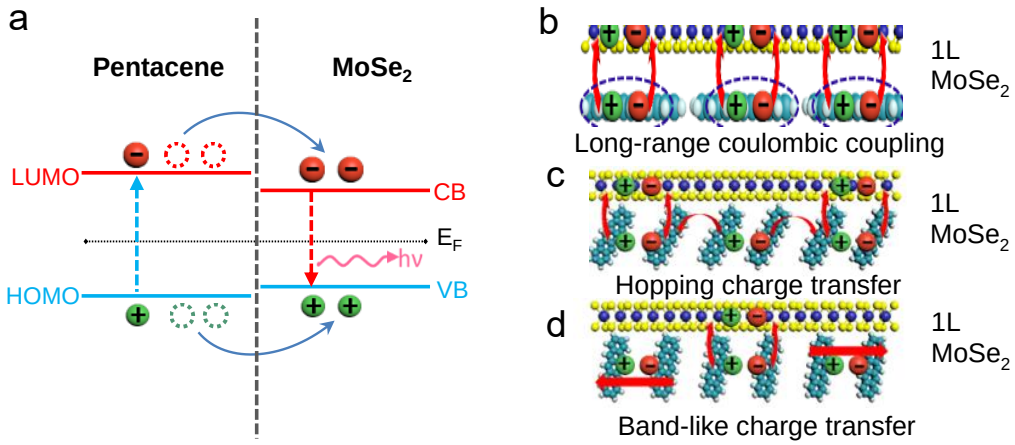

Fig. 1. a, Band alignment diagram of a $MoSe_2$/Pentacene heterostructure, which forms a type I heterostructure. b, Schematic diagram shows the charge transfer between WL PEN (bottom) and 1L $MoSe_2$ (top). The dotted ellipse shows long-range intra-layer coulombic coupling within WL PEN. e, Schematic diagram shows the charge transfer 1L PEN (bottom) and 1L $MoSe_2$ (top). The horizontal crooked arrows show the hopping mechanism of charge transfer within 1L PEN.

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Heavy-metal-free quasi-2D colloidal semiconductor nanoplatelets with atomically uniform thickness

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Atomically thin quasi-two-dimensional (2-D) colloidal semiconductor nanoplatelets are of significant importance. Despite intense interest in these materials, the synthesis of heavy-metal-free semiconductor nanoplatelets is still at primitive stages. The growth mechanism, electronic and optical properties behind their highly anisotropic shape and precisely controlled atomic thickness remains unclear. Here we report a robust approach that produces over ten-grams of zinc chalcogenide nanoplatelets with atomically uniform thickness under ambient conditions. By combining experimental results with the density functional theory simulations, a previously unknown mechanism for the formation of nanoplatelets, which consists of fusion of bundled nanowires, followed by monomer diffusion and reconstructions, and finally oriented attachment, was revealed. The synthesized ZnSe nanoplatelets exhibit an exceptional narrow emission spectrum with full-width at half-maximum as sharp as 90 meV and a 1.9 ns radiative fluorescent lifetime at room temperature. This makes ZnSe nanoplatelets the fastest colloidal fluorescent emitters reported to date, with relevance to applications in light-emitting diodes, catalysis, detectors and lasers.

Multiferroic coupling in novel two-dimensional materials

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Quantum orders typically manifest themselves in collective charge or spin arrangements leading to fascinating properties like ferroelectricity, ferromagnetism, and ferroelasticity. Recent years have seen the rise of a new class of materials possessing exotic quantum orders stemming from the topological nature of electronic band structures. Here We introduce a class of two-dimensional (2D) materials that possess coexisting ferroelectric, ferromagnetic, ferroelastic and topological insulating orders. First of the examples is a prototype 2D FETI in an atomic thin bismuth layers functionalized by CH_2OH, which exhibits a large ferroelectric polarization that is switchable by a ligand molecule rotation mechanism and a strong SOC that drives a band inversion leading to the topological insulating state. In the second example, we have shown the coexistence of ferroelectricity, ferromagnetism and topological insulating orders in CH_2OCH_3 functionalized Ge or As monolayer. Finally, we shown that there is interesting ferroelasticity in hydrogenated boron nanosheets, which is coupled with negative Poisson's ratio and Dirac switch.

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SYMPOSIA 8 – PHYSICS

Remote epitaxy – a new paradigm for stackable electronics

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Ideally, electronic heterostructures from dissimilar materials leads to enhanced functionality. Yet, experimentally forming these heterostructures is challenging due to poor lattice or thermal coefficient of expansion mismatch leading to defect formation or thermally driven atomic diffusion resulting in cross-doping and gradual junction transitions. With the discovery of remote epitaxy and 2D layer transfer [1], these challenges may be overcome. Here, SiC epitaxy is performed on epitaxial graphene as the electrostatic fields from the substrate penetrate the graphene and guide adatom registry. The film is easily peeled away since the graphene is not bonded to either the substrate or epilayer; the epilayer is then van der Waals bonded to a different material enabling new functionality. We will present experimental results on the remote epitaxy of SiC, illustrating potential power electronics and quantum science applications. Experiments to improve remote epitaxy will be reported and progress towards improving layer transfer will be described.

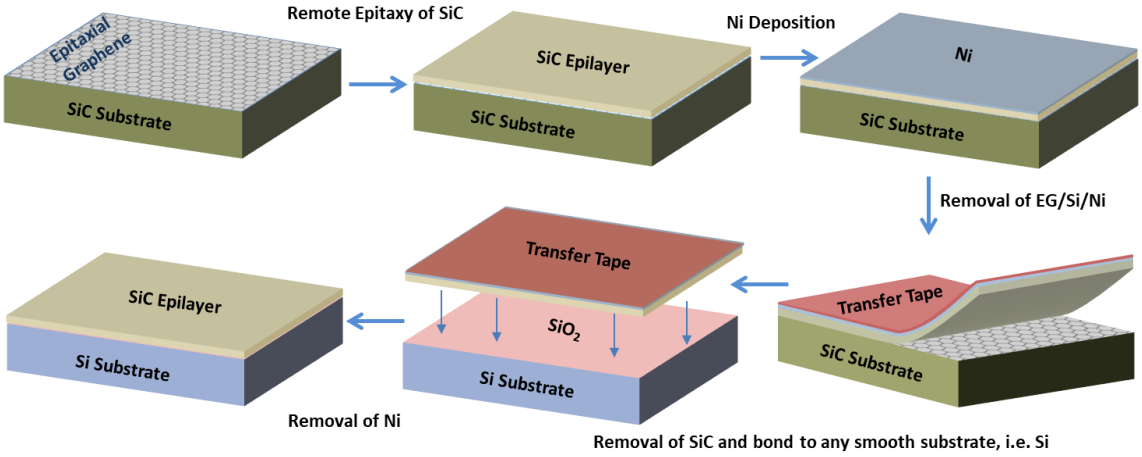

Fig. 1. Process steps for transfer of SiC onto other substrates, e.g. SiO_2/Si.

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Low-dimensional organic nanostructures on surfaces: towards nanoscale control of interfacial (opto) electronic properties

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Electronics and optoelectronics technologies rely on the control of electric charge at the interfaces between active materials of solid-state devices. This behavior is dictated by quantum mechanical phenomena unfolding at the nanoscale and depends strongly on the atomic-scale morphology of these systems. Controlling the atomic-scale structure of such interfaces is hence essential for optimizing the electronic and optoelectronic properties of solid-state systems, and yields potential for developing enhanced nanoelectronics, catalysis, light-harvesting and light-emitting technologies. Here, I will show how supramolecular chemistry on surfaces [1] – where organic molecules and atoms are used as building units for the assembly of well-defined nanostructures – offer compelling avenues for designing materials with atomic-scale precision and tailored electronic properties. I will focus on 1D and 2D organic and metal-organic nanostructures, resulting from on-surface non-covalent and metal-ligand interactions between flat aromatic molecules and transition metal adatoms. The local atomic-scale intramolecular morphology, electronic and chemical structure, and electrostatic properties of these systems are characterized by a combination of low-temperature scanning tunneling microscopy and spectroscopy, non-contact atomic force microscopy, X-ray absorption spectroscopy and density functional theory. This bottom-up on-surface synthesis approach offers means for the synthesis of low-dimensional nanostructures with unusual morphologies and properties, that cannot be achieved via more conventional synthetic chemistry methods, paving the way for nanomaterials with novel functionalities.

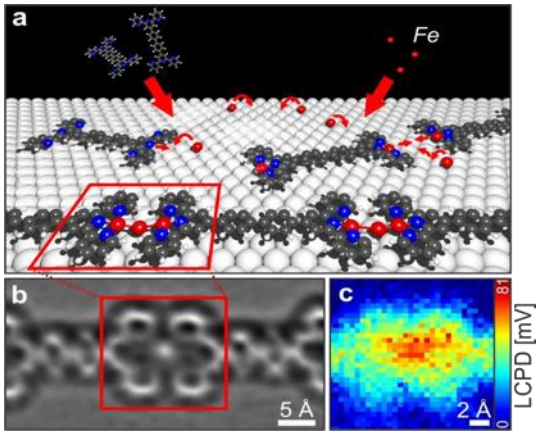

Fig. 1. Self-assembly of 1D coordination nanostructures on a metal surface. a, Bottom-up synthesis of metal-organic nanochains. **b**, Non-contact atomic force microscopy image of iron-based trinuclear coordination motif. **c**, Local contact potential difference map indicating charge accumulation at the tri-iron centre [2].

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Tuning electronic properties of graphene by STM tip

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Scanning Tunneling Microscopy (STM) not only can be used to detect the structure and properties of graphene, but also can tune the electronic properties of graphene by the STM tip [1-3]. Because graphene is a one-atom-thick flake, it is easy to change the interaction between graphene and the substrate. Therefore, we apply the voltage pulse of STM tip to tune the interaction between graphene and the substrate, and realize to turn on/off the electron-phonon coupling in graphene. Our result successfully solves the fundamental contradiction in the reported tunneling spectra of the quasifreestanding graphene monolayer [1]. On the other hand, STM tip could act as a moveable top gate with tip-induced electrostatic potential, owning to the low density of state in the low-energy zone of graphene [2,3]. For the low voltage, tip gating induces a relatively shift of the Landau levels in graphene beneath the tip, and the tunneling between the misaligned LLs results in the magnetic-field-controlled negative differential conductance (NDC) [2]. For the high voltage, edge-free graphene quantum dots are generated by combining the tip-induced electric field with perpendicular magnetic field. STS spectra reveals sequences of charging peaks grouping in quadruplets which correspond to the four-fold degeneracy of graphene. The quadruplet charging peaks here provide a visualized method to detect the broken-symmetry states in graphene [3].

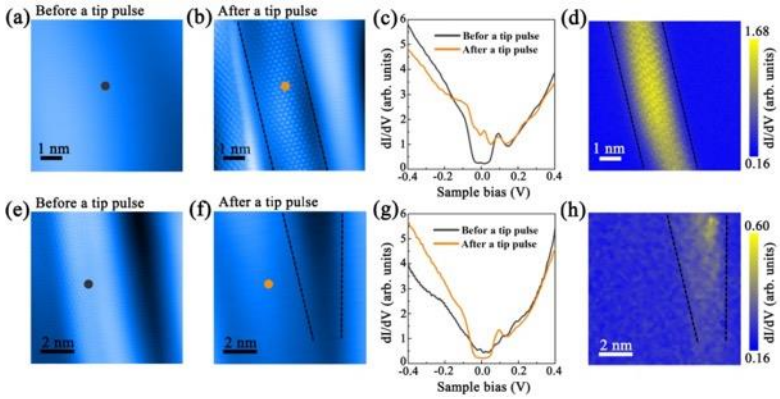

Fig. 1. Turning on and off the electron-phonon coupling of graphene by tip pulse.

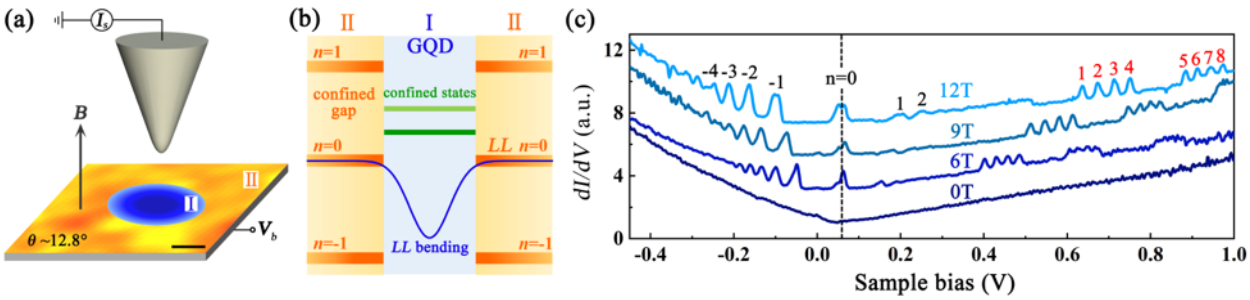

Fig. 2. Realizing the edge-free graphene quantum dot with quadruplet charging peaks in the STS spectra.

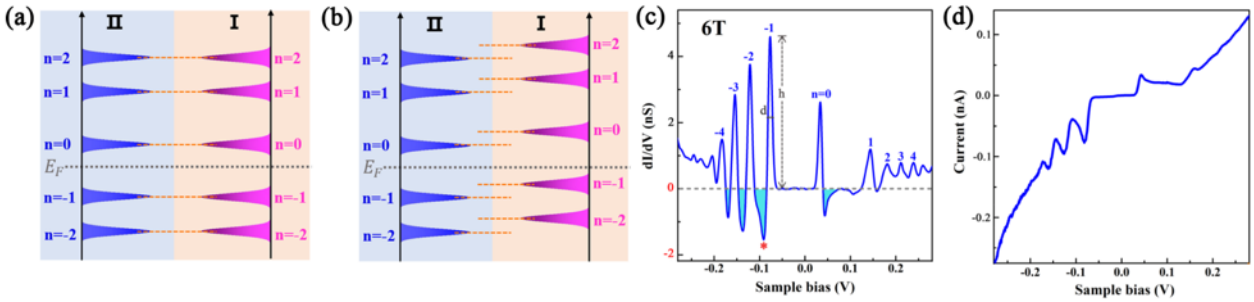

Fig. 3. The magnetic-field-controlled NDC induced by the tunneling between the misaligned LLs.

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Strong light-matter interactions in layered materials

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The realization of low energy-consumption lasers based on atomically thin two-dimensional (2D) transition metal dichalcogenides (TMDCs) are crucial for the development of optical communications, flexible displays, and lasers on the chip level. However, among the as-demonstrated TMDC-based lasers so far, the gain materials are mainly achieved by a mechanical exfoliation approach accompanied with poor reproducibility and controllability. In this work, we report a unique and controlled design for generating lasing from chemical vapor deposition derived high quality monolayer MoS_2 coupled with low-cost silica microsphere cavities. Strong continuous-wave (CW) optically driven lasing is achieved in a wide temperature range from 77 to 400 K, with the wavelength varying from 580 to 750 nm, which can be attributed to transverse electric whispering-gallery-modes (WGMs) of microspheres. On the basis of spectroscopy and theoretical studies, the eminent lasing performances result from the strong spatial confinement of carriers and the enhanced efficiency of spontaneous emission coupling with the cavities. These new findings not only advance the fundamental understanding of 2D lasing effects, but also provide solutions to fabricate low-cost, scalable and integratable TMDC-based lasers.

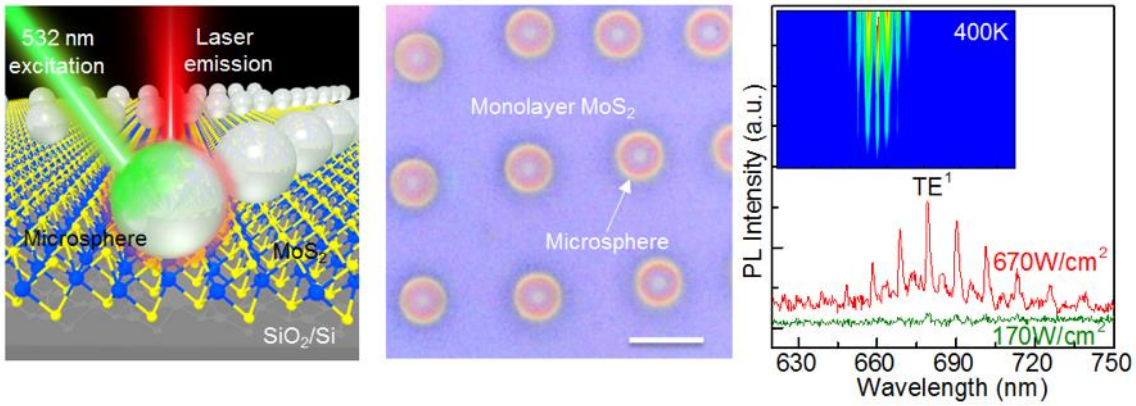

Fig. 1. Schematic of the SiO2 microsphere optical cavity on top of monolayer MoS2 and laser array and lasing behavior even at 400 K.

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Thickness-dependent electronic structure in WTe_2 thin films

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Tungsten ditelluride manifests rich electronic properties from the extremely large and non-saturated magnetoresistance and theoretical predicted type-II Weyl points in the bulk crystals to the two-dimensional topological edge states in the monolayer flakes. The two very different electronic structures between the bulk (semimetals) and monolayer (topological insulators) crystals lead to the question that: Does the sample thickness play an important role on the different electronic structures between the bulk and monolayer crystals? In this work we study electronic structure of WTe_2 thin films over different thicknesses using quantum oscillation measurements. Angle-resolved SdH oscillations show that the WTe_2 thin films cross from three-dimensional to two-dimensional electronic systems at a thickness of ~ 20 nm. Tracing the evolution of SdH oscillation frequencies over different sample thicknesses, it is found that the frequencies dramatically decrease at a thickness of approximately 12 nm, which indicates the onset of finite-size effects on the band structure. Our work pins down two critical length scales of the thickness-dependent electronic structure in WTe_2 thin films [1].

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SYMPOSIA 8 – DEVICES

Nanobubbles and nanotents formed by 2D materials

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Atomically thin crystals, i.e. two-dimensional (2D) materials, are known to be much more stretchable than their bulk counterparts. It is therefore possible to use mechanical strain to dramatically tune their electronic, optical, and magnetic properties. Recently, nano-bubbles and nano-tents formed by two-dimensional (2D) materials have seen a surge of interest because they are able to induce in-plane strain via out-of-plane deformation. Existing MD (molecular dynamics) simulations for those nano-structures are not sufficient in revealing the governing factors or guiding the future design. However, analytical modeling of these nano-structures is a nontrivial task attributing to the atomic thinness of 2D materials, which features intertwined in-plane and out-of-plane deformation as well as unusual 2D materials-to-substrate interaction. By examining experimentally measured profiles of a variety of nano-bubbles and nano-tents, we found all of them to collapse into a simple power law [1]. Using the membrane limit of the Föppl–von Kármán equations, we can analytically unveil what sets the in-plane strains in terms of the shape characteristics. As a validation, our analysis can predict the Raman shift and electromagnetic responses of graphene bubbles and tents, which turn out in good agreement with previous experiments and simulations. Besides pointing to an analytical solution for determining the strain distributions out of measurable profile, our analysis suggests a number of guidelines for the strain engineering of 2D materials. We also show that, both the strain level and the strain distribution can be tuned by the 2D-material-substrate interface adhesion and friction properties. Alternatively, with the measured profiles of nanobubbles and nanotents, interface adhesion and frictional force between the 2D material and the underlying substrate can be extracted (Fig. 1) [1, 2].

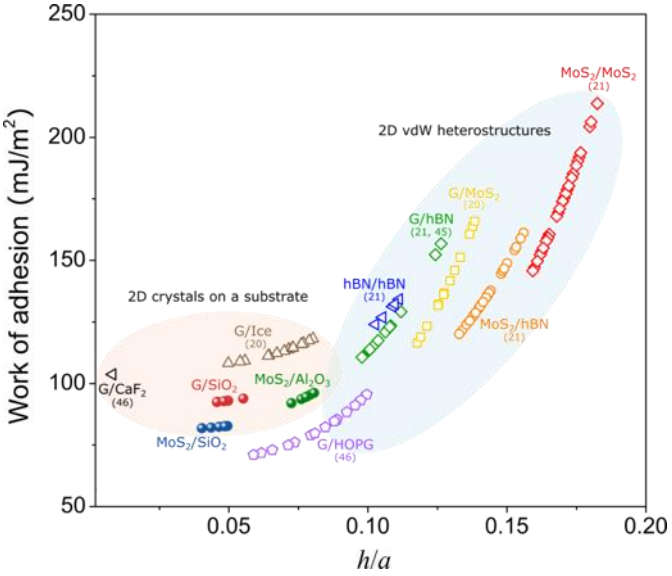

Fig. 1. Work of adhesion values for various 2D material interfaces estimated according to blister profiles, including many interfaces found in 2D heterostructures.

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Solution exfoliated black phosphorus from materials to applications

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Black phosphorus (BP), has recently attracted world-wide attention owing to its great potential in novel nanoelectronics, optoelectronics and electrochemical devices. Solution exfoliation of BP reveals superior advances when compared with mechanical exfoliation [1]. Remarkably, liquid-phase exfoliated BP flakes and quantum dots (QDs) exhibit exciting properties in batteries, solar cells, electronic, and optical devices. The exfoliation of BP in diverse solvents have been demonstrated. The solution exfoliated BP flakes can be an effective electron transport layer in organic photovoltaics (OPVs) [2]. The BP QDs can be incorporated in the active layer of OPV to boost its power conversion efficiencies [3]. Furthermore, it can also enhance the performance of Li-S batteries significantly. In addition, the BP flakes exhibit nonlinear optical properties which can be an excellent saturable absorber for high energy pulse generation in fiber laser.

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Defect engineering in few-layer phosphorene

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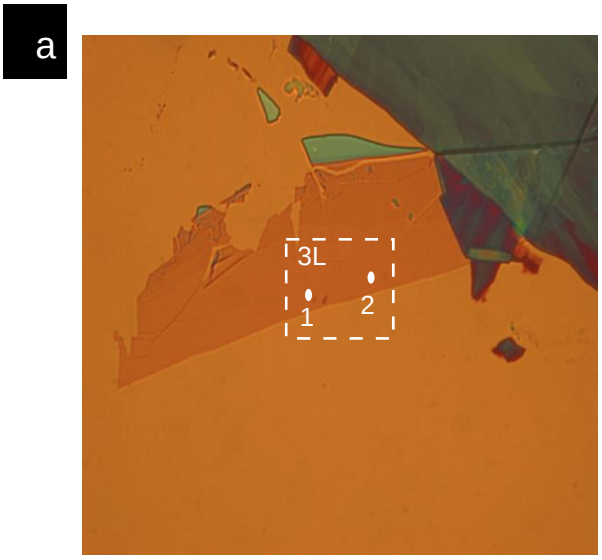
Phosphorene has been demonstrated as a viable option for the two-dimensional (2D) material-based devices and opto-electronic applications because of its universal direct band gap nature and wide-ranging band gaps from 0.3 eV (bulk) to 1.7 eV (monolayer).[1-2] Phosphorene serves as a perfect alternative material to bridge the gap between zero-band-gap graphene and large-band-gap transition metal dichalcogenide (TMD) semiconductors for suitable applications in the infrared wavelength range. Owing to its puckered lattice configuration, phosphorene possesses quasi-one-dimensional (1D) excitons and trions with highly enhanced binding energies [3-4] which is in contrast to other TMD 2D semiconductors [5] and will enable several promising novel optoelectronic and excitonic devices. Defect engineering has been demonstrated to be an important technique to modulate the properties of semiconductors for various applications. [6-7] Particularly, defect engineering in 2D materials is critical and promising for the development of novel optoelectronic devices. However, defect engineered emissions from TMDs have been reported in visible range with energies >1 eV. [8] In contrast, phosphorene, with relatively lower bandgaps, is a perfect candidate to hold defect emissions in infrared wavelength ranges. Particularly, defect emission at the telecommunication band ~1550 nm is critical for future chip-based quantum communication technologies. [9] In this work, we explored the defect engineering in few-layer phosphorene samples, by incorporating extrinsic defects using plasma-enhanced chemical vapor deposition (PECVD) grown oxide substrate. We observed a strong PL peak at ~1430 nm, from localized excitons in three-layer (3L) phosphorene samples. In a three-layer (3L) phosphorene sample, we observed a strong PL emission peak from localized excitons at ~1430 nm, a much lower energy level than free excitonic emissions. Incident power dependent PL measurements were performed to confirm the emission nature of localized excitons, which shows a sub-linear growth with increasing excitation power. Temperature dependent PL measurements were also carried out to explore the thermal stability and activation energy (E_a) of the localized excitons with increasing temperatures. E_a in 3L phosphorene was measured to be ~77 meV, which is a large value indicating relative stability of localized excitons even at higher temperatures (~263 K). This is in sharp contrast to defect states in TMDs, where defect emissions are only visible at cryogenic temperatures.20 The overall quantum efficiency of localized exciton emission in 3L phosphorene was measured to ~3 times higher than that of free exciton peak.



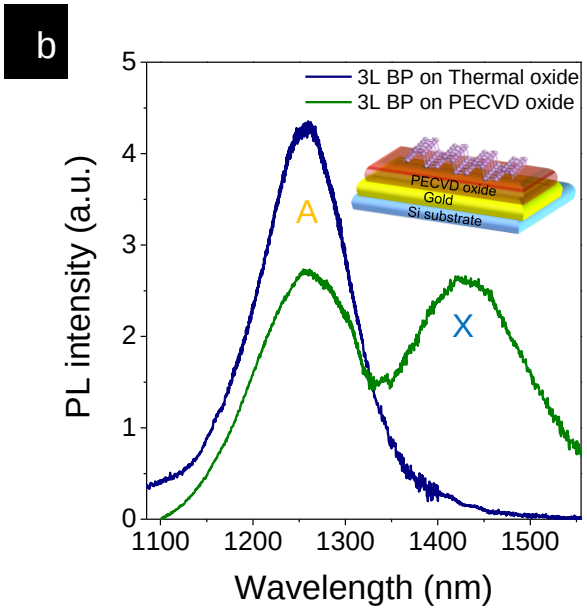


Fig. 1. a, Optical microscope image of the sample used for measurements deposited over PECVD grown oxide layer underneath gold. The dotted square shows the area scanned by PSI to determine the thickness of the sample, hence the layer number (supplementary figure 1b-d). b, Measured PL spectra from 3L phosphorene at room temperature deposited over thermally grown oxide (blue) and 3L phosphorene sample deposited over PECVD grown oxide (green). Designated free (A) and localized (X) exciton peaks have been marked. Inset shows the schematic diagram of the sample.

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Laser printed self-powered textiles

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Stretchable technologies receive a tremendous attention in the current research due to its lightweight and integrability into next-generation textiles and wearable gadgets [1]. The major limitation for the implementation of these technologies in the commercial applications is the lack of long lasting integrable energy storages to power up these devices [2]. In the textile industry, fibre based energy storages are developed as a solution to overcome this issue [3]. However, the technology is limited due to the requirement of uniform thin film coating on a highly curved fibre surface and breaking of the film under deformation. In addition, it is difficult to obtain all of the critical properties like mechanical strength, optical transmittance and electrical conductivity in single optimum textile energy storage [4].

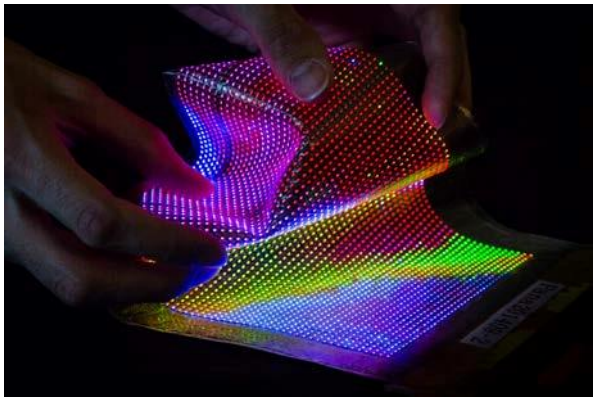

Fig. 1. LED integrated self-illuminating textiles. (Image Courtesy: FUJIFILM).

We developed miniaturised graphene supercapacitors with stretchability up to 150% based on the excitation of two-photon absorption (2PA) in graphene oxide during the laser induced reduction [5]. Based on these supercapacitors, we are introducing the concept of laser printed self-powered textiles for the sensing, health tracking and illumination applications which will have a wide impact towards information processing.

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Strong interlayer coupling in MoS_2 van der Waals homojunction constructed by defect engineering

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With quantum coupling between stacked two-dimensional (2D) materials, atomically thin and sharp van der Waals (vdW) heterostructures are particularly outstanding in optoelectronics, electronics and photovoltaics. However, those applications will be limited by its structural drawbacks including lattice incommensurateness and discontinuous band alignments, which will bring about large-size Moiré patterns, weak interlayer coupling and carrier traps[1, 2, 3]. Since discontinuous band alignments, a large number of carrier trap sites will be produced at the heterojunctions interface[1]. In a word, these two features can hinder electron transport and reduce the separation efficiency of photogenerated electron-hole pairs. Here, we successfully constructed a self-healed/as-grown MoS_2 vdW homojunction. Our pervious poly(4-styrenesulfonate)-induced sulfur vacancy self-healing effect fundamentally changes the electronic structure of monolayer MoS_2[4], makes electron concentration varies 643 times and develops a barrier height difference of ~165 meV between the self-healed/as-grown MoS_2. The ultrafast interlayer charge transfer between the separated MoS_2 monolayers take place, leading to drastic photoluminescence quenching and photovoltaic effect. Such a remarkable rate of ~438 fs is higher than those of vdW heterostructures, due to stronger interlayer coupling. Radiative recombination of interlayer indirect excitons is first detected in 2D homojunctions. This work lays a solid foundation for the structural design of vdW junctions, the clarification of the interlayer excitation principle, the luminescence wavelength widening of 2D materials, the efficient light detection and harvesting.

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SYMPOSIA 8 – CHEMISTRY

Synchrotron radiation X-ray absorption in energy materials

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Main text: With a rising global population and increasing energy demands, a blossoming interest has been raised over the security of our energy future. One of the most effective means is to develop photoelectrochemical conversion processes that can convert molecules in the atmosphere (e.g., water, carbon dioxide, and nitrogen) into higher-value products (e.g., hydrogen, hydrocarbons, and ammonia). To this end, based on the synchrotron radiation X-ray absorption fine structure (XAFS) spectroscopy, we have performed systematic investigations on the structure and performance of energy-related low-dimensional materials. We have designed a series of novel atomically dispersed single-site and atomically thick two-dimensional materials, which exhibited high performance in energy conversion reactions (e.g. photo/electrochemical water splitting, photo/electrochemical CO_2 reduction). By using XAFS as a powerful characterization technique, we report an atomic-level insight, design, and fabrication of single Co site grafted on g-C_3N_4 nanosheets as a prototypical photocatalyst for efficient H_2 production [1]. The composite single-site photocatalyst exhibits steady and high hydrogen production and quantum efficiency. Meanwhile, we have clarified that the unique surface defects and disordered structure in the two-dimensional ultrathin materials can increase the electron density and enhance the charge separation and transportation, thus enhancing the efficiency of solar energy conversion [2]. By using XAFS spectroscopy, we have unveiled the atomic and electronic structures, such as coordination number, structural defects and disorder, and chemical states, of surface active sites of low-dimensional electrocatalysts. Combining the first-principle calculations, we correlated the structures of active site to the reduction of overpotential for the electrocatalytic hydrogen or oxygen evolution in water splitting, as well as the lowered activation energy for carbon dioxide electroreduction [3,4]. Moreover, we have developed in-situ X-ray spectroscopy for the operando investigations of energy materials under photo-/electro-catalytic reactions. The above results can help to guide the design and synthesis of high-performance and low-cost energy conversion materials.

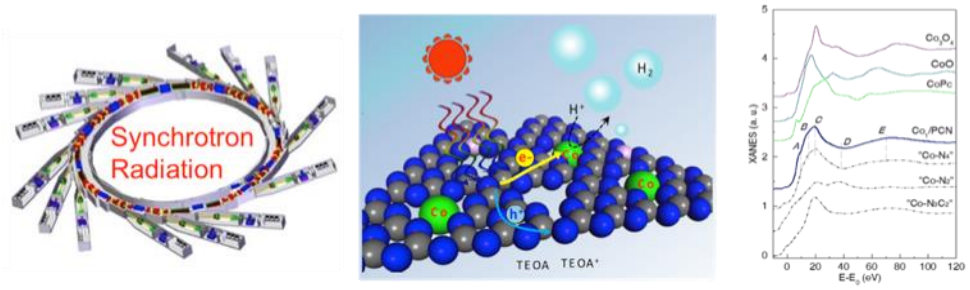

Fig. 1. Atomic characterization and design of low-dimensional energy materials by synchrotron radiation XAFS method.

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Synthesis of 2D materials using liquid metal solvents

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Most metals feature an atomically-thin oxide layer at the metal air interface.[1] This also applies to liquid metals including molten tin, indium, gallium and their alloys. In many cases this oxide layer grows in a self-limiting reaction providing a pathway towards atomically-thin, two-dimensional materials.[2] This talk will discuss different liquid metal-based synthesis strategies for 2D materials and will highlight how large area ultrathin sheets can be isolated form the liquid metal interface. Interestingly, liquid metal-based synthesis strategies allow the isolation of atomically-thin nanosheets of non-stratified materials, providing an opportunity for drastically increasing the number of accessible 2D materials.[2] A variety of liquid metal derived materials will be discussed in this talk, including metal oxides,[2, 3] chalcogenides,[4] nitrides and phosphates. The developed materials are ideally suited for a variety of applications including in electronics, piezotronics and catalysis.

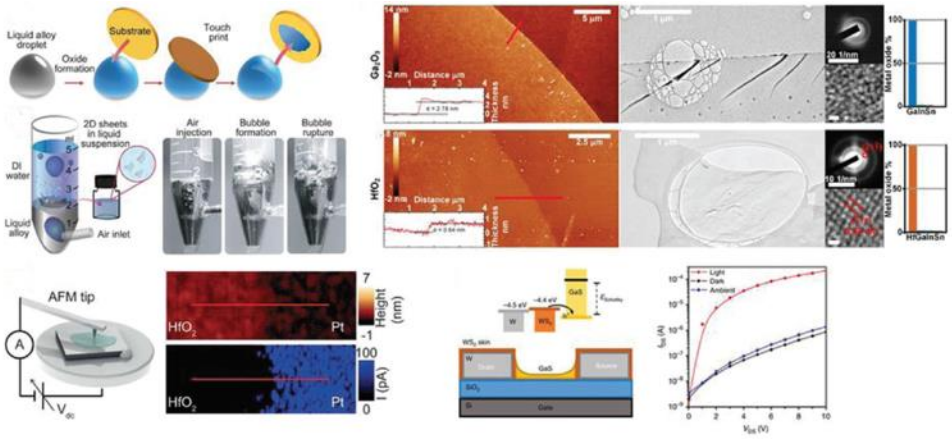

Fig. 1. Overview of liquid metal synthesis approaches, AFM and TEM characterizations of isolated sheets and evaluation of their electronic properties.

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Direct printing in three-dimensions of 2D material inks

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Microsupercapacitors, are a key component for driving miniaturization and providing stable power supply to electronic devices. 2D, planar, electrode configurations common in state-of-the-art microsupercapacitors results in relatively low energy densities limiting device performance. Adding hierarchical 3D structure through such micron-sized electrodes would provide a dramatically increase the energy stored within a single device. 3D printing provides a platform to achieve such 3D hierarchical structured architectures, and it has seen a limited development on the micron size scale. Beyond graphene, 2D materials, including the transition metal dichalcogenide (TMD) family, are exceptionally promising materials for electrochemical devices due to their intercalation capacitance, high mechanical durability, chemical stability, and edge-site density. In order to utilize these attractive properties, spatial structuring is crucial. Here we report the first 3D printed architectures via robocasting of two-dimensional atomically thin transition metal dichalcogenides [1] demonstrating their use as microsupercaacitors. The architectures are fabricated via direct printing of a liquid ink of chemically exfoliated 2D nanosheets. The 3D printed architectures serve as electrodes for microsupercapacitors with mm^2 footprints, 100µm feature size with mechanical robustness and chemical stability. They exhibit areal capacitance of 1450 mF/cm^2 and an exceptionally high energy density of 0.5 mWh/cm^2 which rivals and surpasses comparable devices [1].

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Synthesis of 2D SnS materials for piezoelectric nanogenerator applications

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Piezoelectric properties in two-dimensional (2D) materials, arise due to the breakdown in inversion symmetry as they are reduced to few layer thicknesses[1]. A recent fascination with these types of materials in this context has developed due to their high crystallinity and ability to withstand enormous strain[2]. Potential applications of atomically-thin piezoelectric materials include nano-size sensors, piezotronics, nano-generators[3] and energy-harvesting devices, thus working towards the future goal of portable, low-cost electronic devices. The unique $C2_v$ point symmetry and electronic structures of Group IV monochalcogenides and in particular, 2D tin monosulfide (SnS) are attributed for the large piezoelectric effects predicted by theoretical density functional theory calculations[2]. In this work, we investigate the synthesis of 2D SnS, its characterisation and application to form a 2D nanogenerator. We fabricated atomic layer thick nanosheets to form 2D SnS [4-6], using two methods. Structural, morphological and compositional characterisations were then performed to understand the attributes of the synthesised material. Piezoresponse force microscopy was used to investigate the predicted piezoelectric properties of the 2D SnS, in which a giant d_{33} piezoelectric co-efficient was obtained. The measured value of ~200 pm/V is comparatively much larger than the co-efficients of other low-dimensional materials such as ZnO (~23.7 pm/V) [7] and CdS (~33 pm/V) [8]. Ultimately, the material was then also applied to an energy-harvesting nanogenerator.

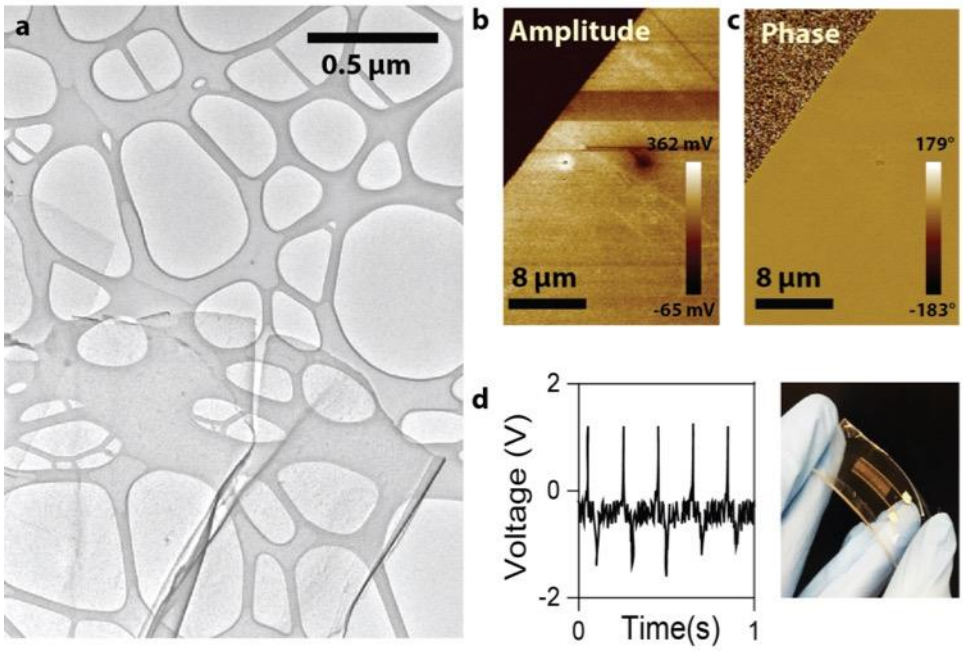

Fig. 1. a) Transmission electron microscopy image of SnS nanosheet **b)** Piezoresponse force microscopy amplitude scan of 2D SnS **c)** Piezoresponse force microscopy phase scan of 2D SnS **d)** Voltage output response from 2D SnS nanogenerator on excitation by force.

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Nano-RuO_2-decorated holey graphene composite fibers for micro-supercapacitors with ultrahigh energy density

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Compactness and versatility of fiber-based micro-supercapacitors (FMSCs) make them promising for emerging wearable electronic devices as energy storage solutions. But, increasing the energy storage capacity of microscale fiber electrodes, while retaining their high power density, remains a significant challenge. Here, this issue is addressed by incorporating ultrahigh mass loading of ruthenium oxide (RuO_2) nanoparticles (up to 42.5 wt.%) uniformly on nanocarbon-based microfibers composed largely of holey reduced graphene oxide (HrGO) with a lower amount of single-walled carbon nanotubes as nanospacers. This facile approach involves (1) space-confined hydrothermal assembly of highly porous but 3D interconnected carbon structure, (2) impregnating wet carbon structures with aqueous Ru^{3+} ions, and (3) anchoring RuO_2 nanoparticles on HrGO surfaces. Solid-state FMSCs assembled using those fibers demonstrate a specific volumetric capacitance of 199 F cm^{-3} at 2 mV s^{-1}. Fabricated FMSCs also deliver an ultrahigh energy density of 27.3 mWh cm^{-3}, the highest among those reported for FMSCs to date. Furthermore, integrating 20 pieces of FMSCs with two commercial flexible solar cells as a self-powering energy system, a light-emitting diode panel can be lit up stably. The current work highlights the excellent potential of nano-RuO_2-decorated HrGO composite fibers for constructing micro-supercapacitors with high energy density for wearable electronic devices.

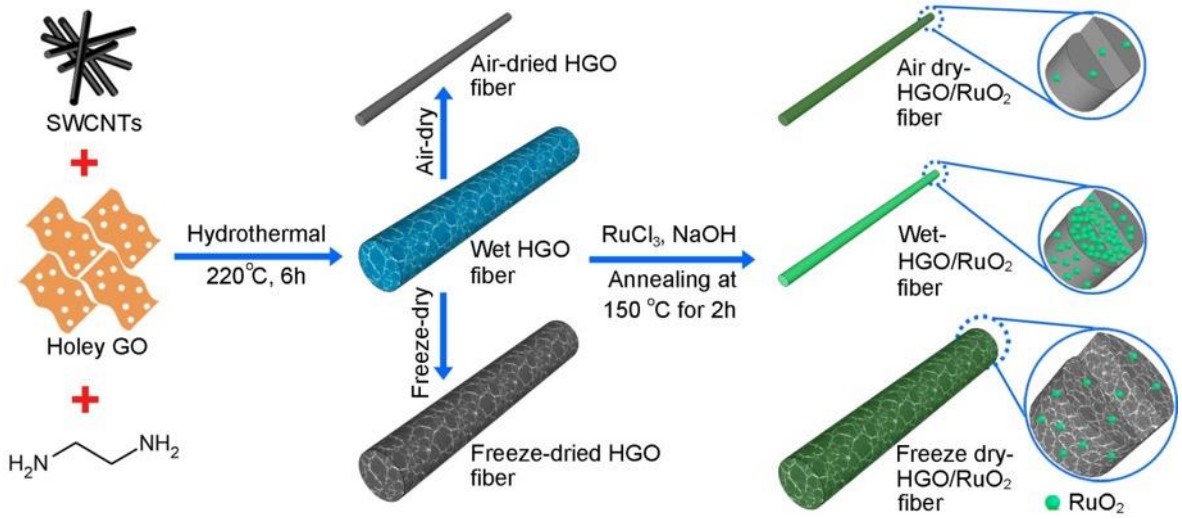

Fig. 1. Facile synthesis of holey graphene oxide / ruthenium composite fibers via different routes for ultrahigh energy density fiber-based micro-supercapacitors.

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SYMPOSIA 8 – SYNTHESIS

Graphene-based materials for environmental protection

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For water purification, we first reported that graphene sponge can be used for the efficient and recyclable adsorption materials for oils and commonly used organic solvents. Then, constantly optimizing the adsorption properties, adsorption capacity can be increased to its own weight more than 800 times; the pore size and pore wall thickness of graphene sponges are continuously adjustable by optimization of structure and preparation method; Further, in order to reduce the cost, cotton and waste paper are selected to use as raw materials to produce carbon sponge with high sorption performance. In addition to the structure of graphene sponge, graphene based metal net is developed, which can be integrated in the filtering system to realize three-phase separation of water, oil and suspended solid particles. For air purification, graphene-based flexible filtering film is developed, which is used for the production of PM2.5 filter masks and have entered the market since November in 2016

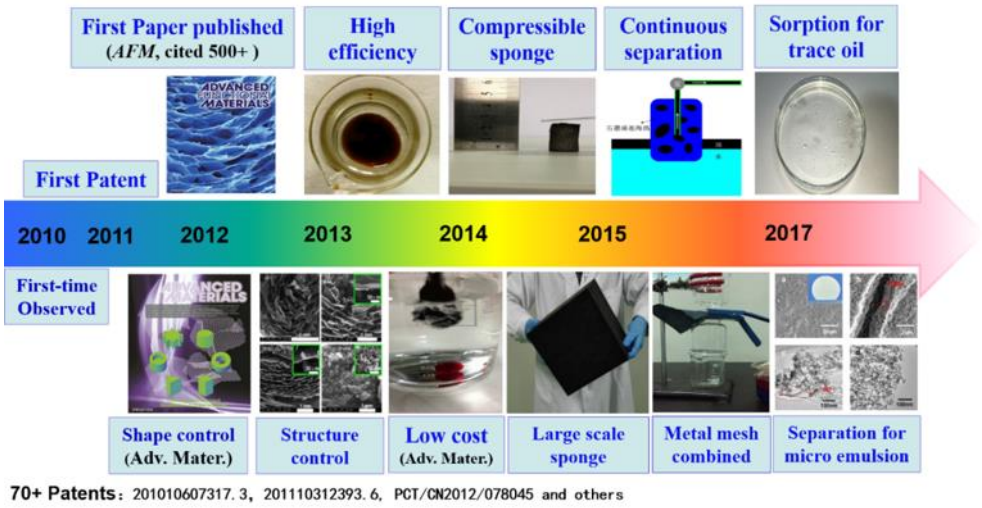

Fig. 1. Research history for oily wastewater treatment

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2D Xenes: a new family of quantum matters

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Two-dimensional (2D) materials, which possess atomic or molecular thickness and infinite planar lengths, are regarded as a novel family of materials that have a great potential to transform modern electronics due to their unique nanostructures and electronic states, especially since the discovery of graphene, which possesses amazing functionalities such as high electron mobility and the quantum Hall effect at room temperature. Silicene and germanene (named Xenes), new allotropes of silicon and germanium in a 2D one-atom-thick honeycomb structure, could have the potential for promising applications in electronics, photonics, and the other related areas because they not only demonstrates essentially the same electronic properties as graphene, such as linear dispersion of the electron band and high Fermi velocity, but they also possess an energy gap at the Dirac point, stronger spin-orbital coupling (SOC) and inherent compatibility with the current semiconductor industry. Moreover, these materials have a great potential to be used in energy storage and catalysis applications.

In this talk, I will review our recent work on silicene and germanene. By molecular beam epitaxial deposition, we successfully synthesized large-scale silicene and germanene layers on metallic substrates. The atomic honeycomb structures have been demonstrated by scanning tunneling microscopy (STM). Dirac fermion characteristics of silicene and germanene were revealed by scanning tunneling spectroscopy (STS) and angle-revolved photoemission spectroscopy (ARPES). We also achieved experimental realization of an electronic Kagome lattice and thereby generation of a flat band in a twisted multilayer silicene. The electrons are localized in the Kagome lattice due to quantum destructive interference, and thus, their kinetic energy is quenched, which gives rise to a flat band peak in density of states. A robust and pronounced one-dimensional edge state has been revealed at Kagome edge. Our observations of the flat band and the edge state in electronic Kagome lattice open up the possibility towards the realization of fractional Chern insulators in two-dimensional materials.

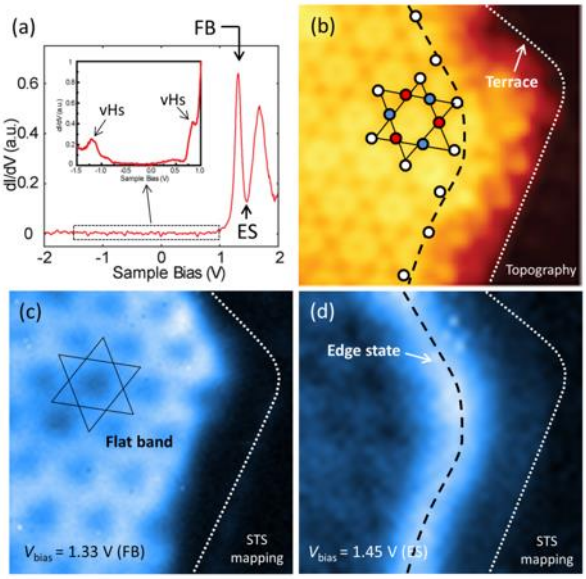

Fig.1 Electronic flat band (FB) in Kagome lattice in twisted silicene bilayer. (**a**) STS measured on Kagome silicene. (**b**) STM image of Kagome silicene with a terrace (white dashed line). The black dashed line indicates the edge of unabridged Kagome lattice. (**c**) STS mapping of FB (V=1.33 V). (**d**) STS mapping of edge state (V=1.45 V).

Graphene coated silicon carbide nanowires

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Silicon carbide (SiC) nanowires (NWs) are of high interest since they combine the physical properties of SiC with those induced by their low dimensionality retaining exceptional mechanical properties, high chemical stability, low thermal expansion coefficients, high thermal conductivity and large band gap, which enable their applications in composite reinforcements, nanodevices and optoelectronics [1]. Although graphene growth on bulk as well as epitaxial SiC has been widely reported in the past decade, to the best of our knowledge graphene growth on SiC NWs is still unavailable in scientific literature. Synthesis of high quality epitaxial graphene on SiC NWs can give rise to a new composite with useful properties and synergisms for the production of next generation electronic/optoelectronic devices, since they combine the best properties of two counterparts in the frame of one hybrid platform. In order to obtain the aforementioned composite, a double layer of Ni(5 nm)/Cu(10 nm) is sputtered on SiC nanowires grown on Si substrate [1] and subsequently annealed in a Carbolite (HT) furnace at 1050°C for one hour. Note that, this method is analogous to our previously developed alloy-mediated catalytic process to grow high quality graphene on heteroepitaxial SiC films [2]. Figure 1 shows scanning electron microscopy (SEM) images and Raman spectra of SiC NWs, before and after graphitization. A notable change in morphology as well as the evolution of D-, G- and 2D- peaks indicate the presence of graphene on SiC nanowires after alloy-mediated graphitization. These graphene coated SiC NWs could contribute to develop a new generation of nano-electronic/optoelectronic devices.

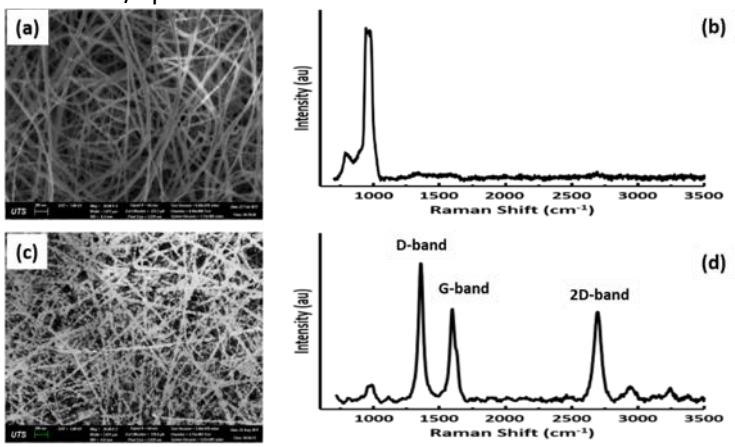

Fig. 1. SEM image of (a) SiC nanowire, and (c) graphitized nanowire. Raman spectra of (b) SiC nanowire, and (d) graphitized nanowire.

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Surface and interface engineering Pd-based ultrathin nanosheets for electrocatalysis

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The intriguing surface-related properties make ultrathin noble-metal nanosheets with few-atomic-layer thickness showing outstanding performances in the field of electrocatalysis. The open double-sided surfaces of ultrathin nanosheets expose the large specific surface area and much active sites. We develop a facile one-pot method, using n-butylamine as a bifunctional agent, to synthesize ultrathin wrinkle-free Pd_4Cu_1 nanosheets with the thickness of 2.71 ± 0.48 nm and the lateral size of 33.8 ± 8.3 nm.[1] The ingenious structure possesses the highest electrochemically active surface area among the reported PdCu nanostructures. The quantum confinement and entrapment effects of Pd_4Cu_1 nanosheets render the modulation of *d*-band electrons and weaken the adsorption of poisoning species that enhance the performance of methanol oxidation. The mass activity of the ultrathin wrinkle-free Pd_4Cu_1 nanosheets is much higher than that of commercial Pd black and Pt black; we design and implement Pd-Pt interfaces with controlled heterostructure features by epitaxial growing Pt nanoparticles on Pd nanosheets.[2] Based on both DFT calculation and experiment results, we demonstrate that the charge transfer from Pd to Pt is highly dependent on the interfacial facets of Pd substrates. Therefore, the Pd-Pt heterostructures with Pd (100) - Pt interfaces exhibits excellent activities and long-term stabilities for hydrogen evolution reaction and methanol/ethanol oxidation reaction in alkaline media, much better than those of the case with Pd (111) - Pt interfaces and commercial Pt/C.

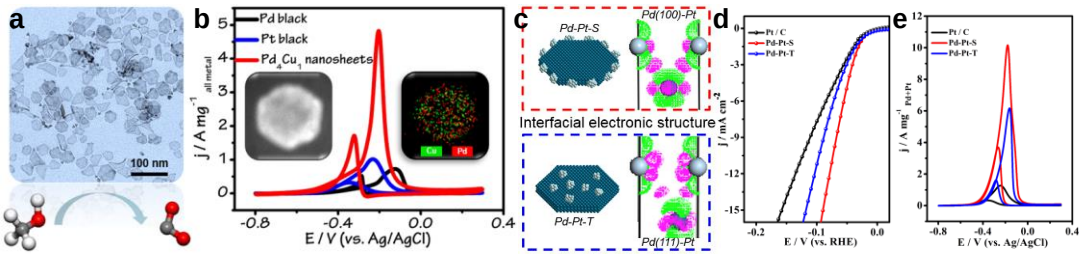

Fig. 1. (a) The TEM and (b) MOR activity of ultrathin wrinkle-free Pd_4Cu_1 NSs. (c) The simulated models and (d-e) electrocatalytic performance of Pd-Pt heterostructures.

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Chemical designing of two diemensioanl materials for renewable energy

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The renewable energy systems are playing major roles in transforming our life style with almost zero CO_2 emission. Where, atomically thin two-dimensional (2D) materials with structural anisotropy, rich surface chemistry and unique electronic structures are technologically intriguing. Importantly their chemical versatility makes them different from their counterparts and potential candidates for number of applications, specifically in the field of renewable energy.
To boost the efficiency of various energy conversion and storage systems, large number of 2D materials are produced. It is found that by playing with the lateral dimensions and thickness, the properties of 2D materials can be changed by manipulating the number of exposed atoms, dangling bonds at surface or/and edges. However, this approach has some limitations due finite limits of thinness and lateral dimensional changes to keep them 2D. Therefore, new chemical designs have been opted like doping of heteroatoms (metallic/non-metallic) or creation of vacancies, which increases the possibilities of defects/charge distribution and enhance the dangling bonds, respectively, which ultimately results new active sites for multiple purposes like catalytic reactions, electrochemical storage of ions, piezoelectric effects *etc*.
Here, we have developed several 2D materials through wet chemistry and physical methods to explain the structural fundamentals at atomic level thickness and change in surface chemistry due to defective structure and/or unsatisfied surface atoms. We further studied that how the catalytic activities/electrode capacities of 2D materials can be enhanced by tuning their aforementioned features, and we have found very exciting results. Recently, we also found that by developing 2D heterostructures with the genuine features of unilamellar sheets of two different materials will be very exciting, which can revolutionize various technological fields, especially the energy sector.

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