Poster Abstracts

Chemistry of 2D materials and applications

Fluorescent detection of mycobacterium tuberculosis via a hybridization-based pull-down assay using semiconductor nanoprobes

Ali Ibrahim, Salwa[1,2,3], Su, Xiaodi[2], Ang, Wee Han[1], Chan, Yin Thai[1,*]

[1]*Department of Chemistry, National University of Singapore, Singapore 117543, Singapore*
[2]*Institute of Materials Research and Engineering, A*STAR, Singapore 117602, Singapore*
[3]*National Institute of Laser Enhanced Science, Cairo University, Giza 12613, Egypt*
**chmchany@nus.edu.sg*

Challenges of controlling infections due to Mycobacterium tuberculosis has led to over ten million cases developing active disease with 1.7 million deaths.[1] Rapid and sensitive diagnosis is very crucial for prompt treatment and isolation of infected patients to prevent further spread of such infection. The conventional diagnostic techniques particularly in resource-limited nations are either time-consuming requiring bacterial culture, or less sensitive relying on microscopic examination.[2]

Here we develop a rapid yet sensitive assay to simultaneously target three different regions of rpoB gene of Mycobacterium tuberculosis exploiting the highly fluorescent semiconductor nanorods as hybridization probes. Three probes of different emission colors are designed through individual interactions of streptavidin-coupled green-, yellow- or red-emitting nanorods with biotin-labeled DNA oligonucleotides complementary to the regions of interest of rpoB gene. Meanwhile, the target gene is amplified through asymmetric solid-phase PCR yielding immobilized amplicons on the surface of microbeads. After denaturation of the immobilized amplicons to single strands, the nanorods-based probes specifically hybridize with their corresponding regions on the microbeads (Fig. 1).

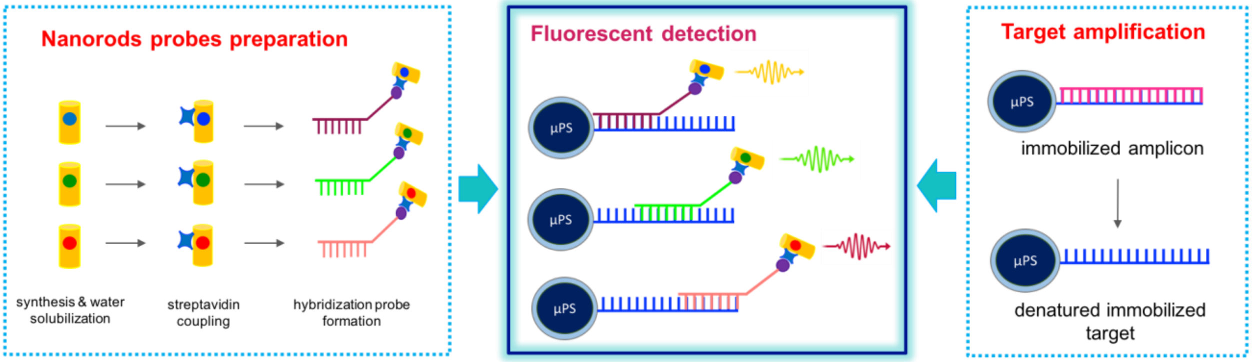

Fig. 1. A graphical representation of the detection scheme used to detect TB target using highly fluorescent semiconductor nanorods as hybridization probes

Successful hybridization of each probe is observed from the beads lit up of samples with wild-type rpoB target while non-template control show no fluorescence. Further optimization of the assay is still ongoing to simultaneously detect drug resistance.

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Cobalt sulfide nanoparticles embedded on nitrogen-doped graphene as bifunctional electrocatalyst for zinc-air batteries

Argurio, Riccardo[1,2], Zong, Yun[2], Guo, Zheng-Xiao[1*]

[1]*Department of Chemistry, University College London, 20 Gordon Street, London, WC1H 0AJ (UK)*
[2]*Institute of Materials Research and Engineering (IMRE), Agency for Science Technology and Research (A*STAR), #08-03, Singapore*
**e-mail: z.x.guo@ucl.ac.uk*

Increasing needs in the energy and control of climate change have raised concerns for new strategies to be adopted to shift from fossil fuels to renewable energy. Due to the rarity of fossil fuels and noble metals, it is important to find low-cost alternative materials. Zinc-air batteries, due to their high energy density and low cost of zinc have attracted much attention as replacements to their respective expensive counterpart Li-ion batteries due to its greater energy. The efficiency of zinc-air batteries is mainly limited by the stability of the catalysts in the cathode oxygen side where the oxygen reduction reaction (ORR, discharge) and oxygen evolution reactions OER (charge) occur [1]. The sluggish ORR kinetics at the cathode of zinc-air batteries limits the overall performance as well as the overpotential in the OER region. Doped reduced graphene oxide (rGO) with heteroatoms (N, S, P) has shown to be able to attain great onset potentials, current densities, high conductivity, and durability compared to the benchmark ORR catalyst, Pt/C. This is due to increase number of functionalities, defects, and porosity obtained from pyrolyzed N-doped rGO (N-rGO-800, N-rGO-900). Though metal-free heteroatom doped graphene has a reasonable ORR performance, it might lack the extra push to drive the OER reaction.

Hence, in this work a strategy to develop highly durable and efficient bifunctional electrocatalysts was adopted where a synergetic effect between CoS nanoparticles on N-doped reduced graphene oxide (CoS@N-rGO-800) allowed to obtain low voltage polarization (<0.7V, after 160 hours) in charge-discharge studies of zinc-air batteries in alkaline electrolyte. This has also been confirmed by three-electrode rotating disk electrode (RDE) studies on glassy carbon electrode (GCE) where great onset potentials, limiting current densities, chronoamperometric stability tests, and overpotentials proving the great potential to apply this catalyst as a low-cost replacement to the benchmark ORR/OER electrocatalysts Pt/C and RuO_2, respectively.

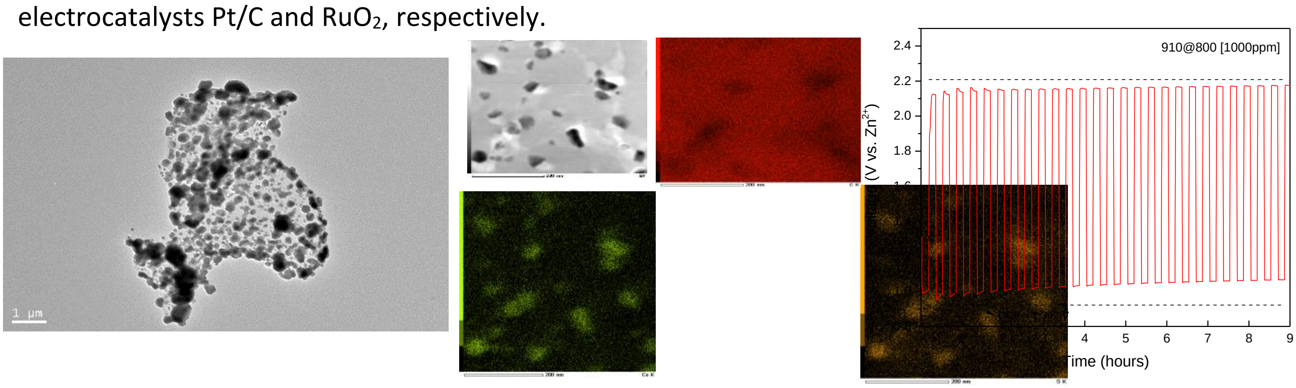

Fig. 1. (a) TEM for CoS-NRG@800, (b) EDX TEM mapping for CoS-NRG@800 and (c) galvanostatic charge-discharge for zinc-air battery cycled at 5 mA/cm^2 with loading 1 mg/cm^2

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Building a DNA nanotube-based 3D DNA walking machine with highly executive efficiency for

ultrasensitive electrochemiluminescence detection of microrna

Jiang Jie, Zhang Pu, Chai Yaqin *, Yuan Ruo *

Key Laboratory of Luminescent and Real-Time Analytical Chemistry, Ministry of Education, College of Chemistry and Chemical Engineering, Southwest University, Chongqing 400715, China.
**e-mail: E-mail:yuanruo@swu.edu.cn (R.Y.).*

Herein, a 3D DNA walking machine based DNA nanotube with improved loading capacity was described and further applied to the ultrasensitive electrochemiluminescence (ECL) detection of microRNA(miRNA) from cancer cells(Fig. 1). The DNA nanotube as 3D track was composed of a rolling circle amplification (RCA)-generated backbone chain in longitudinal extension and numerous triangular rung units (R) in horizontal extension for the abundant loading of ECL emitters, possessing the higher loading capacity compared to traditional track of DNA walking machine.[1]

Moreover, the DNA walker generated from dual target recycling could hybridize with ECL emitters-labeled DNA steps, allowing the formation of sequence-specific domain of 10-23 DNAzyme.[2] In the presence of Mg^{2+} ion, the cleavage of the DNA steps drove an autonomous stepwise locomotion of walker to the nearest neighbor DNA steps along the 3D nanotube track, which leaded to the remarkable reducing of ECL signal since the release of ECL emitters.

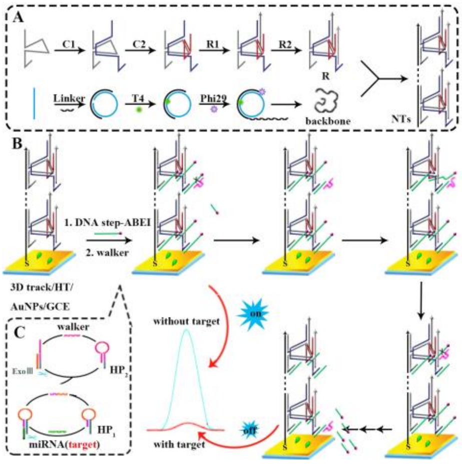

Fig. 1. Schematic Illustration of (A) Preparation of the NTs, (B) the Locomotion Mechanism of the DNA Nanotube-based 3D DNA Walking Machine, and (C) the Formation of DNA Walker Generated from Dual Target Recycling Strategy.

Coupling the DNA nanotube-based 3D DNA walking machine with highly executive efficiency with the target recycling-based dual signal amplification, the biosensor performed an ultra-sensitive detection for miRNA-141 down to 11.5 aM. In general, with highly executive efficiency of locomotion in both longitudinal extension and horizontal extension and excellent biocompatibility, this walking machine initiates a new thought for application of DNA nanostructure for improving the locomotion performance of nanomachine.

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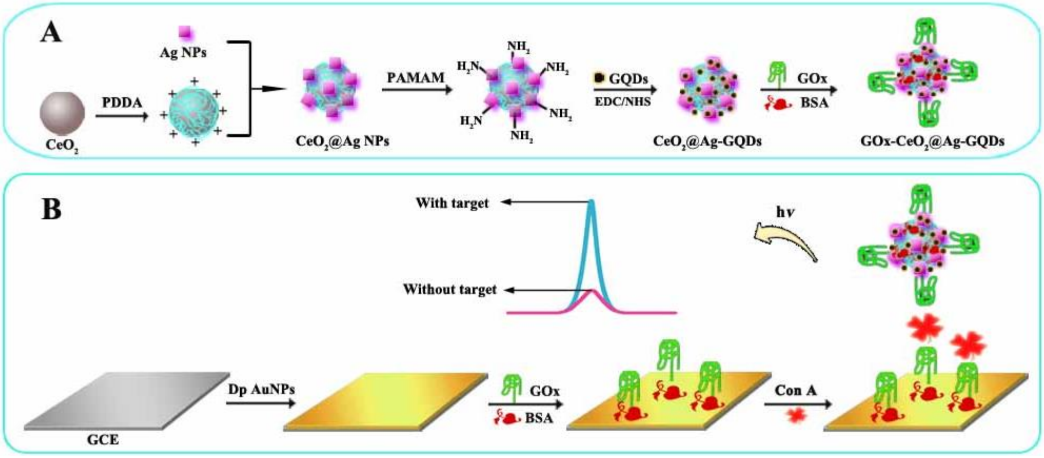
A solid-state electrochemliuminescence biosensor for con a detection based on CeO2@Ag nanoparticles modified graphene quantum dots as signal probe

Fumei Zuo[1], Cong Zhang[1], Han Zhang[1], Xingrong Tan[2], Shihong Chen *[1], Ruo Yuan[1]

[1]Key Laboratory of Luminescent and Real-Time Analytical Chemistry (Southwest University), Ministry of Education, College of Chemistry and Chemical Engineering, Southwest University, Chongqing 400715, China.
[2]Department of Endocrinology, 9 th People's Hospital of Chongqing, Chongqing 400700, China.
**e-mail: cshong@swu.edu.cn*

A solid-state electrochemiluminescence (ECL) biosensor for the detection of concanavalin A (Con A) was constructed using graphene quantum dots (GQDs) [1] as luminophore, which were loaded on polyamidoamine (PAMAM) functionalized CeO_2@Ag NPs by the interaction between the $-NH_2$ of PAMAM and the -COOH of GQDs. The electrodepositing gold layers were used as matrix to immobilize glucose oxidase (GOx). GOx served as recognition elements to further capture Con A by the specific interaction between carbohydrate and Con A. With the increase of the concentration of Con A, the amount of GOx-CeO_2@Ag-GQDs incubated onto the electrode was increased and a higher ECL signal was obtained. The constructed biosensor exhibited a sensitive response towards Con A and a low detection limit of 0.16 pg/mL was obtained. Such a construction strategy provides a new approach for applying GQDs to establish a solid-state ECL biosensor.



Scheme 1. (A) Schematic illustrate of the preparation process of the GOx-CeO_2@Ag-GQDs and (B) the fabrication process of the ECL biosensor.

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Water permeation through metal cation modified atomically thin membranes

Ching, Karin[1], Chen, Xianjue[1], Zhao, Chuan[1,*]

[1]*School of Chemistry, University of New South Wales, Sydney, Australia*
**chuan.zhao@unsw.edu.au*

A new class of materials that are atomically thin have gained increasing attention in membrane-based applications for separation and filtration. Graphene Oxide (G-O), a single-layer oxidised form of carbon, has been at the forefront of two-dimensional membrane research. However, G-O membranes suffer from poor long-term structural stability in water. To enhance G-O membranes' properties, simple modifications such as the introduction small amounts of multivalent cations to crosslink the negatively charged G-O sheet (Fig. 1A) has shown significant improvement in the aqueous stability and mechanical properties of G-O membranes [1].

Currently, there has not been any well-documented relationships between the use of cross-linked ions with the water permeability of G-O membranes. This study aims to fully understand the influence of multivalent cations on the water permeation rate for modified G-O membranes by measuring the vapour transmission rate for a variety of ion modified G-O (Fig. 1B). Previous research has demonstrated that the incorporated ions' different ionic radii changes the interlayer spacing (d-spacing) between G-O sheets [2]. The interlayer spacing and the interaction of water molecules with the intercalated ions are thought to change the permeation rate and water flow through the membrane.

Insights obtained from this investigation will provide another piece of the puzzle on how alterations of G-O membranes will influence the properties of G-O and make it possible to engineer graphene-based membranes with improved physical properties for specific applications in wastewater treatment, desalination and other filtration processes.

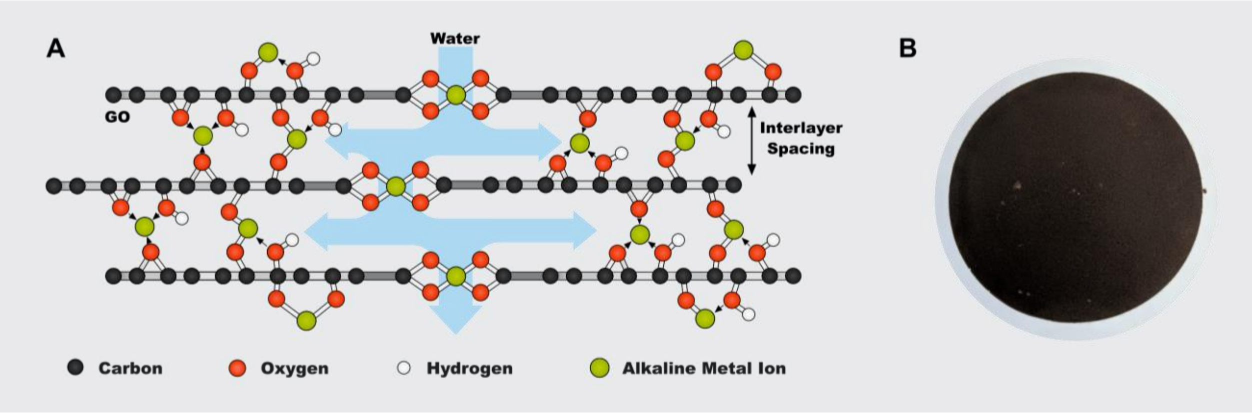

Fig. 1. (**A**) Schematic model of the graphene oxide paper with the metal ions; (**B**) Photograph of a Mn modified G-O membrane on a cellulose nitrate substrate.

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Planar hexagonal molybdenum oxide with intracrystalline molecular pores as an efficient and stable alkaline medium catalyst for HER

Haque Farjana,[1] Bao Yue Zhang,[1] Jian Zhen Ou[1]
Haque, Farjana Presenting[1], Zhang Baoyue Second[1], Ou, Jian zhen

[1]School of Engineering, RMIT University, Melbourne, Victoria, Australia

**e-mail: s3619334@rmit.edu.au*

Alkaline water electrolysis is considered as an economic approach for hydrogen gas production. However, searching a low-cost, high-performance and stable catalyst remains an ongoing request. In this work, we for the first time demonstrate two-dimensional (2D) hexagonal molybdenum oxide as a suitable electrocatalyst for hydrogen evolution reaction (HER) in alkaline medium. Through NH_4^+ doping, the orthorhombic-configured MoO_6 octahedra of α-MoO_3 are transformed to hexagonal coordination, forming one-dimensional intracrystalline tunnels vertical to the 2D lateral domain for facile diffusion of water molecules and formation of HER catalytic sites. Simultaneously, the charge conductivity of the oxide host is increased compared to α-MoO_3, hence improving the reaction kinetics for HER. More importantly, the NH_4^+ dopants are stably accommodated in the corrosion-resisted oxide host, providing an impressive stability in alkaline medium. The synergetic effects leads to an extremely stable HER activity for at least 40 h with a relatively low overpotential of 138 mV and a Tafel slope of 50 mV dec^{-1}, which is superior as a combination to those of single molybdenum compounds and hence provides a great opportunity in developing high-performance alkaline HER catalysts.

Preparation of 1T'-phase $ReS_{2x}Se_{2(1-x)}$ (x = 0 – 1) nanodots for highly efficient electrocatalytic hydrogen evolution reaction

Tran, Thu Ha[1], Lai, Zhuangchai[1], Zhang, Hua[1*]

[1]*School of Materials Science and Engineering, Nanyang Technological University, 50 Nanyang Avenue, Singapore 639798, Singapore*
**e-mail: hzhang@ntu.edu.sg*

Structural engineering of layered transition metal dichalcogenides (TMDs) has become an effective strategy to explore their new properties and significantly enhance their electrocatalytic performance towards the hydrogen evolution reaction (HER). One of the common methods to employ TMDs as a catalyst for HER is through exfoliating the layered materials into nanosheets, along with reducing the dimension and size of TMD nanomaterials and introducing defects and strain within the nanosheets [1, 2]. However, most of the recent studies on TMDs in electrocatalysis field focused on the TMD nanosheets with symmetrical structures such as trigonal prismatic 2H and octahedral 1T phase. Additionally, the preparation of the distorted structure of the commonly used TMD catalysts including MoS_2 and WS_2 has not been well developed, leading to a lack of understanding about the influence of different asymmetrical anion defects on the HER activity of TMD nanomaterials. Here, we successfully prepared a series of 1T'-phase $ReS_{2x}Se_{2(1-x)}$ nanodots using chemical vapor transport followed by Li-intercalation process and investigated the effect of the structural anisotropy on the efficiency of this nanomaterial towards HER [3]. The exfoliation process applied to the distorted structure induces the formation of asymmetrical sulfur vacancies and, together with the alloying effect of chalcogen atoms, results in the superior HER performance of 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 an excellent long-term stability.

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Cobalt oxide/3D Graphene nanosheets composite by the PECVD and hydrothermal-thermal decomposition method for application in supercapacitor

Lei Zhang[1,2] Weitao Zheng[1] Xiaoqiang, Cui[1,*]

[1]*School of Materials Science and Engineering, Jilin University, Changchun, China.*
[2]*College of chemistry, Jilin University, Changchun, China.*
**e-mail: xqcui@jlu.edu.cn*

Graphene is a carbon material with high electrical conductivity, good chemical stability, excellent mechanical strength and large specific surface area.[1][2] As reported, the combination of transition metal oxide and graphene would improve their properties.[3] In this work, we prepared the cobalt oxide/3D graphene nanosheets (GNS) composite electrode materials by the combination of plasma enhanced chemical vapor deposition (PECVD) technique and hydrothermal-thermal decomposition method. The performance of composite electrode materials is confirmed by experimental that indicates more than 2400 F/g with the test of 20 A/g current density and constant current charge and discharge 1000 times, the specific capacitance is maintain 78% of the initial specific capacitance and shows good electrochemical performance. In the meantime, we designed a new system of constraint composite electrode capacitance (Co_3O_4/ GNS-KOH/$K_3Fe(CN)_6$) to improve the specific capacitance. The experimental data reveals that the supercapacitor system shows high specific capacitance, above 10000 F/g, in 1 M KOH solution with 0.08 M $K_3Fe(CN)_6$.

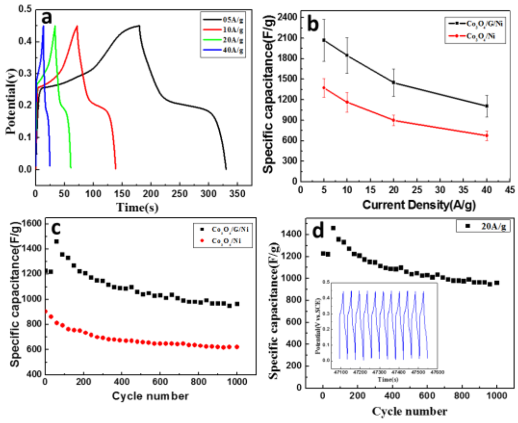

Fig 1. (a) charge-discharge profile at different current densities for Co_3O_4/GNS/Ni foam; and (b) the specific capacitance of under different current density; (c) and (d) presents the results of cycling stability under 20 A/g current density.

References

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Facil band alignment of $C_3N_4/CdS/MoS_2$ sandwich hybrid with high photochemical performance under visible-light

Dantong Zhang [1], Xiaoqiang Cui [1*]

[1]*Institution for example: School of Materials Science and Engineering and Key laboratory of Automobile Materials of MOE, Jilin University, Changchun, China.*
**e-mail: xqcui@jlu.edu.cn.*

Main text: C_3N_4 is a common and promising photocatalyst for degradation of RhB. The superiority of C_3N_4 including low costs, easy preparation, reliable stability, and suitable band gaps to utilize visible-light. However, the fast recombination of photo-excited carriers and inferior carriers' mobility inhibite the industrialization process. We designed the novel sandwich hybrid of $C_3N_4/CdS/MoS_2$ to increase the carriers utilization efficiency according to the well-matched band alignment. The smart arrangement of C_3N_4-CdS-MoS_2 made the step-by-step electron-hole pairs separation. Meanwhile, the conductive layer MoS_2 also support the easily surface transfer of electrons. The coefficient of separation and transfer made the more effective reduction of electron/hole pairs recombination than previous work [1] Compared to the pure C_3N_4, the photodegradation Rhodamine B constant rate of the hybrid is considerably enhanced, from 0.0309 to 0.0533 min^{-1}. The strategy of loading separate/transfer bifunctional cocatalyst can be widely used to maximize the solar utilization efficiency of other photocatalyst.

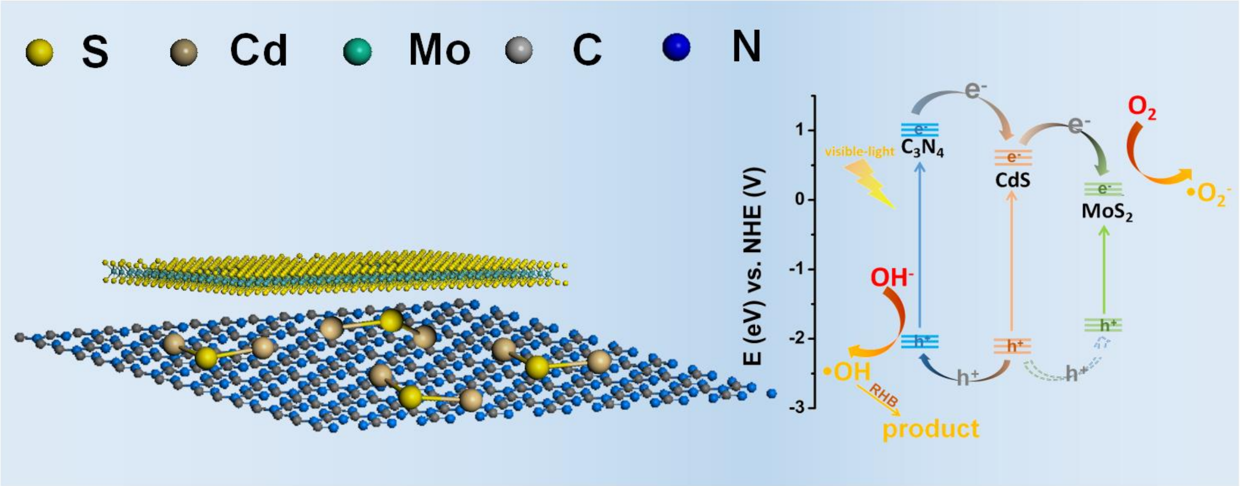

Fig. 1. The sketch map of composite structure and the charge transfer path in the process of degradation of RhB under visible-light illumination.

Reference

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CVD growth of graphene using solvent residing in a PMMA matrix as the carbon source at low temperature condition

Alaa Y. Ali [a,b], Natalie P. Holmes [a], John Holdsworth [a], Warwick Belcher [a], Paul Dastoor [a], Xiaojing Zhou [a]
[a] Center of Organic Electronics, University of Newcastle, Australia
[b] The Higher Committee of Education Development (HCED), Iraq

Abstract:

Multi-layers of graphene have been grown via the chemical vapour deposition (CVD) route by utilising an organic solvent trapped within a polymer film matrix as the carbon source. Chlorobenzene solvent residing in poly(methylmethacrylate) (PMMA) matrix was identified to be a suitable carbon source for the low temperature synthesis of graphene. PMMA dissolved in chlorobenzene was drop cast on quartz glass and heated to 180 °C in the CVD source zone. Importantly, 180 °C being a temperature higher than the boiling point of the solvent and lower than the decomposition temperature of the polymer matrix allowed chlorobenzene to be identified as a suitable carbon source for graphene growth. The graphene was catalytically grown on copper foil substrates, the resultant graphene was found to be multi-layered, as determined by Raman spectroscopy. Further experiments involved varying the growth temperature from 400 °C to 800 °C and also varying the rate of hydrogen gas (H_2) flow between 25 sccm to 100 sccm, which resulted in a significant difference in graphene film quality, as characterised by Raman spectroscopy. The optimal parameters were found to be 1 min at 600 °C growth under a hydrogen flow rate of 75 sccm. From Raman characterisation, G and 2D bands were clearly identified at ~ 1582 cm^{-1} and 2690 cm^{-1}, respectively. Transmission electron microscopy was further used to confirm graphene synthesis. The peak full width at half maximum (FWHM) of the Raman 2D band of ~53.37 cm^{-1} indicated a good quality of graphene layers at 600 °C with a H_2 flow rate of 75 sccm. Comparing to other conditions of H_2 flow rate, the relative intensity ratio of G to 2D band was 0.21, indicative of a few layers of graphene for this growth condition.

Molecular Beam Epitaxy of 1D & 2D Vanadium Diselenide on Molybdenum Disulfide

Chua, Rebekah[1,2], Wong, P.K. Johnny[3], Huang, Yuli[2,4], Wee, Andrew T.S.[1,2,3*]

[1] *NUS Graduate School for Integrative Sciences & Engineering (NGS), National University of Singapore, 28 Medical Drive, Singapore 117456, Singapore*
[2] *Department of Physics, National University of Singapore, 2 Science Drive 3, Singapore 117542, Singapore*
[3] *Centre for Advanced 2D Materials, National University of Singapore, Block S14, Level 6, 6 Science Drive 2, Singapore 117546, Singapore*
[4] *Institute of Materials Research & Engineering (IMRE), A⋆STAR (Agency for Science, Technology, and Research), 2 Fusionopolis Way, Innovis, Singapore 138634, Singapore*
**e-mail: phyweets@nus.edu.sg*

In the era of 2D materials, heterostructures are the next step in producing novel effects and devices for the future [1]. In particular, a stacked system of a ferromagnetic and a semiconducting material has applications in spin-charge conversion effect [2], valleytronics [3], etc. This study will make use of a heterostructure which comprises of VSe_2, a ferromagnetic material [4], and MoS_2, a widely used semiconducting material. To have a systematic study of thickness-dependency, molecular beam epitaxy is the choice fabrication method of VSe_2 for its good controllability in film thickness and other parameters (e.g., flux and temperature). The growth morphology and electronic properties of VSe_2 on a MoS_2 substrate are studied in detail by STM/STS. Interestingly, growth of 1D structures on multiple 2D VSe_2 layers is observed, and phase transition also occurs upon thermal annealing of the 2D VSe_2 crystals. These give insight on the tunability of the crystalline phases and hence the electronic and ferromagnetic properties of VSe_2.

References

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Two Dimensional Lateral Complicated Struture

Duan Xidong1, Duan Xiangfeng[2]

1.State Key Laboratory of Chemo/Biosensing and Chemometrics, College of Chemistry and Chemical Engineering, Hunan University, Changsha, Hunan,410082, China

2.Department of Chemistry and Biochemistry and California Nanosystems Institute,University of California, Los Angeles, California 90095, USA.

Two-dimensional layered materials such as garphene, MoS_2 and WSe_2 have attracted considerable interest in recent times as semiconductor after Si and becoming an important material platform in condensed matter physics and modern electronics and optoelectronics. The studies to date however generally rely on mechanically exfoliated flakes which always be limtited to simple 2D materals, especially 2D lateral complicated structure can not be perpared through exfoliation strategy . Much like the traditional semiconductor technique, complicated structure such as controlling the space distribution of composition and electronic structure of two dimensional semiconductor material is essential to copnstruct all modern electronic and optoelectronic devices, including transistors, p–n diodes, photovoltaic/photodetection devices, light-emitting diodes and laser diodes. And many physics phenomenon can only appear in more complicated structure. To fully explore the potential of this new class of materials, it is necessary to develop rational synthetic strategies of two dimensional lateral complicated struture,such as lateral heterostructure,multiheterostructure, superlattice,quantum well,etc.

With a relatively small lattice mismatch (~4%) between MoS_2 and $MoSe_2$ or WS_2 and WSe_2, it is possible to produce coherent MoS_2–$MoSe_2$ and WS_2–WSe_2 heterostructures through a lateral epitaxial process (Fig. 1a). Our studies indicate that simple sequential growth often fails to produce the desired heterostructures because the edge growth front can be easily passivated after termination of the first growth and exposure to ambient conditions. To retain a fresh, unpassivated edge growth front is important for successive lateral epitaxial growth. To this end, we have designed a thermal CVD process that allows in situ switching of the vapour-phase reactants to enable lateral epitaxial growth of single- or few-layer TMD lateral heterostructures. We used this technique to realize the growth of compositionally modulated MoS_2–$MoSe_2$ and WS_2–WSe_2 lateral heterostructures. From the Fig. 1 b,c,d,e we can see the formation of WS_2–WSe_2 lateral heterostructures clearly. The WS_2–WSe_2 lateral heterostuctures with both p- and n-type characteristics can also allow us to construct many other functional devices, for example, a CMOS inverter. Fig. 1g is the optical image of the invert constructed using the WS_2–WSe_2 lateral heterostuctures and the curves of the output–input and the voltage gain. The voltage gain reaches as large as 24.

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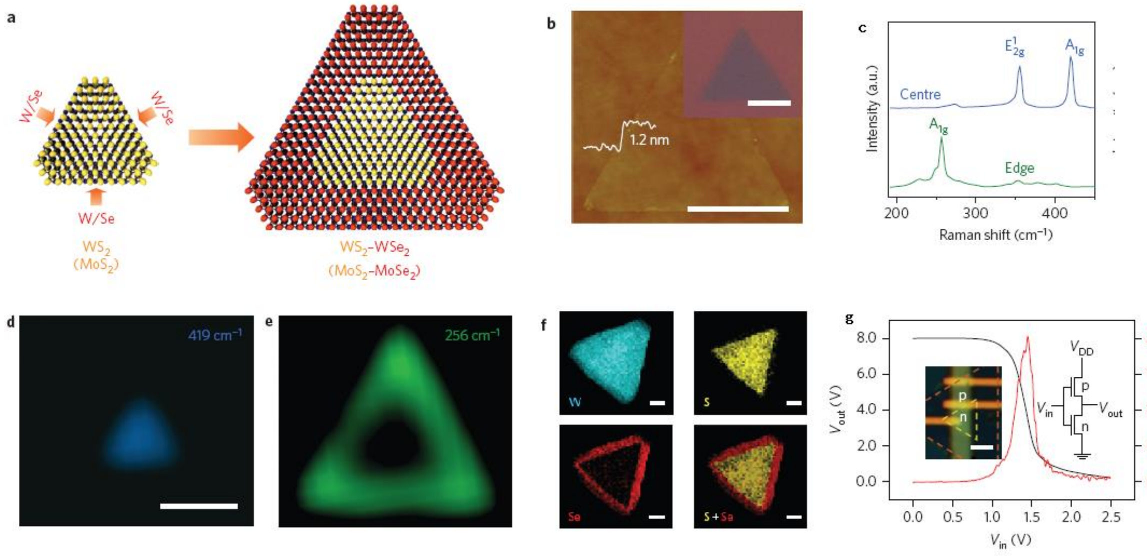

Fig.1a.Schematic of lateral epitaxial growth of WS_2–WSe_2 and MoS_2–$MoSe_2$ heterostructures. b.AFM image

of a triangular domain with a thickness of 1.2 nm. Inset: optical image of a triangular domain. Scale bars, 5 µm. c. Raman mapping at 419 cm^{-1} (WS$_2$ A^{1g} signal), demonstrating that WS$_2$ is localized at the centre region of the triangular domain. Scale bar, 5 µm. d. Raman mapping at 256 cm^{-1} (WSe$_2$ A^{1g} signal), demonstrating that WSe$_2$ is located in the peripheral region of the triangular

In a typical sequential-growth process for 2D lateral heterostructure, the excessive thermal degradation or uncontrolled nucleation duringthe temperature swing between sequential growthsteps represents the key obstacle to reliable formation of monolayer heterostructure or other lateral complicated structure .We designed a modified CVD system.We used a reverse flow from the substrate to the source during the temperature swing between successive growth steps A forward flow fromt he chemical vapor sourcewas only applied at the exact growth temperature. With such reverse flow, the existing monolayer materials will not exposure to high temperature and chemical vapor source at the tempreture increasing and decreasing steps to minimize thermal degradation and eliminate uncontrolled homogeneous nucleation. With a high degree of controllability in each step, the integrity and quality of monolayer heterostructures can be well preserved after multiple sequential growth steps. We used our approach initially for the general synthesis of a wide range of 2D crystal heterostructures. We also grew more complex compositionally modulated superlattices or multiheterostructures, the number of periods and repeated spacing can be readily varied during growth. HADDF-STEM analysis of the atomic structure of the lateral heterostructures and Multiheterostructures show the atomically sharp interface can be clearly observed.

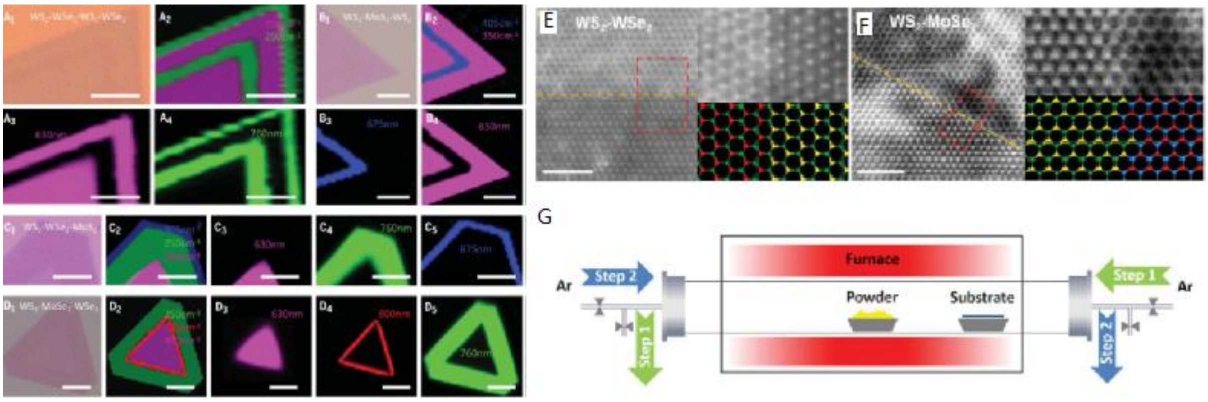

Fig.2 (A1-A4) Optical microscope image RamanMapping, PL mappingWS$_2$-WSe$_2$-WS$_2$-WSe$_2$ superlattice on SiO$_2$/Si substrate. (B1 to B4)Optical microscope image, Raman mapping, and PL mapping images ofthe WS$_2$-MoS$_2$-WS$_2$ multiheterostructure on SiO$_2$/Si. (C1 to C5) Optical microscope image, Raman mapping, and PLmapping of the WS$_2$-WSe$_2$-MoS$_2$ multiheterostructure on SiO$_2$/Si. (D1 to D5) Optical microscope image,Raman mapping, and PL mapping of the WS$_2$-MoSe$_2$-WSe$_2$ ultiheterostructure on SiO$_2$/Si. All scale barscorrespond to 5 µm. (E-F) Atomic structure of the WS$_2$-WSe$_2$ lateral heterostructures and WS$_2$-MoSe$_2$ lateral heterostructures,showing atomically sharp interface.(G) Schematic illustration of a modified CVD system for the robust epitaxial growth of lateral heterostructures.

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Identifying the Non-Identical Outermost Selenium Atoms and Invariable Bandgap across the Grain Boundary of Anisotropic Rhenium Diselenide

Hong, Min[1], Zhang, Yanfeng[1*]
[1]*College of Engineering, Peking University, Beijing, China*
**e-mail: yanfengzhang@pku.edu.cn*

Rhenium diselenide ($ReSe_2$) is a unique transition metal dichalcogenides (TMDCs) possessing distorted 1T structure with a triclinic symmetry, strong in-plane anisotropy and promising applications in optoelectronics and energy-related fields. So far, the structural and physical properties of $ReSe_2$ are mainly uncovered by transmission electron microscopy and spectroscopy characterizations. Herein, by combining scanning tunneling microscopy/spectroscopy (STM/STS) with first-principles calculations, we accomplish the on-site atomic-scale identification of the top four non-identical Se atoms in a unit cell of the anisotropic monolayer $ReSe_2$ on the Au substrate. According to STS and photoluminescence results, we also determine the quasiparticle and optical bandgaps, as well as the exciton binding energy of monolayer $ReSe_2$. Particularly, we detect a perfect lattice coherence and an invariable bandgap across the mirror-symmetric grain boundaries in monolayer and bilayer $ReSe_2$, which considerably differ from the traditional isotropic TMDCs featured with defect structures and additional states inside the bandgap (Fig. 1). Such essential findings should deepen our understanding of the intrinsic properties of two-dimensional anisotropic materials, and provide fundamental references to their applications in related fields [1,2].

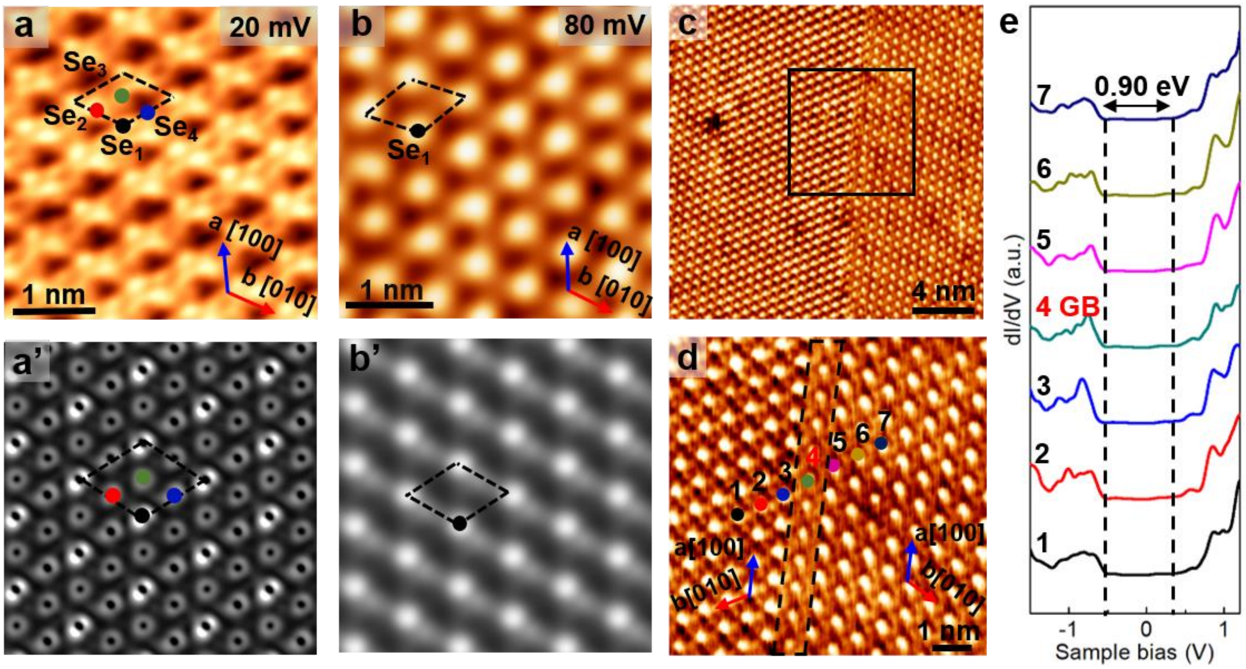

Fig. 1. STM/STS characterizations of the atomic structure and electronic property of $ReSe_2$ and its mirror-symmetry grain boundary on Au. (a-b') Bias-dependent STM images and the corresponding simulation results of monolayer $ReSe_2$ lattice. (c-e) STM images and STS spectra captured at a mirror-symmetric grain boundary of $ReSe_2$/Au.

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Fast synthesis and covalent modification of black phosphorus and graphene

Hossain Md. Zakir*

International Research and Education Center for Element Science
Graduate School of Science and Technology, Gunma University, Gunma, Kiryu, Japan
**e-mail: zakir@gunma-u.ac.jp*

Since the graphene appear as the emerging material for varieties of applications including sensor, electronics, optoelectronics, composite and energy storages, other two dimensional materials such as MoS2, WS2 and hexagonal boron nitride (h-BN) got renewed interest for utilization in next generation technologies. Very recently, another two-dimensional material, black phosphorus (BP), the most stable allotrope of phosphorus, has drawn tremendous interest because of its tunable direct band gap, high carrier mobility, and intrinsic anisotropic electrical and optical properties. [1] Similar to that of graphite, the BP is also a layered material where the different layers are held together by weak Van der Waals force. The single layer of BP is widely known as phosphorene. Because of its electronic and optoelectronic properties, BP has also emerged as a promising semiconductor material for nanoelectronics and nanophotonics devices. Among the various challenges in realization of graphene and BP based applications, the easy synthesis of high quality material and it's chemical modification is highly desirable. In this presentation I will focus on the chemical routes for the safe and fast synthesis of high quality BP and its modification through the methods developed for graphene.

To date, BP are synthesized by three major methods such as high-pressure (~1.2 GP) transformation of red phosphorus (red-P) to BP at 200 oC, bismuth flux and transport reaction [2-4]. Transport reaction method (TRM) became popular for small scale synthesis of high quality BP crystal or ribbon [4]. In TRM, red-P, tin and I2 or SnI4 are sealed in evacuated silica ample (typical inner diameter of 10 mm and length ~ 10 cm) and heated to ~ 600 oC in controlled way for about 24 h. We found that there is a danger of exploding the silica ample during the heating of a naked ample into the furnace, which may causes the damage of the tube and muffle furnaces. Hence as the safely measure during the BP synthesis, we enclosed the silica ample into a flange fitted stainless steel tube, which is then programmed heated to the desired temperature in a tube furnace or muffle furnace. With this kind of secured set-up, we have grown the pure BP crystal with more than 90 % yield within 4-6 hours. With the variation of heating and cooling patters, ratios of reactants, and inner diameters of the silica ample, we found that cooling down pattern is the crucial for synthesis of BP through TRM. Details of the experimental procedure and the results will be presented.

As prepared BP gradually undergoes oxidation in atmospheric condition. Hence it is necessary to chemically modify the upper BP layers so that it can withstand against oxidation. We have employed the different chemical functionalization methods developed for graphene to functionalize BP. Recently we have developed different methods for organic modification of graphene using as prepared Grignard reagent [5], Grignard synthesis reaction [6] and in-situ diazotization of primary amine [7]. In this presentation, I will also focus on the effective routes for chemical functionalization of BP.

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Stability and electronic properties of 2D tetraoxa[8]circulene nanosheets

Kuklin, Artem[1,*], Baryshnikov, Gleb[2]

[1]Department of Chemistry, Kyungpook National University, 80 Daehakro, Bukgu, Daegu 41566, Republic of Korea
[2] Division of Theoretical Chemistry and Biology, School of Biotechnology, KTH Royal Institute of Technology, SE-10691 Stockholm, Sweden
**e-mail: artem.icm@gmail.com*

Two-dimensional covalent organic frameworks (2D-COFs) are rapidly increasing area of interest due to the unique structure of the polymers and enormous potential for optoelectronics. In addition to existing linear polymers, two-dimensional lattices consisting of heterocyclic molecules become to attract a lot of attention providing a flexible variation of their electronic and topological properties. Heterocyclic circulenes represent a specific class of polyaromatic compounds due to their highly symmetrical structure and promising luminescent properties and can be considered as building blocks of a perfect 2D nanosheet. On the basis of first-principle calculations we report a new family of 2D lattices based on tetraoxa[8]circulene molecules with different possible types of fusing. All nanosheets demonstrate high thermodynamic stability and unique electronic properties depending on the fusing type. Among three types of nanosheets, only two demonstrate semiconducting properties exhibiting 1.37 and 1.84 eV direct band gaps calculated at the HSE06 level of theory, while one is found to be semimetal, which hosts strong topological states induced by spin-orbit coupling. Using quadratic polynomial fitting of band structures all compounds are predicted to be good organic semiconductors due to relatively low effective masses, which result in high carrier mobility. Clearly observable quantum confinement effect on the band gap size in oligomers contained 1, 4 and 9 monomers is also discussed. Owing to the versatility of chemical design, these materials have the potential to expand applications beyond those of graphene.

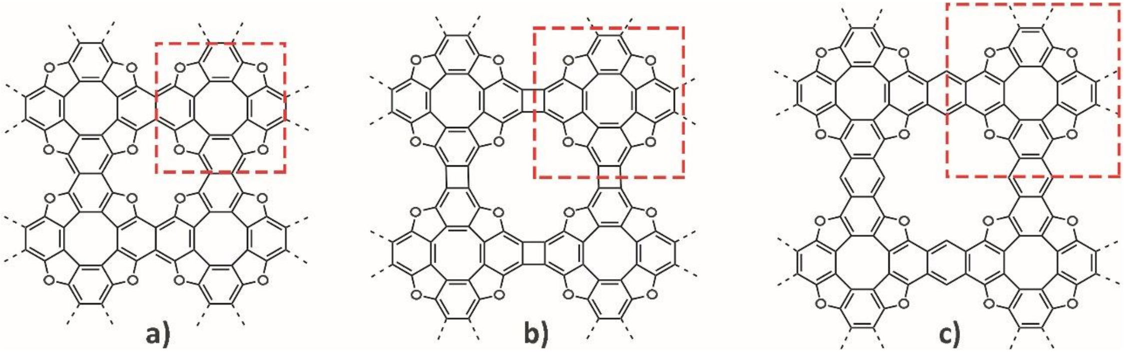

Fig. 1. Illustration of 2D tetraoxa[8]circulene formation via attaching the same monomers in different ways (from left to right: polymer #1, polymer #2 and polymer #3).

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Transferring graphene with paraffin

Leong, Wei Sun[1], Wang, Haozhe[1], Hong, Jin-Yong[1], Kong, Jing[1,*]

[1]Department of Electrical Engineering and Computer Science, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA
**e-mail: jingkong@mit.edu*

Field-effect electron mobility as high as 200 000 cm^2/V-s has been reported for graphene exfoliated from bulk crystal at 5 K. Nevertheless, mobility values reported for large-area graphene is still several orders of magnitude lower, which has been attributed to four factors: polycrystalline structure, effect of surrounding medium, contamination from transfer support layer, and wrinkles present in graphene. Any of these factors greatly decrease the carrier mean free path in graphene, which act as a central cause of extrinsic scattering, and hence limiting the carrier mobility. Here, we report a paraffin wax-enabled transfer method that simultaneously addresses both the transfer support layer contamination and graphene wrinkling issues. Specifically, we use paraffin wax as a support layer for graphene based on two rationales: paraffin has a very simple chemical structure and its thermal expansion coefficient is high. Compared to poly (methyl methacrylate) (PMMA), paraffin is unlikely to leave any problematic residues on graphene as it has no reactive carbonyl functional groups. Moreover, paraffin radicals cannot covalently bond to graphene. Furthermore, our density functional theory (DFT) calculations confirm that wax has lower adsorption energy with graphene compared to PMMA, which supports the observation of much lesser contamination in our wax-transferred graphene. To solve the graphene wrinkling issue, we fish the wax-coated graphene stack with a targeted substrate from DI water at a higher temperature of 40 °C, instead of the usual room temperature. At 40 °C, the wax support layer is thermally expanded, which stretches the graphene film underneath and hence unleashing wrinkles in graphene. Through atomic force microscopy and Raman studies, we prove that wax-assisted transfer processes noticeably reduce polymer contamination and wrinkling in graphene compared to PMMA. Thus, field-effect transistors fabricated on wax-transferred graphene exhibit near-zero Dirac voltage and the electron mobility that is higher that of PMMA-transferred graphene. Our wax-assisted transfer technique could open a new avenue for the development of high-performance large-area graphene-based electronics by minimizing the charge carrier scattering centres in graphene (*i.e.* polymer residues and wrinkles in graphene).

Quantum imaging of 2D materials using nitrogen-vacancy centres in diamond

Lillie, Scott[1,2,*], Dontschuk, Nikolai[1,2], Broadway, David[1,2], Hollenberg, Lloyd[1,2], Tetienne, Jean-Philippe[1]

[1]School of Physics, The University of Melbourne, Melbourne, Australia.
[2]CQC2T, The University of Melbourne, Melbourne, Australia.
**e-mail: slillie@student.unimelb.edu.au*

Sensing and imaging techniques utilising the nitrogen-vacancy (NV) colour centre in diamond [1] are used routinely to interrogate condensed matter systems [2]. The properties of the NV centre make it particularly sensitive to magnetic and electric properties of its nano-scale environment, and allow non-invasive sensing and imaging to be performed under a wide-range of conditions [1]. Recent works have applied these techniques to 2D materials, including NMR spectroscopy of h-BN mono-layers [3], and, in our group, magnetic imaging of current flow in graphene (Fig. 1a,b) [4].

Here, we highlight the capabilities of NV-diamond as a sensing and imaging platform for the characterisation of 2D materials and ultra-thin systems. The near-field optical coupling of NV centres and 2D flakes allows imaging by simple fluorescence measurements, provided they are metallic in nature or have an appropriate band structure, as has been demonstrated with graphene [5]. The magnetic and electric properties of 2D materials can be mapped by magnetic resonance experiments. Ferromagnetism and electric fields can be probed via their effect on the electron spin resonance transitions of proximal NV centres [6], whereas magnetic noise, associated with either charge dynamics or spin fluctuations within the material, is observed via its effect on the NV relaxation rate [7]. We have demonstrated the sensitivity of imaging such magnetic noise from ultra-thin metallic systems deposited on the diamond surface, towards this goal (Fig. 1c) [8].

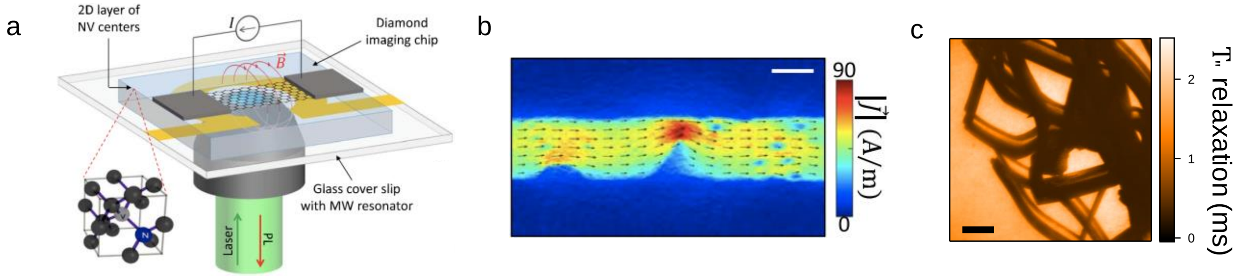

Fig. 1. a, Schematic of NV imaging platform with a fabricated graphene device [4]. b, Reconstructed current density map of a graphene ribbon by magnetic resonance measurement, scale bar 10 m [4]. c, Magnetic noise imaged from an ultra-thin (down to < 1 nm) metallic deposition on diamond measured via quenching of the NV relaxation time, scale bar 20 m [8].

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Phase-Selective Synthesis of 1T' MoS_2 Monolayers and Hetero-phase Bilayers

Liu L[1], Wu J[2], Wu L[3], Ye M[4], Liu X[5,6], Wang Q[3], Hou S[3], Lu P[3], Sun L[1], Zheng J[1], Xing L[1], Gu L[5,6,7], Jiang X[4], Xie L[2,5*] and Jiao L[1*]

[1]Department of Chemistry, Tsinghua University, Beijing, China
[2]CAS Key Laboratory of Standardization and Measurement for Nanotechnology, CAS Center for Excellence in Nanoscience, National Center for Nanoscience and Technology, Beijing, China
[3]State Key Laboratory of Information Photonics and Optical Communications, Beijing University of Posts and Telecommunications, Beijing, China
[4]State Key Laboratory of Superlattices and Microstructures, Institute of Semiconductors, Chinese Academy of Sciences, Beijing, China
[5]University of Chinese Academy of Sciences, Beijing, China.
[6]Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing, China
[7]Collaborative Innovation Center of Quantum Matter, Beijing, China.
**e-mail: lyjiao@mail.tsinghua.edu.cn*

Two-dimensional (2D) MoS_2, whose potential is being explored for optoelectronic and other applications, is thermodynamically stable and hence easily synthesized in its semiconducting 2H phase [1]. In contrast, growth of its metastable 1T and 1T' phases is hampered by their higher formation energy [2]. Here, supported by theoretical calculations, we designed a potassium-assisted chemical vapor deposition method for the phase-selective growth of 1T' MoS_2 monolayers and 1T'/2H hetero-phase bilayers. This is realized by tuning the concentration of K in the growth products to invert the stability of the 1T' and 2H phases. The synthesis of 1T' MoS_2 monolayers with high phase purity allows to characterize its intrinsic optical and electrical properties, revealing peculiar in-plane anisotropy. This phase-controlled bottom-up synthesis offers a simple and efficient way for manipulating relevant device structures, and provides a general approach for producing other metastable-phase 2D materials with unique properties.

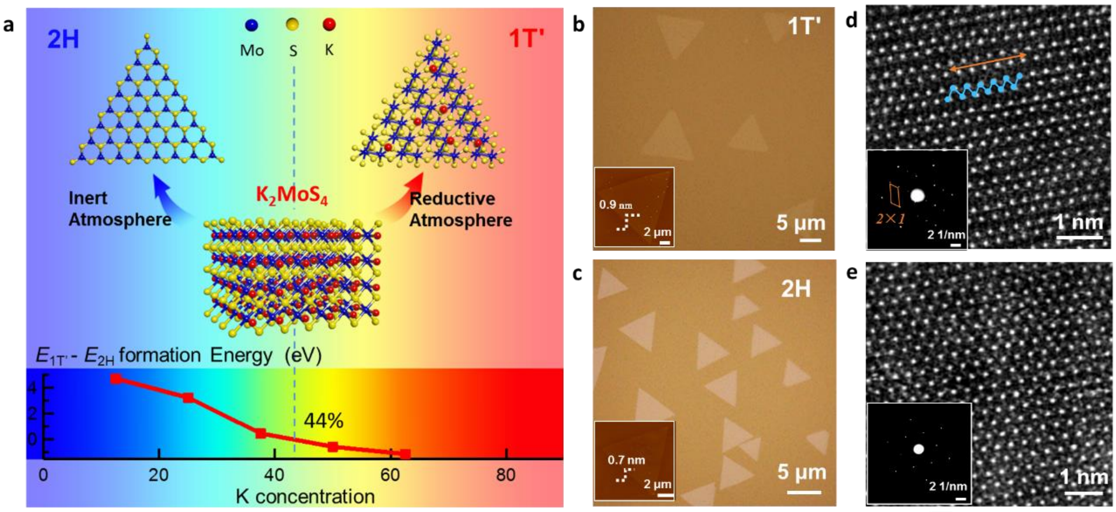

Fig. 1. Schematics for the phase-controlled synthesis strategy. **a**. Blue, yellow, and red spheres represent Mo, S, and K atoms, respectively. The inset plot at the bottom shows the calculated formation energy difference between 1T' and 2H phase K_xMoS_2 as a function of K concentration. 1T' phase becomes more stable than 2H phase at K concentration of > 44%. **b**, **g**, Optical images of 1T' and 2H MoS_2 monolayer flakes grown on mica, respectively. Insets of **b** and **g**: AFM images of 1T' and 2H MoS_2 monolayers, respectively. **c**, **h**, Atomically resolved filtered STEM images of 1T' and 2H MoS_2 flakes, respectively. Insets of **c** and **h**: SAED patterns of 1T' and 2H MoS_2 flakes, respectively.

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A tunable single-monochromator raman system based on the supercontinuum laser and tunable filters for resonant raman profile measurements

Xue-Lu, Liu[1,2], He-Nan, Liu[1,2], Ping-Heng, Tan[1,2,*]

[1]State Key Laboratory of Superlattices and Microstructures, Institute of Semiconductors, Chinese Academy of Sciences, Beijing 100083, China.
[2]College of Materials Science and Opto-Electronic Technology, University of Chinese Academy of Sciences, Beijing 100049, China.
**e-mail: phtan@semi.ac.cn*

Resonant Raman spectroscopy requires that the wavelength of the laser used is close to that of an electronic transition. A tunable laser source and a triple spectrometer are usually necessary for resonant Raman profile measurements. However, such a system is complex with low signal throughput, which limits its wide application by scientific community. Here, we construct a tunable micro-Raman spectroscopy system based on the supercontinuum laser, transmission grating, tunable filters, and single-stage spectrometer for the measurement of resonant Raman profile. The supercontinuum laser in combination with transmission grating makes a tunable excitation source with a bandwidth of sub-nanometer. Such a system exhibits continuous excitation tunability and high signal throughput. Its good performance and flexible tunability are verified by resonant Raman profile measurement of twisted bilayer graphene, which demonstrates its potential application prospect for resonant Raman spectroscopy.[1]

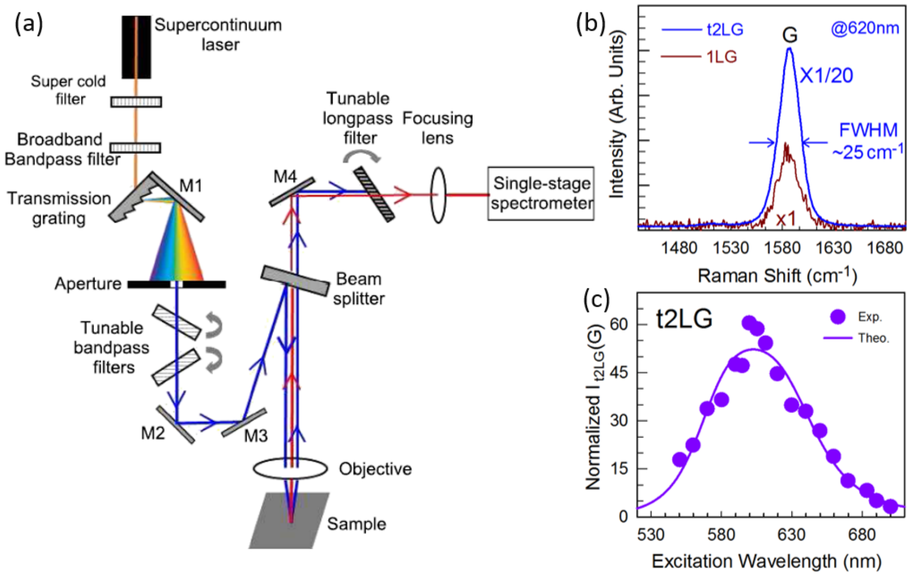

Fig.1. (a) Schematic diagram of the tunable Raman system. (b) Raman signal of monolayer Graphene(1LG) and twisted bilayer Graphene(t2LG) excited by 620 nm. (c) Resonant Raman profile of the G mode (solid circles) of t2LG and the corresponding fitting results(solid line).

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Ultrathin two-dimensional metallic nanosheets as highly efficient (electro)catalysts

Liu, Jiawei[1], Yang, Nailiang[1], Zhang, Zhicheng[1], Zhang, Hua[1*]

[1]*Center for Programmable Materials, School of Materials Science and Engineering, Nanyang Technological University, Singapore*
**e-mail: hzhang@ntu.edu.sg*

The past few years have witnessed the blossom and rapid development of novel two-dimensional (2D) nanomaterials beyond graphene and transition metal dichalcogenides. Among them, ultrathin 2D metallic nanosheets have attracted extensive research interest due to their anisotropic structures, fascinating properties and potential applications in vast fields. Particularly, owing to their high surface area-to-volume ratio and high density of unsaturated atoms exposed on their surface, 2D metallic nanosheets stand out as promising (electro)catalysts. To prepare 2D metallic nanosheets, wet-chemical synthesis is a facile method 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. Impressively, to maximize the exposure of catalytically active sites, the capping agent, oleic acid, is removed through a post-treatment with ethylenediamine (EN). 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 thickness of about 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, our Pd@Ru nanosheets expose both core and shell atoms, i.e., the Pd nanosheets are incompletely covered by the submonolayered Ru. Impressively, the obtained 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 offer opportunities in the employment of wet-chemical synthesis strategy to prepare 2D metallic nanosheets, as well as the exploration of 2D metallic nanosheets as efficient (electro)catalysts.

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Wafer scale monolayer Bi_2O_3 from liquid metal bismuth with UV photodetector application

Messalea Kibret[1] *and Daeneke Torben*[1]

[1] School of Engineering, RMIT University, 124 La Trobe Street, 3001 Melbourne, Victoria, Australia

Two dimensional (2D), semiconducting transition and post transition oxides are emerging as a promising category of materials for high-performance oxide optoelectronic applications. 2D ultrathin oxides feature superior stability in ambient atmosphere when compared with other chalcogenides, can have excellent carrier mobility and are easily doped via oxygen vacancies. However, the wafer-scale synthesis of crystalline atomically thin samples has been a challenge, since most of transition and post transition oxides are not layered. Herein we use a facile, scalable method to synthesise ultrathin bismuth oxide nanosheets using a liquid metal facilitated synthesis approach. Monolayers of α-Bi_2O_3 featuring sub-nanometre thickness, high crystallinity and large lateral dimensions could be isolated from the liquid bismuth surface. The nanosheets were found to be n-type semiconductors with a direct band gap of 3.5 eV and were suited for developing UV-photodetectors where direct bandgap wold allow high absorption and efficient electron-hole pair generation under UV excitation. The developed devices featured a high UV responsivity of ~400 AW^{-1} when illuminated with 365 nm UV light and fast response times of 70 µs. The developed methods and obtained nanosheets can likely be developed further towards the synthesis of other bismuth based atomically thin chalcogenides that hold promise for electronic, optical and catalytic applications.

Electric Field Exfoliation of Piezoelectric Two Dimensional Materials

Mohiuddin, Md[1], Ou, Jianzhen[1], Kalantar-zadeh, Kourosh [1,2*]

[1] School of Engineering, RMIT University, Melbourne, Victoria 3001, Australia
[2]School of Chemical Engineering, University of New South Wales, Sydney, New South Wales 2052, Australia
**e-mail: k.kalantar-zadeh@unsw.edu.au*

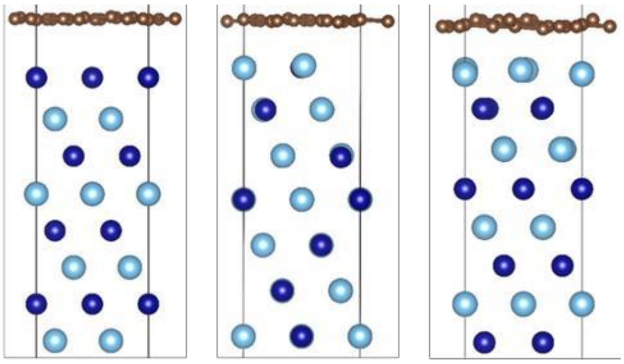
Conversion of mechanical energy into electrical energy, and *vice versa* in piezoelectric materials have a wide range of applications in energy harvester, sensors, and actuators. Antiparallel stacking sequence in semiconducting transition metal dichalcogenides (TMDs) bulk crystal makes it centrosymmetric thus nonpiezoelectric. Contrary, piezoelectricity in mono or odd layers arises from broken inversion symmetry in many two-dimensional (2D) TMDs can be utilized for efficient exfoliation processes. Owing to distinctive physical properties and emerging applications, 2D tungsten disulfide (WS_2) has become one of the most extensively studied TMDs in the recent years. Here we demonstrate an experimental process to improve exfoliation efficiency of WS_2 using an external electric field. We successfully able to thin down and enhance the exfoliation efficiency by exploiting the intrinsic piezoelectric nature of WS_2. The nanosheets produced in the liquid phase by our developed method are relatively small in size and free from any apparent defects. The developed approach can lead to new possibilities of large-scale production of non-centrosymmetry 2D layered materials for the applications in electronics, optoelectronics, and energy harvesting devices.

Bimetallic alloys for graphene/CNTs CVD growth

Parishudda Babu Movva and Alister J. Page*

Discipline of Chemistry, School of Environmental & Life Sciences, The University of Newcastle, Callaghan, 2308 NSW, Australia
e-mail: alister.page@newcastle.edu.au

Low dimensional carbon nanomaterials such as graphene/carbon nanotubes (CNTs) have been the focus of research interest due to their remarkable physicochemical properties and potential industrial applications.1-2 Bimetallic alloy catalysts are novel materials for chemical vapour deposition growth of graphene and CNTs, due to their heteronuclear metal-metal bonding, geometrical structure and catalytic properties.3-4



Type-1 catalyst

Type-2 catalyst

Type-3 catalyst

Fig.1 Three types of alloy catalyst ● Cr ● Ti ● C

In this work, first principles calculations were performed to examine the strength of the graphene-catalyst interaction for bimetallic transition metal alloy catalysts (Figure 1). Results indicate that alloys composed of a strongly interacting metal and a weakly interacting metal produce yield alloys with ideal graphene interaction strengths, and vice-versa. We show also that the surface layer structure plays a major role in determining the overall graphene-metal interaction for these alloy catalysts. These findings will assist in the future experimental development of new alloy CVD catalysts for more controlled graphene/carbon nanostructure growth.

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Electronic and optical properties of doped ReS_2 and $ReSe_2$ mono-layer

Obodo Kingsley Onyebuchi,*[1] Ouma Cecil Napthaly Moro,[2] Obodo Joshua Tobechukwu[3] and Braun Moritz[4]
[1]*University of South Africa, Pretoria, 0001, South Africa. E-mail:*
[2]*Natural Resources and Environment, Council for Scientific and Industrial Research, P. O. Box 395, Pretoria, 0001, South Africa*
[3]*Institute of Physics, RWTH Aachen, Germany*
[4]*University of South Africa, Pretoria, 0001, South Africa*
**e-mail: obodokingsley@gmail.com*

We investigate the structural, electronic and optical properties of transition metal doped triclinic monolayered rhenium disulfide and diselenide (ReS2 and ReSe2) by means of quantum mechanical calculations. The calculated electronic band gaps for ReS2 and ReSe2 monolayers are 1.43 eV and 1.23 eV, respectively, with both having a non-magnetic ground state. The calculated dopant substitutional energies under both Re-rich and X(S or Se)-rich conditions show that it is possible to experimentally synthesize transition metal doped ReX2 (where X is S or Se) monolayer systems. We found that the presence of dopant ions (such as transition metals and lanthanides) in the ReS2 and ReSe2 monolayers significantly modifies their electronic ground states with consequent introduction of defect levels and modification of the density of states profile. It was found that Mn doped structures show a very minute reduction of the electronic band gap. We found that a ferro- or a non- magnetic ground state configuration was obtained depending on the choice of dopant ions in ReS2 and ReSe2 monolayers. Cr, Fe, Co, etc. doping result in a ferro-magnetic ground state configuration for the ReX2 structures. The calculated absorption and reflectivity spectra show that certain class of dopants causes a general increase in the absorption spectral peaks but only a minute influence on the reflectivity. Optical anisotropy was observed depending on whether the direction of polarization in the xy-plane is either parallel or perpendicular.[1]

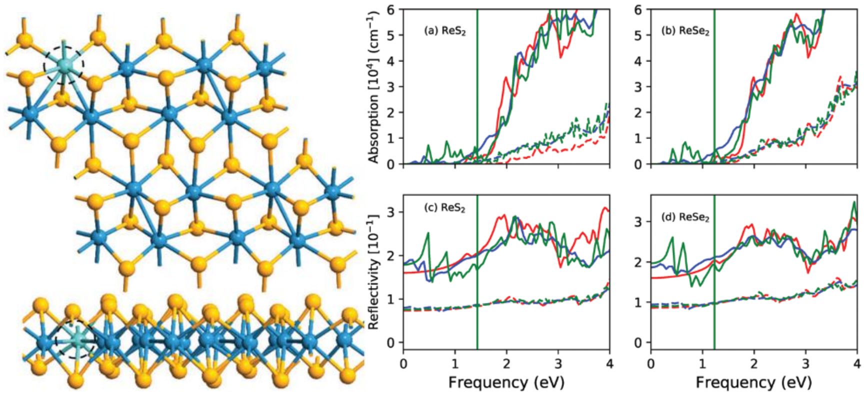

Fig. 1. The top and side view of the doped ReX2 mono-layer crystal structure is shown (dark blue, light green and orange ball represent Re atoms, transition metal dopant and X (either S or Se) atoms respectively) is presented in the left-hand side. The circled black dotted line represents the position of the dopant transition metal ion. The calculated Absorption and Reflectivity as a function of the frequency for the pristine, Co and V doped monolayered ReX2 structures is presented on the right hand side. The solid red, dashed red, solid blue, dashed blue, solid green and dashed green line represent ReS2(010), ReS2(001), Co-ReS2(010), Co-ReS2(001), V-ReS2(010), V-ReS2(001) direction respectively for the doped structures.

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Non-Stoichiometric WO_3 Precursor Tuning the Growth and Crystallinity of WS_2

Mei Er, Pam [1], Yumeng, Shi [1, 2, 3*], Hui Ying, Yang [1*]

[1] *Pillar of Engineering Product Development, Singapore University of Technology and Design, 8 Somapah Road, Singapore 487372, Singapore.*
[2] *International Collaborative Laboratory of 2D Materials for Optoelectronic Science & Technology of Ministry of Education, Engineering Technology Research Center for 2D Material Information Function Devices and Systems of Guangdong Province, College of Optoelectronic Engineering, Shenzhen University, Shenzhen 518060, China.*
[3] *Engineering Technology Research Center for 2D Material Information Function Devices and Systems of Guangdong Province, College of Optoelectronic Engineering, Shenzhen University, Shenzhen 518060, China*
**e-mail: yumeng.shi@szu.edu.cn (Y. Shi); yanghuiying@sutd.edu.sg (H. Y. Yang)*

Abstract: The extraordinary electrical, optical, thermal and mechanical properties, which exist in monolayer transition metal dichalcogenides (TMDC) materials, offer various promising applications in future ultrathin logic devices, nanogenerators, flexible electronics and optoelectronic devices.[1-4] Transition metal oxide powders have been widely used as the growth precursors for monolayer transition metal dichalcogenides (TMDCs) in chemical vapor deposition (CVD). [5-7] It has been proposed that the metal oxide precursors in gas phase undergo a two-step reaction during the CVD growth, where the transition metal sub-oxides are likely formed first and then the sulfurization of these sub-oxides leads to the formation of TMDCs. [5, 8] However, the effects of stoichiometry of transition metal oxide precursors on the growth of TMDC monolayers have not been studied yet. In this contribution, we report the critical role of WO3 precursor pre-annealing process on the growth of WS2 monolayer. Besides, several WO3 precursors with different types of oxygen vacancies have also been prepared and determined by X-ray powder diffraction (XRD), X-ray photoelectron spectroscopy (XPS) as well as the density functional theory calculation. Among all the non-stoichiometric WO3 precursors, the thermal annealed WO3 powder exhibits the highest oxygen vacancies concentration and produces WS2 monolayers with significantly improved quality in term of lateral size, density, and crystallinity. Our comprehensive study suggests that the chemical composition of transition metal oxide precursors would be fundamentally critical for the growth of large-area and high-quality WS2 monolayers, which further pave the way for revealing their intrinsic properties and unique applications.

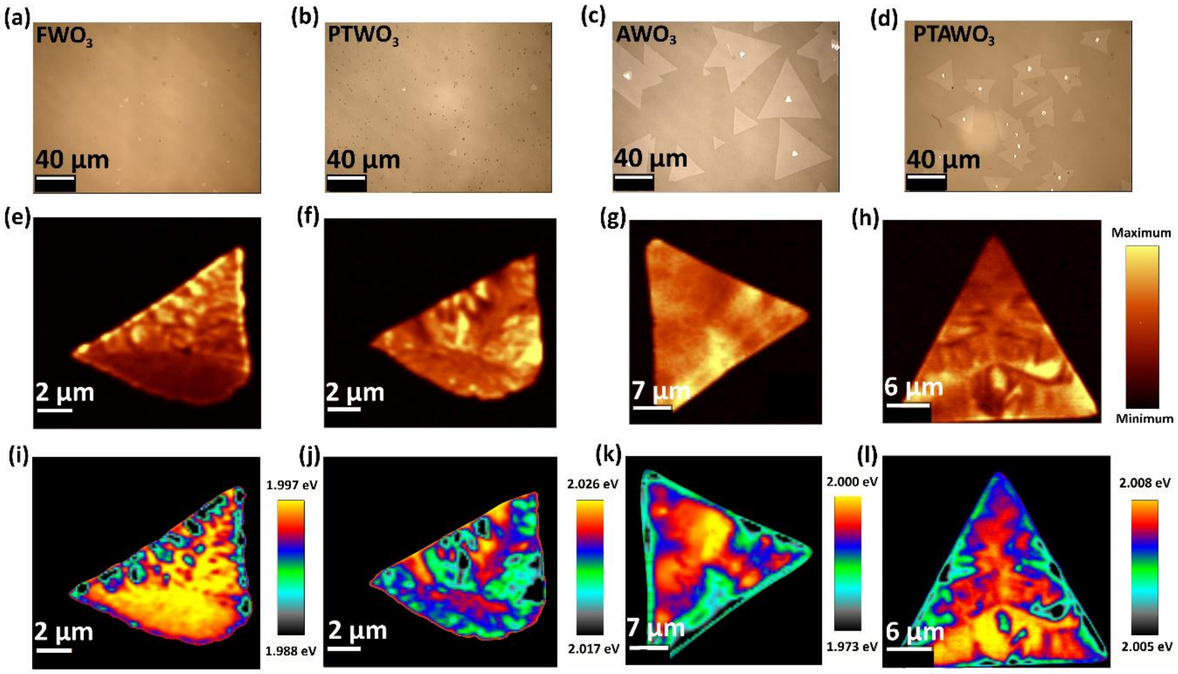

Fig. 1. Optical characterizations of the monolayer WS2 that were obtained from various types of pretreated WO3 powder. (a-d) Optical image of monolayer WS2 monolayer that were grown from FWO3, PTWO3 powder, AWO3, PTAWO3 powder, respectively. (e-h) PL intensity mapping for the monolayer WS2 that were synthesized from FWO3, PTWO3, AWO3 and PTAWO3 powders, respectively. (i-l) PL position mapping of the monolayer WS2 that were synthesized from FWO3, PTWO3, AWO3 and PTAWO3 powders, respectively.

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Laser induced micro-patterning of upconversion nanoparticles on molybdenum disulphide monolayer

Eng Tuan, Poh[1], Xiaogang, Liu[2,*], Chorng Haur, Sow[3,*]

[1] NUS Graduate School for Integrative Science and Engineering, National University of Singapore, Singapore 117456, Singapore
[2] Department of Chemistry, National University of Singapore, 3 Science Drive 3, Singapore 117543, Singapore
[3] Department of Physics, National University of Singapore, 2 Science Drive 2, Singapore 117551, Singapore
**e-mail: xiaogangliu@nus.edu.sg; physowch@nus.edu.sg*

The ability to micropattern lanthanide – doped upconversion nanoparticles (UCNPs) has always been highly valued for its optical potential in crafting photodetectors, [1, 2] microdisplays, bioassays, as well as security and anti-counterfeiting readouts. [3, 4] Through the use of a focused laser beam, UCNPs were deposited *in – situ* directly from the colloid suspension onto the surface of MoS_2 monolayers (Fig. 1). The laser induced effect resulted in the formation of ring and sponge – like microstructures arising from nanoparticle aggregation. The facile technique was well endowed with high spatial resolution and substrate selectivity, paving the way for MoS_2 based full color display. Furthermore, through a holistic analysis of the microstructure developed, a detailed insight to the critical role of the laser beam along with the dynamics of the deposition mechanism at play was acquired.

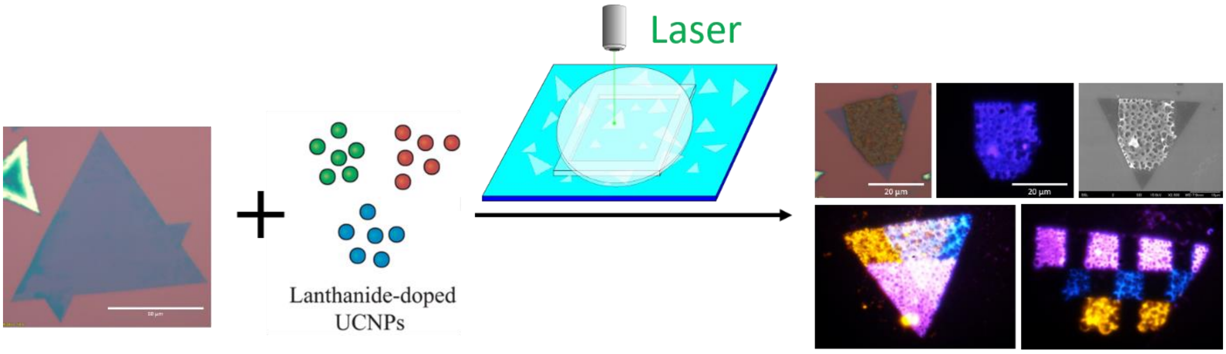

Fig. 1 General schematics for laser assisted nanoparticle deposition onto a MoS_2 monolayer, leading to multicolor display for various applications.

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Two-Dimensional Metallic Tantalum Disulfide as a Hydrogen Evolution Catalyst

Jianping Shi[1,2], Zhongfan Liu[2], Yanfeng Zhang[1,2*]

[1]*Department of Materials Science and Engineering, College of Engineering, Peking University, Beijing, China*
[2]*Center for Nanochemistry (CNC), Beijing Science and Engineering Center for Nanocarbons, Beijing National Laboratory for Molecular Sciences, College of Chemistry and Molecular Engineering, Peking University, Beijing, China*
**e-mail: yanfengzhang@pku.edu.cn*

Two-dimensional metallic transition metal dichalcogenides are emerging as prototypes for uncovering fundamental physical phenomena, such as superconductivity and charge-density waves, as well as for engineering-related applications. However, the batch production of such envisioned transition metal dichalcogenides remains challenging, which has hindered the aforementioned explorations. Herein, we fabricate thickness-tunable tantalum disulfide flakes and centimetre-sized ultrathin films on an electrode material of gold foil via a facile chemical vapour deposition route. Through temperature-dependent Raman characterization, we observe the transition from nearly commensurate to commensurate charge-density wave phases with our ultrathin tantalum disulfide flakes. We have obtained high hydrogen evolution reaction efficiency with the as-grown tantalum disulfide flakes directly synthesized on gold foils comparable to traditional platinum catalysts. This work could promote further efforts for exploring new efficient catalysts in the large materials family of metallic transition metal dichalcogenides, as well as exploiting their applications towards more versatile applications.

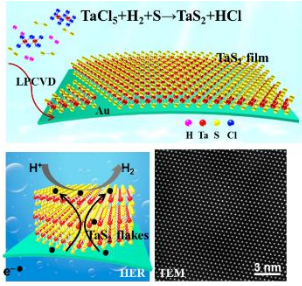

Fig. 1. Two-dimensional metallic tantalum disulfide as a hydrogen evolution catalyst

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Synthesis and photochemistry of gallium oxide nanoflakes featuring trap state absorption

Syed, Nitu[1], Daeneke, Torben[1], Kalantar-Zadeh, Kourosh[1,2,*]

[1]*School of Engineering, RMIT University, Melbourne, VIC 3001, Australia*
[2]*School of Chemical Engineering, University of New South Wales, Kensington, NSW 2033, Australia*

**e-mail: k.kalantar-zadeh@unsw.edu.au*

Main text: The most striking behavior of liquid metal gallium stems from the existence of the ultrathin surface oxide skin on exposure to air. Taking advantage of this unique surface oxide, this work introduces a novel and inexpensive technique to synthesize gallium oxide (Ga_2O_3) nanostructures at high yield. The synthesis process follows a facile and very inexpensive two-step method comprising liquid gallium metal sonication in DI water and subsequent annealing.The obtained nanoflakes are next used as a functional material for the photocatalytic mitigation of organic pollutants and waste. It has been shown in our work that the synthesized porous Ga_2O_3, despite its relatively wide bandgap (4.7 eV), exhibits enhanced photocatalytic performance under solar light irradiation. The superior properties of Ga_2O_3 nanoflakes as a photocatalyst can be explained by its electronic band structure. Here the improvement of the photocatalytic activity of Ga_2O_3 is achieved by shifting its photo-response towards the visible range by introducing trap states into its wide band gap. The presence of these trap states provides an effective strategy to reduce the electronic bandgap and enhances the optical absorption of the material.
Overall, the findings are relevant for developing effective and environment friendly solar light driven photocatalysts following a facile and inexpensive synthesis route enabling practical future electronic and optical applications. This work can be a high benchmark to present a novel route for synthesizing oxide nanostructures that can be extended to other low melting temperature metals and their alloys. The developed method furthermore has great potential for scaling up and high yield synthesis.

Morphology engineering in monolayer MoS_2-WS_2 lateral heterostructure

Tang, Bijun[1], Zhou, Jiadong[1], Liu, Zheng[1,2,3, *]
[1]Center for Programmable Materials, School of Materials Science and Engineering, Nanyang Technological University, Singapore 639798, Singapore.
[2]Centre for Micro-/Nano-electronics (NOVITAS), School of Electrical & Electronic Engineering, Nanyang Technological University, 50 Nanyang Avenue, Singapore 639798, Singapore
[3]CINTRA CNRS/NTU/THALES, UMI 3288, Research Techno Plaza, 50 Nanyang Drive, Border X Block, Level 6, Singapore 637553, Singapore
** e-mail: z.liu@ntu.edu.sg*

In recent years, heterostructures formed in transition metal dichalcogenides (TMDs) have attracted significant attention due to their unique physical properties beyond the individual components. Atomically-thin TMD heterostructures, such as MoS_2-WS_2, MoS_2-$MoSe_2$, MoS_2-WSe_2 and WSe_2-WS_2, have been synthesized so far via chemical vapor deposition (CVD) method [1-6]. Engineering the morphology of domains including size and shape, however, still remains challenging. Here, we report a one-step CVD strategy on the morphology engineering of MoS_2 and WS_2 domains within the monolayer MoS_2-WS_2 lateral heterostructures through controlling the weight ratio of precursors, MoO_3 and WO_3, as well as tuning the reaction temperature. Not only can the size ratio in terms of area between WS_2 and MoS_2 domains be easily controlled from less than one to more than twenty, but also the overall heterostructure size can be tuned from several to hundreds of microns. Intriguingly, the quantum well structure, a WS_2 stripe embedded in the MoS_2 matrix, is also observed in the as-synthesized heterostructures, offering opportunities to study quantum confinement effects and quantum well applications. This approach paves the way for the large-scale fabrication of MoS_2-WS_2 lateral heterostructures with controllable domain morphology, and shall be readily extended to morphology engineering of other TMD heterostructures.

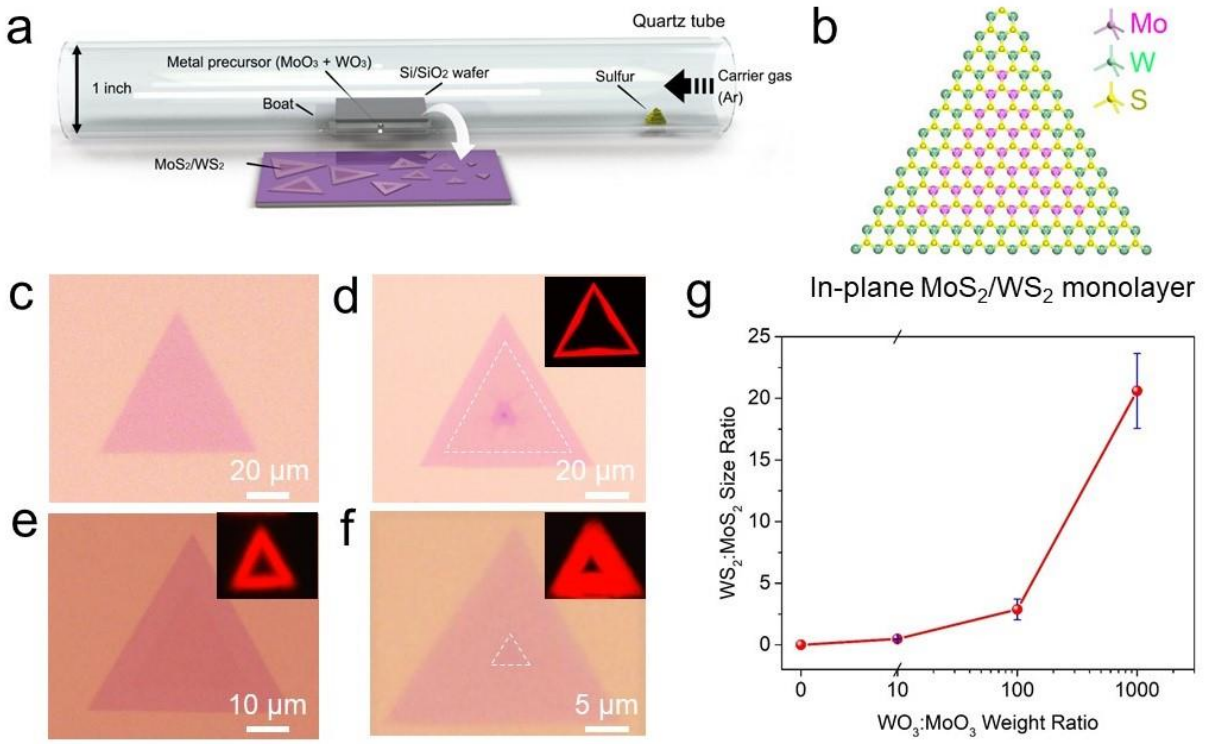

Fig. 1. Schematic of the experimental setup and the overall morphologies of the MoS_2-WS_2 lateral heterostructures synthesized.
a) Schematic of the synthesis process for lateral heterostructures. b-f) Crystal structure and optical images of the MoS_2-WS_2 lateral heterostructures grown at 650 °C with WO_3:MoO_3 weight ratio of 0, 10, 100 and 1000, respectively. The inset images in d-f are the corresponding fluorescence images, showing different sizes of the WS_2 in the shell and MoS_2 in the core. g) The size ratio of WS_2 to MoS_2 at different source weight ratios.

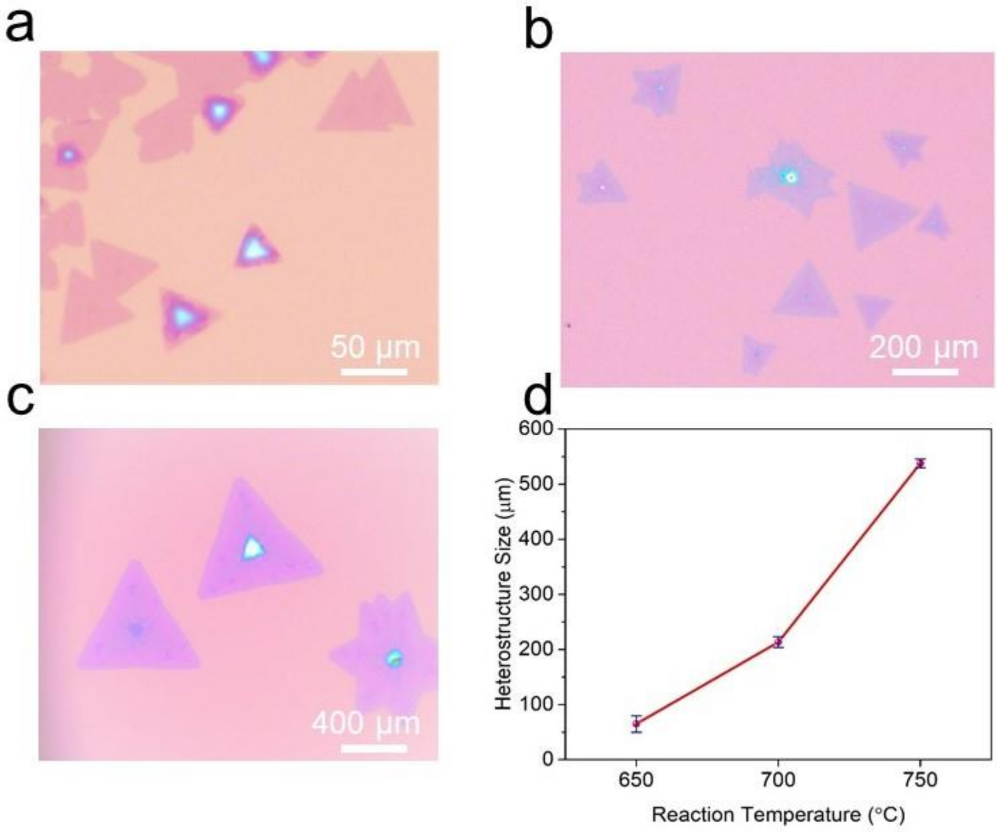

Fig. 2. Optical images of the MoS_2-WS_2 lateral heterostructures grown at the temperature of a) 650 °C, b) 700 °C and c) 750 °C. Especially, at high temperature of 750 °C, the size of the lateral heterostructures reaches about 560 µm. d) The size of the heterostructures grown at different reaction temperatures with error bars of 15, 10, and 8, respectively.

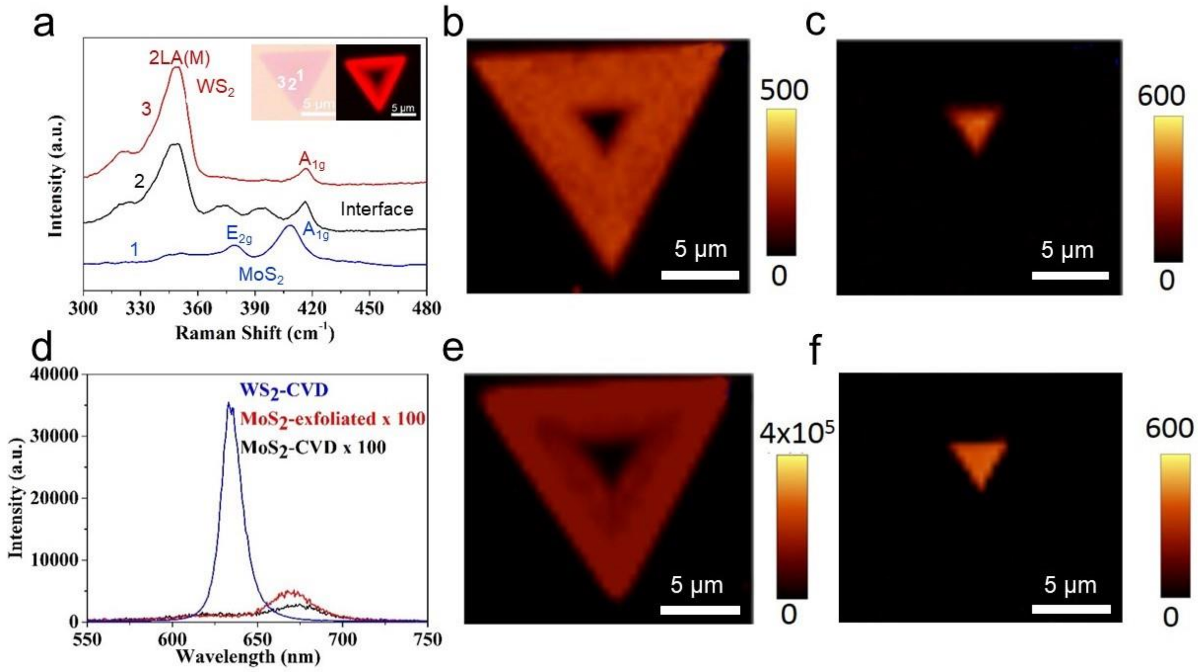

Fig. 3. Raman and photoluminescence (PL) characterizations of the MoS$_2$-WS$_2$ lateral heterostructures.

a) Raman spectra taken from the core, shell and the interface of the heterostructure, showing characteristic peaks of MoS$_2$ and WS$_2$ in the inner and outer triangles, respectively, as well as their superposition at the interface region. Insets are the optical and fluorescence image of the MoS$_2$-WS$_2$ lateral heterostructures. b-c) Raman intensity mapping at 381 cm^{-1} and 351 cm^{-1}, showing the core–shell structure with MoS$_2$ as the core and WS$_2$ as the shell. d) PL spectra of the heterostructure with peaks at 630 nm and 680 nm, indicating pure WS$_2$ and pure MoS$_2$, respectively. The peak at the interface is between 630 nm and 680 nm. e-f) PL intensity mapping at 680nm and 630 nm, corresponding to the characteristic PL peaks of MoS$_2$ and WS$_2$, respectively.

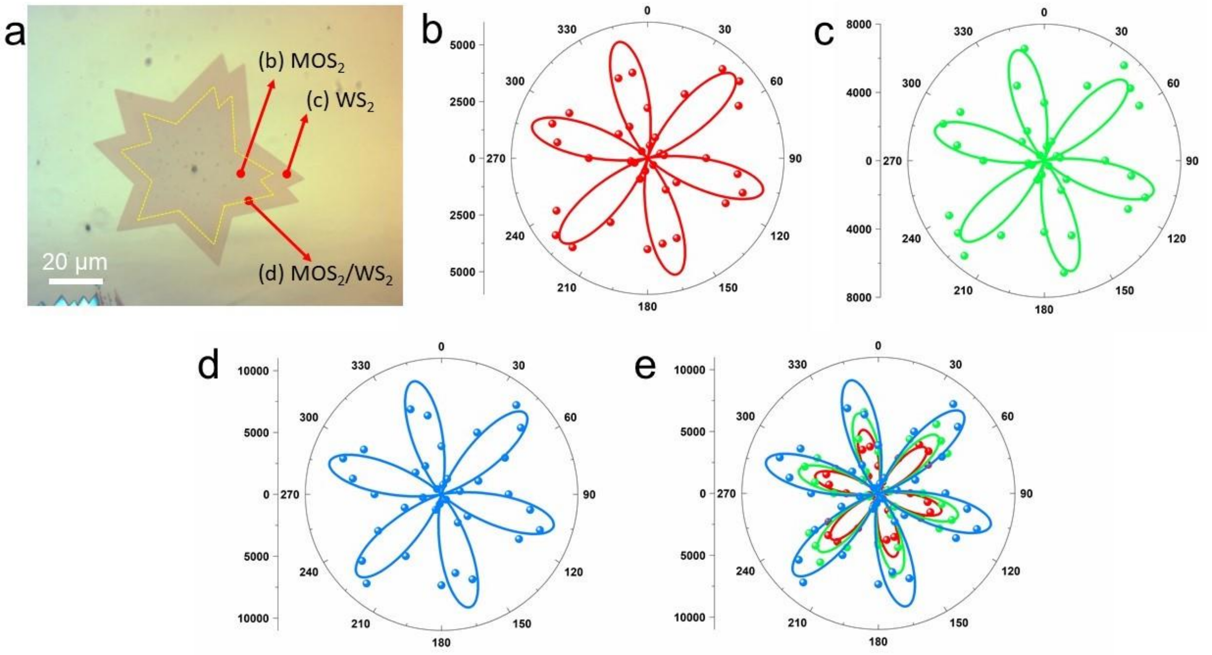

Fig. 4. Second-harmonic generation (SHG) characterization of the MoS$_2$-WS$_2$ lateral heterostructures.

a) The optical image of the heterostructure. b-d) SHG signals obtained from MoS$_2$ in the core, WS$_2$ in the shell and the interface. e) The overall signals of the lateral heterostructure.

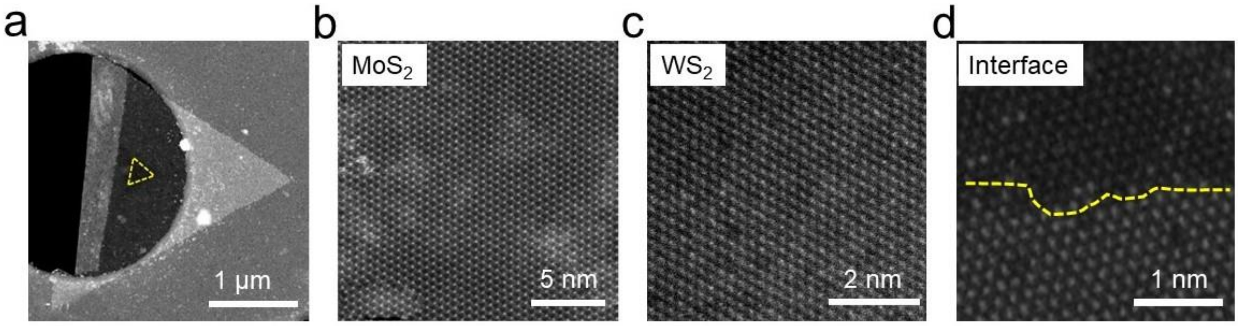

Fig. 5. Annular dark-field scanning transmission electron microscope (ADF-STEM) characterization of the MoS$_2$-WS$_2$ lateral heterostructures.

a) A low-magnified ADF-STEM image of the MoS$_2$-WS$_2$ lateral heterostructures with the side length of the inner MoS$_2$ triangle at about 300 nm. b-d) Atomic-resolution ADF-STEM images of MoS$_2$, WS$_2$ and the interface, respectively.

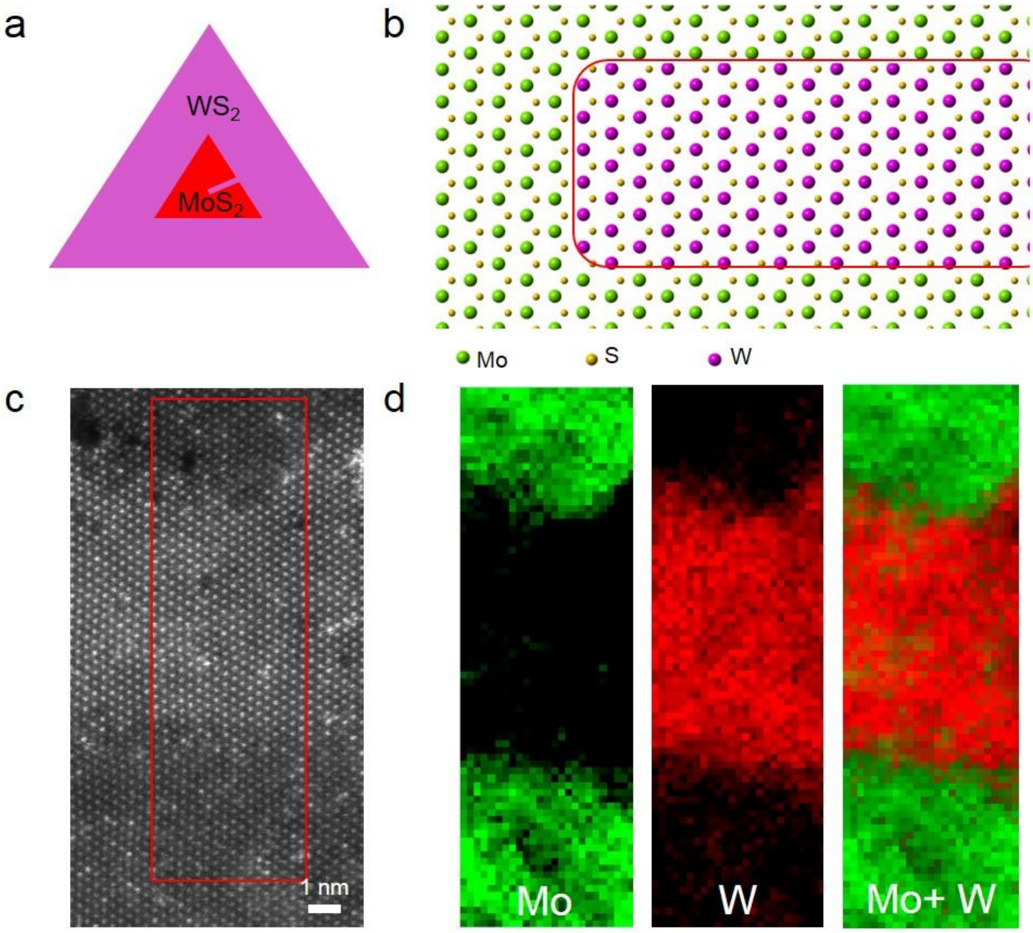

Fig. 6. Schematic and ADF-STEM characterization of the WS$_2$ quantum well in the MoS$_2$-WS$_2$ lateral heterojunctions.

a-b) The schematic and crystal structure of the heterostructure synthesized at 800 °C. The WS_2 quantum well shown in (b) is highlighted in-red. c) Atomic-resolution STEM images of the MoS_2-WS_2-MoS_2 lateral heterojunctions structure and the WS_2 quantum well structure. d) The electron energy loss spectroscopy (EELS) mapping of Mo, W and both, respectively.

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Disorder and dissipation in delta-doped phosphorus-in-silicon

Jesse A. Vaitkus[1*], Jackson S. Smith[1], Nicolas Vogt[1], and Jared H. Cole[1]
[1]*Chemical and Quantum Physics, School of Science, RMIT University, Melbourne 3001, Australia*
**e-mail: jesse.vaitkus@rmit.edu.au*

Delta-doped (δ-doping) phosphorus-in-silicon nanostructures are novel electronic devices that exhibit Ohmic scaling all the way down to the nanoscale[1]. These 'wires' are made using a δ-doping technique that combines scanning-probe lithography with molecular-beam epitaxy [2]. This technique achieves both high-density carrier concentrations and excellent two-dimensional (2D) confinement of donor atoms[3] giving rise to physics directly analogous to a two-dimensional electron gas (2DEG). Despite being an excellent candidate for patterned devices, details of the origin of elastic and inelastic scattering mechanisms is left wanting. Efforts hitherto have been completely bottom-up [4,5] utilizing fully atomistic models which are extremely computationally expensive. In contrast, we use a top-down approach using the so-called effective-mass approximation in which the lowest lying conduction band is approximated by a parabola with an effective electron mass. Using this method, the problem reduces to standard 2DEG physics and is extremely computationally cheap in comparison. Using our in-house codebase we can include disorder (Fig. 1) with given statistics[7], dissipation [8], and demonstrate fully quantum magnetotransport in mesoscopic systems using Non-Equilibrium Green's Functions (NEGF) [9].

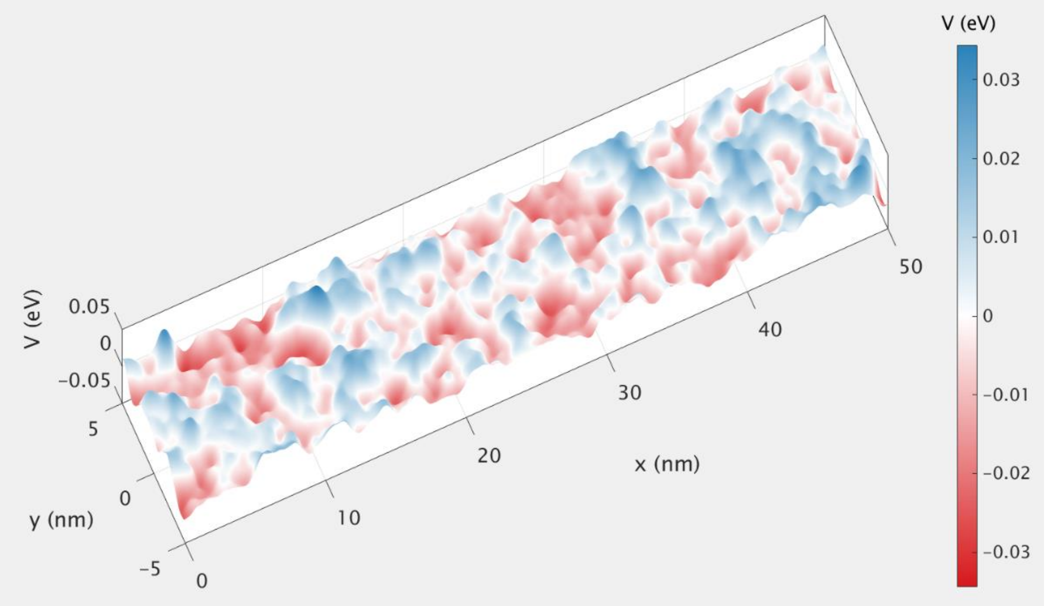

Fig. 1. Random potential disorder configuration calculated with disorder with a Gaussian correlation function with correlation length 1nm and RMS of 10meV.

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Improved Homogeneity and Performance of Field Effect Transistors Based on Wafer-Scale Continuous MoS2 Film towards Practical Application

Hu Xu, Haima Zhang, Zhongxun Guo , Peng Zhou, David Wei Zhang, Wenzhong Bao*

State Key Laboratory of ASIC and System, School of Microelectronics, Fudan University, Shanghai 200433, China

Atomic thin transition-metal dichalcogenides (TMDs) such as MoS_2 has been considered as an emerging platform to build next generation semiconductor devices. However, to date most device investigations are still based on exfoliated TMD sheets in micrometer scale. Here we propose a novel chemical vapor deposition (CVD) synthesis strategy by introducing the multilayer (ML) MoS_2 islands to improve the contact and high-*k* dielectric deposition. A four-probe method is applied to confirm that the contact resistance decreases by one order of magnitude. It can be attributed to the extra amount of exposed edges from ML-MoS_2 islands to guarantee a conformal contact with evaporated metal electrodes. Based on such wafer scale (2-inch) continuous MoS_2 films synthesized on an insulating substrate, top-gated field effect transistor (FET) array is also fabricated to explore key metrics such as threshold voltage (V_T) and field effect mobility (μ_{FE}) for hundreds of MoS_2 FETs (Fig. 1). The statistical results exhibit surprisingly low variability of these parameters. An average effective field effect mobility of 70 $cm^2V^{-1}s^{-1}$ and subthreshold swing (*SS*) about 150 mV/dec are extracted from these MoS_2 FETs, which are comparable to the best top gated MoS_2 FETs achieved by mechanical exfoliation. The result is a key step towards scaling 2D-TMDs into functional systems and paves the way for the future development of 2D-TMDs integrated circuits.

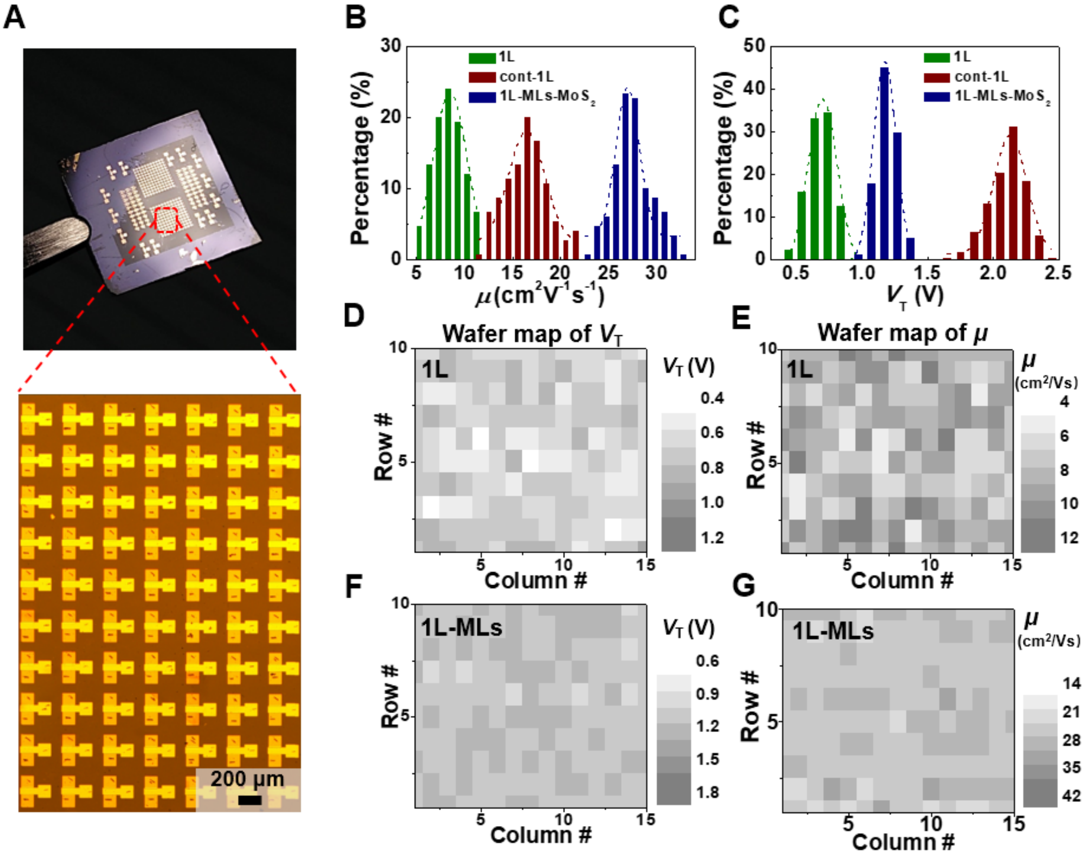

Fig. 1. Batch fabrication and uniformity characterization of MoS_2 FETs. (**A**) Batch-fabricated MoS_2 FET array on a diced 1×1 cm^2 wafer. (**B** to **C**) Histogram and Gaussian distribution fits of statistical data for 1L, cont-1L and 1L-MLs-MoS_2 FETs. (B) Field effect mobility μ extracted from linear regime of transfer curves. (C) Threshold voltage V_T calculated by the linear extrapolation method. (**D** to **G**) Mapping of V_T (**D** and **F**) and μ (**E** and **G**) according to the device location on the chip, for 1L (**D** and **E**) and 1L-MLs-MoS_2 (**F** and **G**). The range of gray scale is set as the mean value with ±50% offset, for convenience of comparison.

Large-area and Layer-controlled Synthesis of few layer MoS_2 assisted by sodium chloride

Pengfei Yang[1], Yanfeng Zhang [1,*]

1 Center for Nanochemistry (CNC), Academy for Advanced Interdisciplinary Studies, Department of Materials Science and Engineering, College of Engineering, Peking University, Beijing 100871, P. R. China
**e-mail: yanfengzhang@pku.edu.cn*

Atomically layered two-dimensional transition metal dichalcogenides (TMDCs) have opened new perspectives for the future electronics and optoelectronics owing to their thickness-dependent physical and chemical properties. A method for the synthesis of large-area and layer-controlled TMDCs is of vital importance. Herein, by assist of commercial sodium chloride, we develop a controllable low-pressure CVD method to grow large-area few layer MoS_2. Raman, UV, and PL are performed to show highly uniform thickness with areas exceeding hundreds of micrometers. In addition, by using glass as substrate, the sample can be detached free of etching and damage. The chemically homogenous junctions arising from neighboring MoS_2 domains that vary in layer thickness exhibits rectification behavior. The fabrication of photodectors present high performance. This work provides a promising future for the layer-engineering and applications of two-dimensional TMDCs.

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Plasma-assisted fabrication of ‘in-depth’ doped mos$_2$ vertical homostructure for optoelectronics application

Zhang, Xiao-Mei Presenting Corresponding[1,2,*]

[1]*Department of Mechanical Engineering,* [2]*Department of Chemical Science and Engineering; Tokyo Institute of Technology, Tokyo, Japan.*
**e-mail: zhang.x.as@m.titech.ac.jp*

Two-dimensional (2D) atomic layered crystals are believed to be the most promising candidates for optoelectronic applications, due to their unique properties such as their optimum thickness scalability, superior intrinsic strain limit and near ideal transparency. Large-bandgap transition metal dichalcogenides (TMDs) (for example, MoS_2) offer experimental mobility approaching single-crystal silicon thin-film transistors, with two orders of magnitude thinner profile and high strain limits (up to 20-30%). [1] In this work, I report a large-area growth of MoS_2 atomic layers on SiO_2 substrates via Vapor-Phase deposition. The growth of MoS_2 is carried out by chemical vapor deposition (CVD) method in a tube furnace via codepositing MoO_3 and S on a heated substrate in a flowing Ar ambient. Fig.1 shows an optical image of one local section with MoS_2 over 500 µm in size on the SiO_2 substrate. The MoS_2 vertical homostructure is fabricated via an ‘In-Depth’ doping process by plasma surface treatment. To generate a p-n homojunction in multilayer (ML)-MoS_2, an effective doping depth control is a challenging due to their atomistically thin dimensions. Compared to surface functionalization and substitutional CVD doping, plasma treatment emerges as the most effective doping technique for layered MoS_2 due to a wide range of doping that can be achieved with good control and selectivity. Fluorine (F)- and oxygen (O) atoms are the critical dopants responsible for the p-doping in MoS_2, due to a surface charge transfer processes between the strong electronegativity dopants and MoS_2 layers. [2] Additionally, such surface charge transfer processes induced by the dopant atoms can only affect the top few layers due to the screening of electric field in MoS_2. The ‘In-Depth’ plasma-assisted doping process can realize a vertical p-n homojunction in the ML-MoS_2. The MoS_2 vertical homojunction demonstrates a potential of doped MoS_2 for quasi-transparent optical components in light harvesting cells and nanoscale optoelectronics.

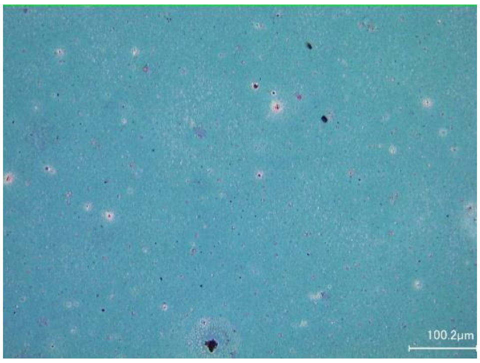

Fig. 1. Optical image of one local section with MoS_2 on the SiO_2 substrate

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Device applications in electronoics, photonics and optoelectronics

Optoelectronic devices based on few-layer black phosphorus

Taimur Ahmed[1,*], Sruthi Kuriakose[1], Vipul Bansal[2], Sharath Sriram[1], Madhu Bhaskaran[1] and Sumeet Walia[1]
[1]*Functional Materials and Microsystems Research Group and Micro Nano Research Facility, RMIT University, Melbourne VIC 3001, Australia*
[2]*Ian Potter NanoBioSensing Facility and NanoBiotechnology Research Laboratory, School of Science, RMIT University, Melbourne VIC 3001, Australia*
**e-mail: Taimur.ahmed@rmit.edu.au*

Black phosphorus (BP) has recently emerged as an exciting elemental two–dimensional (2D) material with exotic electronic and optoelectronic properties that are easily tunable [1, 2]. Owing to the broadband photoabsorption in BP, covering from ultraviolet (UV) to infrared [3, 4], and strong light-matter coupling [5] render it an ideal 2D material for opto-electronic devices which can manipulated their photoresponse under different excitation wavelengths. Here we show that ambient oxidation induced trap sites lead BP to exhibit a unique photoresponse in different UV wavelengths, *i.e.*, positive photocurrent under 280 nm (UV-B, Fig. 1a) and negative photocurrent in 365 nm (UV-A, Fig. 1b) excitations. We exploit this unique photoresponse of BP for selective sensing of UV band radiation. Also, we employ positive and negative photocurrent of BP to mimic excitatory and inhibitory action potentials, respectively, in a biological synapse. Furthermore, we demonstrate all-optical BP synaptic devices capable of imitating key neural behaviors such as psychological learning and forgetting, pulsed-pair facilitation and spatiotemporally correlated dynamic logic.

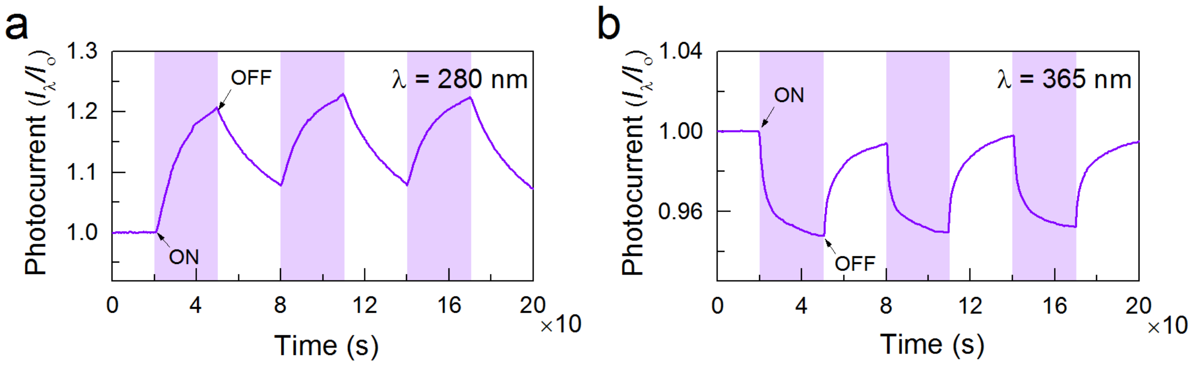

Fig. 1. Photoresponse of a BP photo-transistor under UV excitation wavelengths. Transient photocurrent of BP under (a) 280 nm illumination, exhibiting a positive photocurrent, and (b) 365 nm illumination, exhibiting a negative photocurrent.

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Synthesis of Large Area Quasi-2D MoO_{3-x} for High Performance Optoelectronic Devices

Arash, Aram[1], Bhaskaran, Madhu [1], Sriram, Sharath [1], Balendhran, Sivacarendran[1,*]

[1]School of Engineering, RMIT University, Melbourne, Australia
**e-mail: shiva.balendhran@rmit.edu.au*

Two-dimensional (2D) molybdenum trioxide has been attracting research interest due to its band gap tunability and a wide variety of its optoelectronic properties [1]. However, the lack of a reproducible synthesis process for large coverage quasi-2D MoO$_3$ has limited its progress. Here we report on the synthesis of large area quasi-2D MoO$_{3-x}$ via physical vapor deposition, using MoO$_3$ powder as the precursor. The as-grown layers are directly grown on SiO$_2$/Si, eliminating the necessity for any transfer process. The quality of the crystal growth is controlled by varying precursor amount, growth temperature and pressure. These as-grown MoO$_{3-x}$ layers allow for the fabrication of low power UV sensor arrays with rapid response times (200 µs) and responsivity up to 98 µA/W.V, at a bias voltage of 0.1 V, which is at least 400 times power efficient than the next best contender.

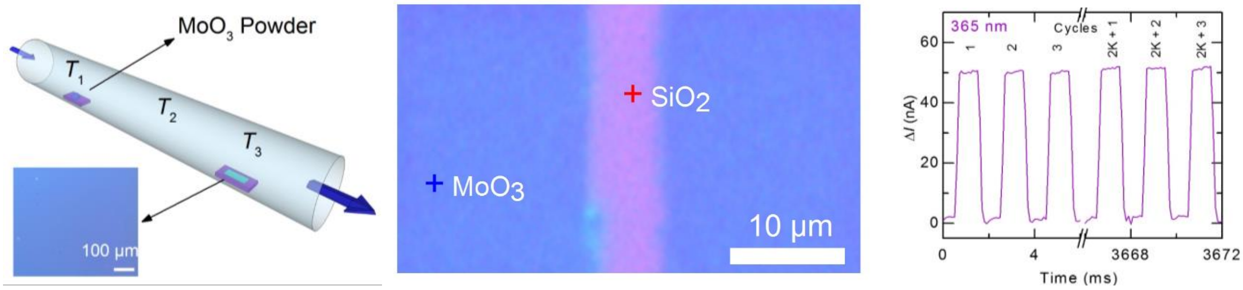

Fig. 1. Left to right: Schematic of CVD process, optical image of as-grown MoO$_{3-x}$ layers, UV photocurrent response for as-grown based device

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Integration of graphene nanofibers to achieve an efficiency breakthrough in hole blocking layer-free perovkite solar cells

Xi Chen*, Min Gu*

Laboratory of Artificial-Intelligence Nanophotonics, School of Science, RMIT University, Melbourne, 3000, Australia
**e-mail: xi.chen5@rmit.edu.au; min.gu@rmit.edu.au*

Hole blocking layer (HBL)-free perovkite solar cell (PSC), an innovative photovoltaic device getting rid of complex and high-temperature fabrication processes [1-2], has been regarded as promising strategies for renewable energy conversion. However, HBL-free PSCs suffer from low energy conversion efficiencies. In this paper, we realize an efficiency breakthrough in such solar cells via the incorporation of an innovative nanomaterial - graphene nanofibres, A remarkable 16.64% efficiency has been achieved through the nanofibre integration into PSCs. This value is significantly higher than that of the state-of-the-art HBL-free PSCs fabricated by simple procedures (around 15%) [1-2].

The graphene nanofibres, containing an inner amorphous core and outer crystalline walls, are synthesized through longitudinal wall cutting of carbon fibres by wet chemical method [3], in which the average diameter of the fibre decreases from 250 nm to 75 nm (Fig. 1a). The graphene nanofibres are sprayed above a Spiro-MeOTAD layer in a HBL-free PSC (without an Au back contact), and then another Spiro-MeOTAD layer is spin-coated followed by thermal evaporation of the Au back contact (Fig. 1b).

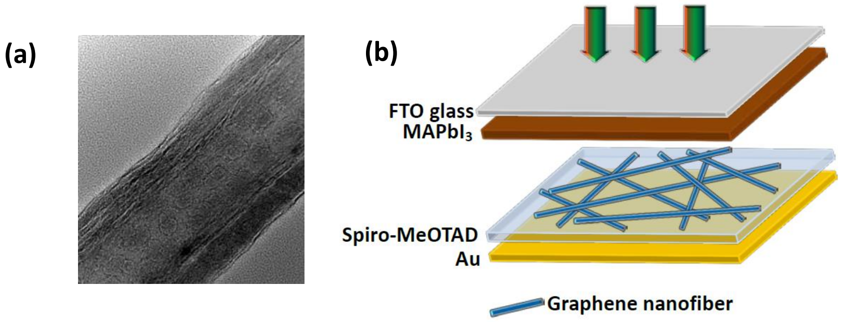

Fig. 1. (a) TEM image of a grapene naofibre. Scale bar: 50 nm. (b) Structure of a HBL-free PSC with the integration of grapene naofibres.

The nanofibre exhibits an excellent electrical property for the performance boost in PSCs, which electrical conductivity is much higher than that of Spiro-MeOTAD. The sheet resistances of a 200 nm nanofibre-integrated Spiro-MeOTAD layer decrease substantially with the increase of the integration coverages, from 563 Ω/sq of the particle-free layer to 368 Ω/sq under 20% coverage. Under such coverage the nanofibre-integrated HBL-free PSC delivers a J_{sc} of 21.36 mA/cm^2, a V_{oc} of 1.093 V, and a fill factor of 0.713, leading to an efficiency of 16.64% under standard AM1.5G illumination. The efficiency is 19.8% higher than that of the nanofibre-free PSC with an efficiency of 13.89%.

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Graphene FET based detection of the non-zero planar dipole moment of cytosine

Dontschuk, Nikolai[1,2,*], Taditch, Anton[2], Stacey, Alastair[1,2]

[1]School of Physics, The University of Melbourne, Parkville VIC 3010, Australia
[2]CQC2T, School of Physics, The University of Melbourne, Parkville VIC 3010, Australia
[3]The Australian Synchrotron, 800 Blackburn Rd Clayton VIC 3168, Australia
**e-mail: dontschuk.n@unimelb.edu.au*

The interactions of fundamental bio-molecules and solid surfaces provides a~~nd~~ rich and important field of study, with implications ranging from single molecule sensing [1,2] to deciphering the origins of life [3]. Graphene provides a powerful substrate upon which the interactions of planar bio-molecules, such as DNA nucleobases, can be investigated with unmatched sensitivity. Here we present work that combines electrical measurements from exposed channel graphene field effect transistors (FETs) and synchrotron based soft x-ray measurements to probe the interactions of cytosine with graphene in an ultra high vacuum environment. We show that at low coverages the cytosine adsorbs in a planar π-π stacking arrangement. Surprisingly this allows us to directly observe that cytosine has an intrinsic planar component to its dipole moment (μ_z). Changes to the graphene work function and Fermi level, measured with both electrical and x-ray techniques, were induced by the combined dipole field of a quantifiable coverage of cytosine molecules, which we were able to measure as $\mu_z \approx 0.16$ eÅ per molecule. This result agrees with *ab-initio* modelling of the expected intrinsic planar dipole component [4,5].

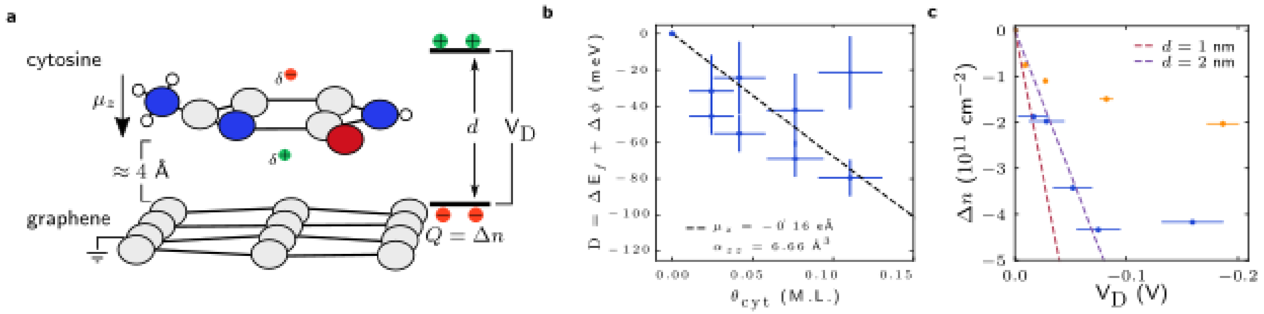

Fig. 1. (a) A schematic of cytosine adsorbed on graphene indicating the vital parameters that dictate changes to the graphene work function via the cytosine dipole field (V_D) and graphene doping. **(b)** Cytosine coverage induced changes to the graphene work function, with the expected relationship for $\mu_z \approx 0.16$ eÅ shown as a black dashed line. **(c)** Measured relationship between dipole field and graphene doping.

We have also explored the limits of sensitivity of graphene field effect transistors, showing the surprising result that the per-cytosine current response of a graphene FET based sensor has a super-linear relationship to the carrier density within the graphene. Even with the modest values of carrier density that could be achieve in our devices with a 90 nm back gate we show that single molecule detection of cytosine would be possible with a 100 x 100 nm device geometry.

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Ultrasensitive Two-dimensional Bi_2O_2Se Phototransistors on Silicon Substrate

Qundong Fu[1], Chao Zhu[1], Xiaoxu Zhao[2], Stephen John Pennycook[2], and Zheng Liu[1,*]

[1]School of Materials Science and Engineering, Nanyang Technological University,
Singapore 639798,
Singapore
E-mail: z.liu@ntu.edu.sg.
[2]National University of Singapore, Department of Materials Science and Engineering,
Block EA 07-14, 9 Engineering Drive 1, 117575,
Singapore

Two-dimensional (2D) materials have been considered as intriguing building blocks for next generation optoelectronic devices. However, their photoresponse performances still need to be improved for practical applications. We demonstrated ultrasensitive 2D phototransistors employing CVD-grown 2D Bi_2O_2Se transferred onto silicon substrate with a non-corrosive transfer method. The as-transferred Bi_2O_2Se preserved a high quality in contrast to the serious quality degradation in the HF-assisted transfer. The phototransistors showed a responsivity of 3.5×104 AW^{-1}, a photoconductive gain of more than 10^4, and a time response in the order of sub-millisecond. With the back gating of silicon substrate, the dark current could be reduced to several pA. This yields an ultrahigh sensitivity with the specific detectivity of 9.0×10^{13} Jones, which is one of the highest values among 2D material photodetectors and two orders of magnitude higher than that of other CVD-grown 2D materials.[1,2] The high performances of the phototransistor shown here together with the developed unique transfer technique are promising for the development of novel 2D material based optoelectronic applications, as well as integrating with state-of-the-art silicon photonic and electronic technologies.

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Enhancing charge density wave driven resistance switching through gate control

Mahajan, Mehak, Murali, Krishna, and Majumdar, Kausik*
Department of Electrical Communication Engineering, Indian Institute of Science, Bangalore 560012, India.
*email: kausikm@iisc.ac.in

1T-TaS_2 is a unique layered material that exhibits temperature dependent resistivity switching resulting from different charge density wave (CDW) phases. The nearly-commensurate (NC) to incommensurate (IC) phase transition is of high practical interest which can be driven electrically while operating at room temperature. This has attracted several applications such as fast broadband photodetection, neuromorphic computing, fast oscillator [1-3]. However, the resistivity switching ratio due to this phase transition is small () and cannot be tuned by a gate voltage thereby limiting its widespread usage.

In this work, by using a 1T-TaS_2/2H-MoS_2 heterojunction (Fig. 1a), we achieve a gate-controlled resistivity switching during the NC-IC phase transition of TaS_2 (Fig. 1b), and the switching ratio is enhanced by a factor of (Fig. 1c) compared to the isolated 1T-TaS_2 control (dashed line in Fig. 1c). We show that in addition to the resistivity switching in TaS_2, the NC-IC phase transition brings about a suppression of the Schottky barrier height (SBH) at the 1T-TaS_2/2H-MoS_2 contact interface. The change in the SBH during the phase transition results in a gate voltage dependent carrier injection from TaS_2 to MoS_2 (Fig. 1d), allowing us to control the resistance switching ratio by a back-gate voltage. Further, another SBH change is observed in the same structure due to the commensurate (C) to triclinic (T) phase transition during the heating cycle, from which the Mott gap opening in the C phase of 1T-TaS_2 is extracted to be ± 7 meV. The results show a promising pathway to modulate the CDW induced resistivity switching which is attractive for a variety of device applications.

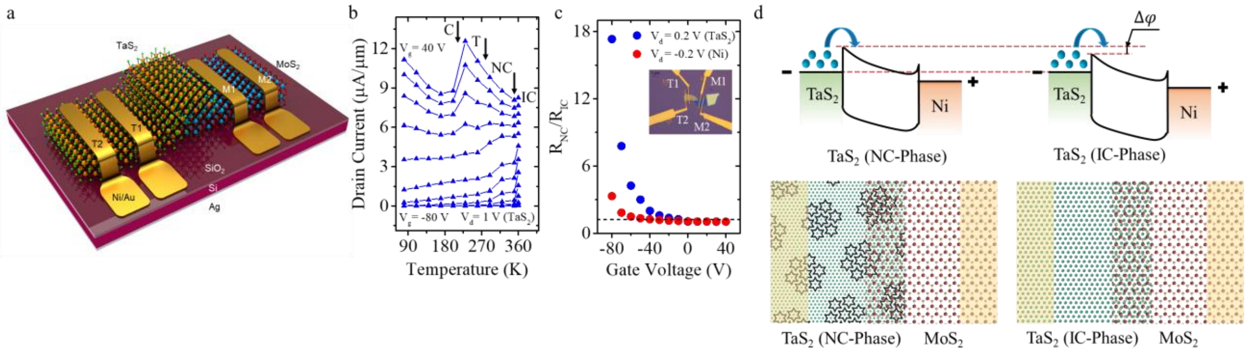

Fig. 1. (a) Schematic of the heterojunction device. (b) Temperature dependent drain current (probing terminals T1 and M1) under (electron injection by TaS_2). (c) Gate voltage dependent resistance switching ratio for TaS_2 injection and Ni injection . Dashed line shows data from TaS_2 control. Inset: Optical image of the fabricated device. (d) Schematic explanation of the mechanism illustrating SBH suppression due to NC-IC phase transition.

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Stable and scalable 1T MoS_2 with low temperature-coefficient of resistance

Sharma, Chithra H[1], Surendran, Ananthu P[1], Thalakulam, Madhu[1,*]

[1] *School of Physics, Indian Institute of Science Education and Research, Thiruvananthapuram, Kerala, India*
**e-mail: madhu@iisertvm.ac.in*

Among the van der Waals systems MoS_2 is a highly tunable and easily available choice with robust electrical and mechanical properties. The presence of 2D polymorphic phases with distinct electrical properties makes MoS_2 a potential candidate for all-2D monolithic circuits. While the semiconducting 2H phase is widely studied for device applications, the electrical characteristics of 1T MoS_2 is relatively unexplored. A method for engineering a stable 1T phase from the 2H phase in a scalable manner is wanting at large. Here we demonstrate a controllable and scalable 2H to 1T phase engineering technique for MoS_2 using microwave plasma. Our method allows lithographically defining large-area 1T regions in a 2H sample. Structural characterizations of these phases performed using HR-TEM and Raman scattering experiments, the electrical characterizations of the 2H, 1T and the 1T/2H junctions down to 4 K will be discussed. The 1T samples show excellent temporal and thermal stability making it suitable for standard device fabrication techniques. We conduct both two-probe and four-probe electrical transport measurements on devices with back-gated field effect transistor geometry in a temperature range of 4 K to 300 K. The 1T samples exhibit Ohmic current-voltage characteristics in all temperature ranges without any dependence to the gate voltage, a signature indicative of a metallic state. The sheet resistance of our 1T MoS_2 sample is considerably lower and the carrier concentration is a few orders of magnitude higher than that of the 2H samples. In addition, our samples show negligible temperature dependence of resistance from 4 K to 300 K ruling out any hoping mediated or activated electrical transport

Near-Infrared Photoresponse Excitations at WSe_2–Organic Molecules Interfaces

Haining, Liu [1,2], Liming Xie [1,2*]

[1]*CAS Key Laboratory of Standardization and Measurement for Nanotechnology, CAS Center for Excellence in Nanoscience, National Center for Nanoscience and Technology, Beijing 100190, P. R. China*
[2]*University of Chinese Academy of Sciences, Beijing 100049, P. R. China.*
**e-mail: Xielm@nanoctr.cn*

The interface between molecules and two-dimensional materials has attracted broad interest and is becoming emerging technologies in photoelectronic applications. Here, we have found near infrared (NIR) interface excitations at the interfaces of two-dimensional transition metal dichalcogenides/organic molecules, in which there are tightly bound electron-hole pairs due to charge-transfer (CT). Our electrical measurements have revealed low-energy CT bands in the near infrared (NIR) region up to 1200 nm for WSe2-TCNQ (tetracyanoquinodimethane) complex and 1300 nm for WSe2-F4TCNQ (2,3,5,6-Tetrafluoro-tetracyanoquinodimethane) complex, respectively. Meanwhile, the dark current of the complexes is extremely low which can be dowm to pA. The photoresponse property of the WSe2-organic CT complexes can be tuned by electrical gating of WSe2.

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Broadband photodetectors based on graphene-charge transfer complexes (CPX) hybrid structure with ultra high photoresponsivity

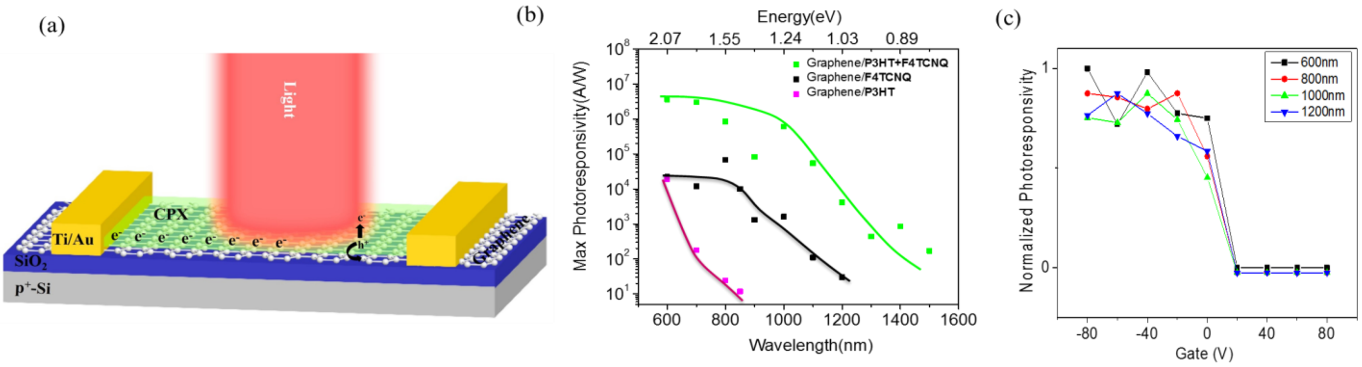
Iqbal, Muhammad Ahsan[1, 2], Liming, Xie [1, 2,*]

[1]*CAS Key Laboratory of Standardization and Measurement for Nanotechnology, CAS Center for Excellence in Nanoscience, National Center for Nanoscience and Technology, Beijing 100190, P. R. China.*
[2]*University of Chinese Academy of Sciences, Beijing 100049, P. R. China.*
**e-mail: xielm@nanoctr.cn*

Infrared photodetectors have widespread applications in telecommunication, thermal imaging and bio-medical imaging, etc. [1]. Organic charge transfer complexes (CPXs) have been developed as promising materials for the near infrared (NIR) photodetecion applications [2-4] .However, the low mobility have limited the photoresponsivity of organic CPX based photodetectors[5] [6]. Here, thin layer of organic CPX are integrated on graphene transistor channel to form hybrid phototransistors with ultra-high photoresponsivity of $\approx 10^6$ A W^{-1} in NIR region.

Fig. 1. (a) Schematic sketch for hybrid phototransistor structure and (b) Wavelength dependent photoresponsivity of Graphene/ P3HT +F4TCNQ, Graphene/P3HT & Graphene/F4TCNQ. (Vbais=1V, Vg= -40V) (c)Gate-dependent normalized photoresponsivity of graphene/ (P3HT +F4TCNQ) at different wavelengths (fix power intensity for each wavelength) (Vbais=1V).

Our study reveals graphene-organic CPX have shown a broadband photoresponse from the visible to NIR range. A high photoelectric gain resulting from the photogating effect at the graphene/CPX interface. In addition, the photoresponse property of graphene-organic CPX can be regulated by electrical gating of graphene [7] [8]. Our findings pave the way toward the implementation high performance in the IR wavelength regime with potential applications in optoelectronics.



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Comparing the second harmonic generation on MoS_2 with different stacking orders

Jungcheol Kim[1], Woongki Na[1], Hyeonsik Cheong[1]

[1]Department of Physics, Sogang University, Seoul 04107, Korea

The effects of stacking order in the second harmonic generation (SHG) of molybdenum disulfide (MoS_2) are investigated. 2H-MoS_2 is representative of semiconducting transition metal dichalcogenides (TMDCs). Although 2H-MoS_2 is most common in nature, the 3R phase can exist due to a small difference in the formation energy. However, most studies so far have focused on the 2H phase, and only few studies are reported for the 3R and mixed phases[1]. We found the 2H, 3R and mixed phase of exfoliated MoS_2 from natural molybdenite crystals. We compared the SHG of samples with different stacking orders in detail. Moreover, we estimate the value of the second order susceptibility which can be beneficial for developing realistic 2-dimensional nonlinear optical devices using each stacking order.

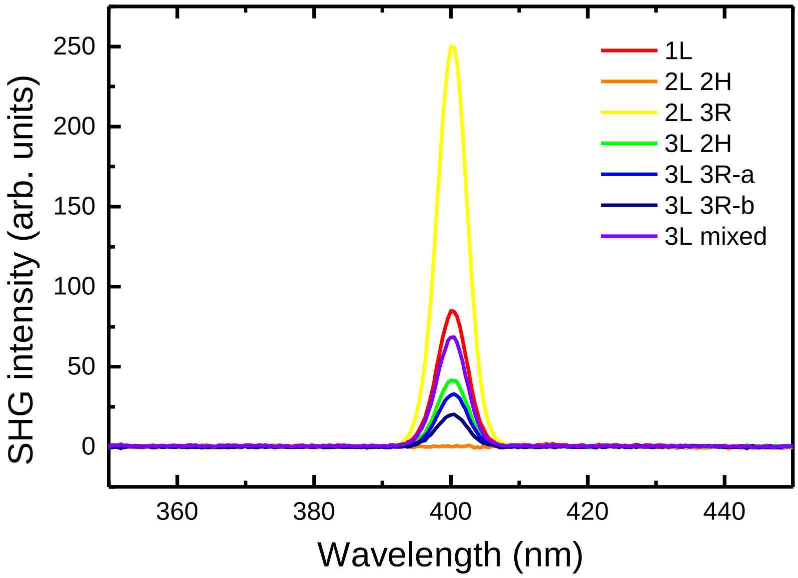

Fig. 1. SHG response using 800 nm excitation source on MoS_2 with different stacking orders

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Graphene reflective microlens

Han Lin[1]* and Baohua Jia[1]

[1]Centre for Micro-Photonics, Faculty of Science, Engineering and Technology, Swinburne University of Technology, P.O. Box 218, Hawthorn VIC 3122, Australia.

*Correspondence to: hanlin@swin.edu.au

Modern technology relies on multifunction devices that combine integrated optical, mechanical, and electrical systems. Optics and optoelectronics play an important role in communication, processing, sensing, and display systems. Micro-optics is important in this context because it enables the miniaturization of photonic systems and enhances the integration, precision, multifunctionality, and energy saving characteristics of these devices. Micro-optics, microlenses and microlens arrays become increasingly important[1].

Conventional microlenses are transmission lenses, which have strong chromatic aberration due to the dispersion of the materials. In comparison, reflective lenses are able to focus light at different wavelength to the same focal spot without chromatic aberration. However, no reflective microlens has been demonstrated due to the difficulty in fabrication[1].

In this work, we discover that graphene microbubble can be used as an efficient reflective microlens due to the highly symmetric near perfect curvature, which is able to focus laser beam into a diffraction-limited ultra-long photonic jet (Fig. 1) using the versatile direct laser fabrication technique in graphene oxide (GO) material. It is envisaged that the GO microbubbles may find applications in many micro-biophotonic devices [2] for in-situ imaging, spectroscopy and sensing at positions on-demand.

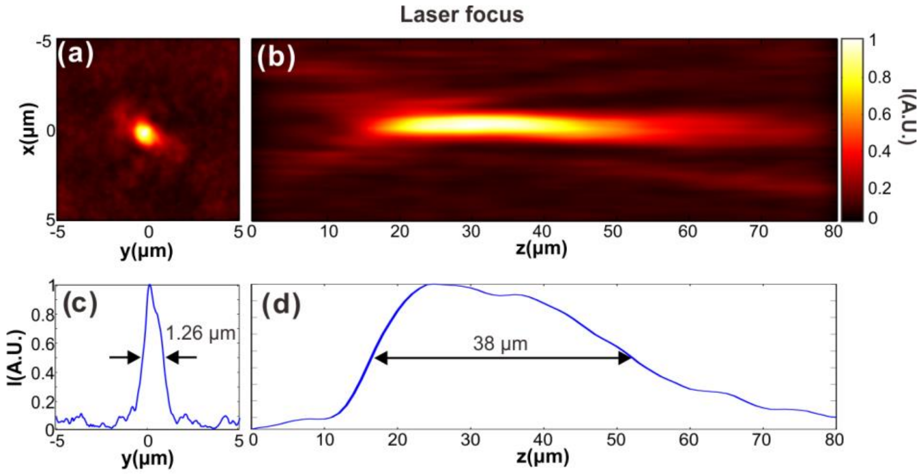

Fig. 1 Measured ultra-long graphene photonic jet illuminated by He-Ne laser. Intensity distribution of the ultra-long photonic jet in the x-y focal plane (a) and x-z focal plane (b), and the intensity plots along the y-direction (c) and z-direction (d).

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Flexible and highly sensitive strain-pressure sensor based on TMDs-assisted graphene foam/polymer hybrid nanostructures

Mondal Shuvra [1,2], Kim Seong Jun [1], Min Bok Ki [1], and Choi Choon-Gi [1, 2,*]

[1] *Graphene Research Lab., Emerging Devices Research Group, Electronics and Telecommunications Research Institute (ETRI), Daejeon, Korea*
[2] *School of ETRI (ICT-Advanced Device Technology), University of Science and Technology (UST), Daejeon, Korea*

**e-mail: cgchoi@etri.re.kr*

Strain-pressure sensors for health monitoring and biomedical application have gained considerable attention in recent years due to their feasible functionality on flexible electronics and superior electronic properties. Recently, connected 3D structure of graphene with microporous network structure forming graphene porous network (GPN) assisted with Ecoflex as a graphene supporting polymer exhibited excellent electrical and mechanical stability. In addition, transition metal dichalcogenides (TMDs) such as MoS_2-based piezo-resistive sensors are well known for their excellent mechanical properties and high gauge factor.

Herein, we introduce a flexible and highly sensitive strain-pressure sensor based on TMDs-assisted graphene foam/Ecoflex composite hybrid nanostructures. The hybrid nanostructures consist of a molybdenum disulfide (MoS_2) with different concentration of $(NH_4)_2MoS_4$ formed as nanoflakes on MoS_2 planner sheets for the enhancement of sensing performance. The MoS_2 planner sheets were uniformly arranged with a cracked-paddy shape on the GPN, and the size of nanoflakes formed on MoS_2 planner sheets was gradually enlarged by increasing the concentration of $(NH_4)_2MoS_4$ solution. In our finding, these conformal nanostructures of MoS_2 on the GPN can produce improved resistance variation against external strain and pressure. The presence of the graphene and MoS_2 were confirmed in MoS_2/GPN/Ecoflex by X-ray photoelectron spectroscopy (XPS) and Raman analysis. Consequently, our MoS_2/GPN/Ecoflex sensor exhibited noticeably improved sensitivity compared to previously reported GPN/PDMS sensors in a pressure test due to the existence of the MoS_2 nanoflakes. Notably, the MoS_2/GPN/Ecoflex sensor showed a high sensitivity of ~6 kPa^{-1} at MoS_2 synthesized using 1.25 wt% $(NH_4)_2MoS_4$. Additionally, it showed excellent durability even under repeated loading-unloading pressure over 4000 cycles. This study paves the way to apply as pressure-strain sensor for human motion detection and healthcare applications.

Photodetection Study in Bilayer MoS_2 using Pd Schottky Contact

Moun, Monika*, Singh, Aditya, Tak, B.R., Singh Rajendra

Department of Physics, Indian Institute of Technology Delhi, Hauz Khas, New Delhi-110016, India
**e-mail: monikamoun18@mail.com*

Two-dimensional (2D) materials based devices have been investigated with great interest in recent past for their potential application in electronic and opto-electronic devices. Molybdenum disulfide (MoS_2) has been considered as a promising candidate due to its unique properties such as presence of both indirect and direct bandgap and high ON/OFF ratio. Photodetection is one of the main aspects of MoS_2 based opto-electronic devices.

In the present work, uniform bilayer MoS_2 flakes were grown on SiO_2/Si substrate using chemical vapor deposition method. Characterization of as synthesized MoS_2 flakes were carried out using Raman, PL and AFM. Metal electrodes on MoS_2 flake were patterned using electron beam lithography and deposited using thermal evaporation system followed by lift off in acetone. Palladium being a high work function metal makes Schottky contact with MoS_2. Pd/Au was patterned on MoS_2 flake in MSM geometry. Further, the fabricated device was electrically characterized in dark and illumination condition using a DC probe station. Spectral response of the device was recorded and maximum responsivity of 0.8 A/W was observed at 650 nm which corresponds to bandgap of monolayer MoS_2. Saturation in the responsivity was observed when the device was further illuminated with higher laser energy than 650 nm wavelength. Power dependent electrical measurements ranging from 0.1 mW/cm^2 to 2 mW/cm^2 were performed at 650 nm incident light and photocurrent was observed to enhance with increasing power. In addition to this, persistent photoconductivity was also observed in the device. This may be due to the defects and vacancies present in as synthesized MoS_2 flakes or at MoS_2/SiO_2 interface which can lead to photocharge trapping.

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The effect of gamma irradiation on HBN encapsulated graphene field effect transistors

Narayanan Kutty, Maya[1*], Koybasi,Ozhan[2], Dahl,Øystein[3], Azar, Amin S.[3], Taniguchi, T.[4], Watanabe, K.[4], Monakhov Edouard[1], and Belle, Branson D.[2]
[1]*Centre for Materials Science and Nanotechnology, Department of Physics, University of Oslo, P.O. Box 1048, Blindern, N-0316 Oslo, Norway.*
**m.n.kutty@smn.uio.no*
[2]*SINTEF DIGITAL, Forskeningsveien 1, NO-0314 Oslo, Norway.*
[3]*SINTEF INDUSTRY, Forskeningsveien 1, NO-0314 Oslo, Norway.*
[4]*Advanced Nanomaterials Laboratory, High Pressure Group, National Institute for Materials Science, 1-1 Namiki, Tsukuba, Ibaraki 305-0044, Japan.*

Graphene field effect transistors (GFETs) provide a vehicle to investigate radiation effects as the field effect mobility and charge neutrality (Dirac) point are highly sensitive to surrounding environment traps, fixed charges at oxide/substrate interface. Prior studies have shown that Gamma radiation can cause electrically active defects in the substrate, increase trap density at the interfaces while causing displacement damage resulting in p-doped behavior [1]. We report Co_{60} (Gamma rays) radiation induced defects by evaluating the material and electrical response of hBN encapsulated exfoliated graphene and unencapsulated CVD GFETs. The Raman spectra (at 532nm) of unencapsulated CVD and hBN encapsulated devices pre and post irradiation (total dose of 5kGy) shows an upshift of both G and 2D peaks by about $5cm^{-1}$ in unencapsulated CVD graphene. This is in contrast to hBN encapsulated exfoliated graphene which only showed a small upshift in the 2D peak by $1cm^{-1}$ (see Fig.1). This slight upshift can be attributed to an increase in doping. The transport characteristics measured at 300K for hBN encapsulated GFET shows shift in dirac voltage from -2.72V pre-irradiation to +4V post-irradiation as shown in Fig.2 along with degradation of mobilities from $36x10^3cm^2$/V.s pre-irradiation to $21x10^3cm^2$/V.s post-irradiation. We infer that the energy deposited by radiation creates electrically charged defects in the substrate thereby affecting device performance. Furthermore, we will present the electrical and material study of the effects of increasing total dosage of gamma radiation providing further insight into creating radiation hardened graphene sensors.

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Figures

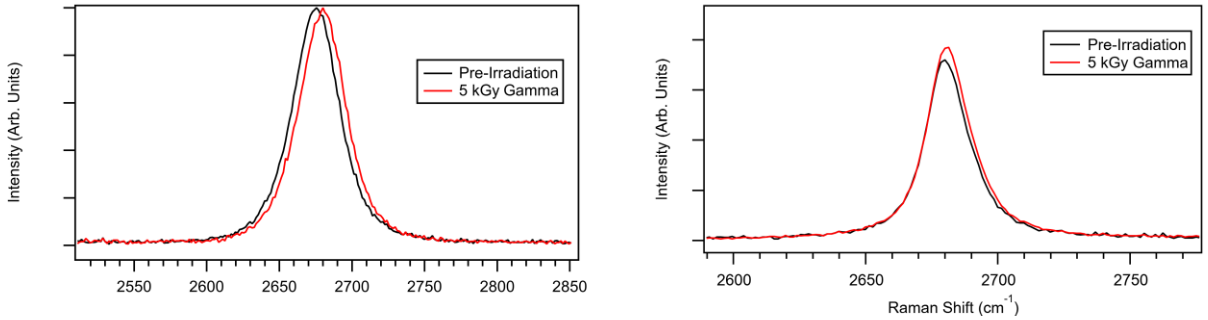

Fig. 1: 2D peak of Raman Spectrum for unencapsulated CVD graphene (left), hBN encapsulated GFET(right) pre and post irradiation

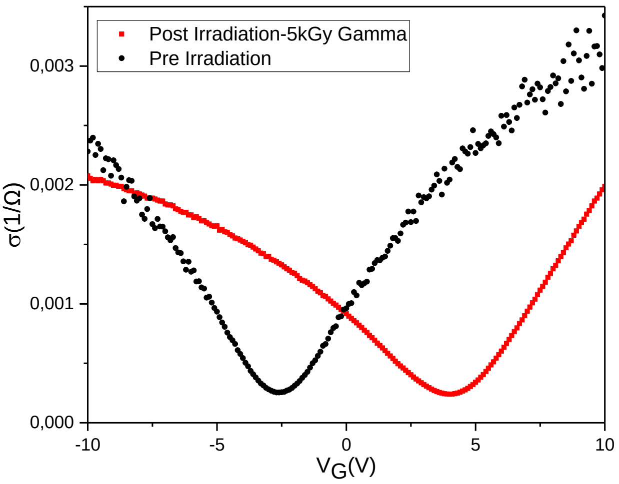

Fig. 2: Conductivity versus gate voltage of hBN encapsulated GFET pre and post irradiation.

Strong depletion in hybrid perovskite p-n junctions induced by local electronic doping

Ou, Qingdong[1,]*, Bao, Qiaoliang[1]

[1]Department of Materials Science & Engineering, ARC Center of Excellence in Future Low-Energy Electronics Technologies (FLEET), Monash University, Clayton, Victoria
**E-mail: qingdong.ou@monash.edu*

Organic-inorganic hybrid perovskites, a class of crystalline ionic semiconductors, are promising semiconductors because of their direct bandgap, long diffusion length and large dielectric constant.[1-4] Here, we would like to highlight our recent progress on carrier depletion in the lateral p-n junction induced by local electronic doping at the surface of individual $CH_3NH_3PbI_3$ perovskite nanosheets.[5]

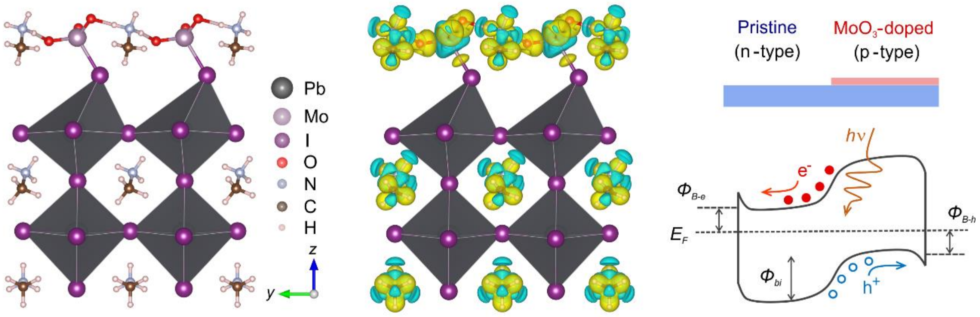

Fig. 1. Structure of MoO_3 doped lateral perovskite nanosheet p-n junctions.

Unlike conventional surface doping with a weak van der Waals adsorption, covalent bonding and hydrogen bonding between a MoO_3 dopant and the perovskite are theoretically predicted and experimentally verified. The strong hybridization-induced electronic coupling leads to an enhanced built-in electric field. The large electric permittivity arising from the ionic polarizability further contributes to the formation of an unusually broad depletion region up to 10 microns in the junction. Under visible optical excitation without electrical bias, the lateral diode demonstrates unprecedented photovoltaic conversion with an external quantum efficiency of 3.93% and a photodetection responsivity of 1.42 A W^{-1}. The p-n junctions presented may provide insight into new approaches for developing high-performance optoelectronic devices based on this family of materials.

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Electrical characteristics of epitaxial graphene on silicon

Pradeepkumar, Aiswarya[1], Mishra, Neeraj[1], Gaskill, D. Kurt[2], Iacopi, Francesca[1,*]

[1]School of Electrical and Data Engineering, University of Technology Sydney, Broadway, NSW 2007, Australia
[2]US Naval Research Laboratory, Washington, DC 20375, USA
**e-mail: francesca.iacopi@uts.edu.au*

Graphene can be a promising material for next generation nano-integrated devices owing to its extraordinary electronic properties [1]. Large-scale fabrication and exploitation of the outstanding electrical properties of graphene-based micro- and nano-devices has been held back so far by the cost and lack of a suitable method to synthesize graphene in a way that is compatible with existing semiconductor technology infrastructure and processes.

We have demonstrated a transfer free, self-aligned synthesis of high quality, uniform bilayer graphene directly on silicon wafer through cubic silicon carbide at temperatures compatible with conventional semiconductor processing [2]. This approach allows for easy wafer level patterning by self-alignment, and as such would represent an ideal test vehicle to explore and integrate the appealing electrical properties of graphene. However, the use of heteroepitaxial SiC on silicon should be approached carefully as we have recently shown that the 3C-SiC/Si electrical junction is unstable and prone to severe leakage because of the diffusion of interstitial carbon into the silicon matrix [3], leading to great difficulties. In this work, we aim to isolate and understand the electrical characteristics of graphene grown directly on cubic silicon carbide/silicon over large areas. With the help of room temperature Hall effect measurements as well as cryogenic transport measurements on van der Pauw structures of the graphene/3C-SiC/Si, we aim at establishing a general description of electrical behavior of the graphene on 3C-SiC/Si system.

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Investigation of Doping Effect by High-k Dielectric via Atomic Layer Deposition

Yaochen Sheng, Hu Xu, Wenzhong, Bao*

School of Microelectronics, Fudan University, Shanghai, China.
**e-mail: baowz@fudan.edu.cn*

Atomically thin transition metal dichalcogenides (TMDs) with appropriate bandgap show promising potential in electronics and optoelectronic applications. However, the serious doping after high-k dielectric deposition causes a nonnegligible shift of voltage threshold (V_T), which hinders the future circuit application. Here, we systematically investigate the doping effect caused by dielectric deposition for both exfoliated and Chemical Vapor Deposition (CVD) synthesized MoS_2 sheets.MoS_2 with various thickness, Optimizing ALD temperature, and different types of seeding layer are tested to minimize the doping effect. Additionally, deep learning algorithm is introduced to analyse key processing parameters and adopted as guidelines for future optimization of device processing.

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Heterogeneous copper nanowire-graphene oxide thin films: a cost-effective platform for transparent conductive electrodes

Thekkekara V Litty1,2*, Jason N Naveen2, Chen Wenlong2, Gu Min1

1Laboratory of Artificial Intelligence Nanophotonics, School of Science, RMIT University, Melbourne-3000, Australia
2 Department of Chemical Engineering, Monash University, Clayton-3800, Australia
.
**e-mail:*
littyvarghese.thekkekara@rmit.edu.au

Next generation technologies demand for the light-weight cost-effective integrable materials with maximum output efficiency [1]. Graphene is one of the most commonly used material towards this goal, but the lack of optical bandgap limits its real-life applications [2]. Widely used materials like gold and silver on the other hand are known for the excellent properties in the visible region [3]. However, the cost of these materials makes them less usable in the largescale applications. Graphene oxides [4] and copper nanowires [5] are the preferential alternatives in this context to overcome the issues of opening an optical bandgap and cost-effectiveness.

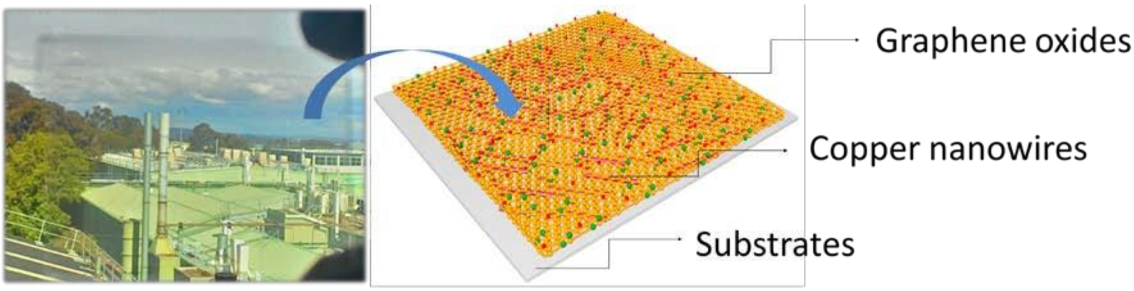

Fig. 1. Transparent conductive electrodes from copper nanowire-graphene oxide thin film.

Here, we report the use of a heterogeneous thin film from copper nanowires and graphene oxides as transparent conductive electrodes (TCEs) with transmission upto 90% and electrical resistance reduced to 101 Ω/sq (Fig.1). We will further discuss the use of graphene oxides has a protective oxidation barrier for the copper nanowires.

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Radiation tolerance of 2D material based devices for space applications

Vogl, Tobias1,*, Sharma, Ankur2, Sripathy, Kabilan1, Zhang, Linglong2, Karouta, Fouad3, Buchler, Ben C.1, Lu, Yuerui2, Lam, Ping Koy1

1Centre for Quantum Computation and Communication Technology, Department of Quantum Science, Research School of Physics and Engineering, The Australian National University, Acton ACT 2601, Australia
2Research School of Engineering, The Australian National University, Acton ACT 2601, Australia
3Department of Electronic Materials Engineering, Research School of Physics and Engineering, The Australian National University, Acton, ACT 2601, Australia
**e-mail:*
tobias.vogl@anu.edu.au

Characteristic for all devices based on 2D materials is that they have very low size, weight and power (SWaP) requirements, making them feasible for mobile employment, especially on satellites in space. The applications in space technology are versatile, including solar cells, batteries and electronic circuits as well as sensors and non-classical light sources for ultra-secure long-distance quantum communication.
Here we present a comprehensive study on the effects of radiation in the Earth's atmosphere on various devices based on 2D materials. Using theoretical modelling packages we first calculate relevant radiation levels in the low Earth orbit (LEO) and expose various different devices (field-effect transistors in MoS_2 and WSe_2 as well as single-photon emitter in hBN[1] and blank monolayers in WS_2 and $MoSe_2$) to gamma rays, energetic protons and electrons. At the fluence levels which are comparable to LEO, no big change was expected. While this assumption held true for most devices, however, WS_2 monolayers showed decreased defect densities after the gamma ray exposure, characterised by a 3-fold increase in PL intensity and lifetime as well as change in doping ratio which was proportional to the photon flux. Measurements at liquid He temperatures confirm the disappearing defect peak. The mechanism was traced back to oxygen-related vacancy healing. Oxygen molecules from the ambient air or the substrate can be dissociated by the highly energetic photons and then fill in for sulfur vacancies as DFT calculations show. Other radiation sources did not have an impact on any of the more than 100 devices under investigation. In conclusion, novel 2D materials are suited for space applications.

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Quantum-correlated photons from semiconductor cavity polaritons

Guillermo Munoz-Matutano[1], Andrew Wood[1], Mattias Johnsson[1], Xavier Vidal Asensio[1], Ben Baragiola[1], Andreas Reinhard[1], Aristide LeMaitre[3], Jaqueline Bloch[3], Alberto Amo[3], Gilles Nogues[2], Benjamin Besga[1,2], Maxime Richard[2] and Thomas Volz[1,*]

[1]ARC Centre of Excellence for Engineered Quantum Systems, Department of Physics & Astronomy, Macquarie University, Sydney, New South Wales, Australia.
[2]Institution Institut Néel, Université Grenoble Alpes - CNRS:UPR2940, 38042 Grenoble, France.
[3]Centre de Nanosciences et de Nanotechnologies, CNRS, Univ. Paris-Sud, Université Paris-Saclay, C2N-Marcoussis, 91460 Marcoussis, France.
**e-mail: thomas.volz@mq.edu.au*

Over the past decade, quantum-well exciton-polaritons in semiconductor microcavities have attracted a great deal of interest as driven-dissipative quantum fluids. Polaritons offer themselves as a versatile platform for performing Hamiltonian simulations with light, as well as for experimentally realizing nontrivial out-of-equilibrium phase transitions. In addition, polaritons exhibit a sizeable mutual interaction strength that opens up a whole range of possibilities in the context of quantum state generation. While squeezed light emission from polaritons has been reported previously, the granular or quantum nature of polaritons has not been observed to date. Here we report on the observation of quantum correlated photons from tightly confined quantum-well polaritons in a semi-integrated tunable fiber cavity [1]. From the characteristic dispersive shape of the second-order autocorrelation function at zero time delay around the polariton resonance, we are able to extract a value for the non-linear polariton-polariton interaction constant. Our results act as a door opener for accessing the newly emerging field of quantum polaritonics.

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Hybrid polaritons in a monolayer $MoSe_2$-GaAs-microcavity leading to monolayer induced bosonic condensation

Wurdack, Matthias[1], Lundt, Nils[2], Klass, Martin[2], Estrecho, Eliezer[1], Betzold, Simon[2], Baumann, Vasilij[2], Waldherr, Max[2], Nalitov, Anton[3,4,5], Cherotchenko, Evgenia[4,5], Cai, Hui[6], Kavokin, Alexey V.[5,7,8], Tongay, Sefaattin[6], Ostrovskaya, Elena A.[1,*], Klembt, Sebastian[2], Höfling, Sven[2,9] &
Schneider, Christian[2]

[1]ARC Centre of Excellence in Future Low-Energy Electronics Technologies and Nonlinear Physics Centre, Research School of Physics and Engineering, The Australian National University, Canberra, ACT 2601, Australia.
[2]Technische Physik and Wilhelm-Conrad-Röntgen-Research Center for Complex Material Systems, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany.
[3]Science Institute, University of Iceland, Dunhagi 3, 107 Reykjavik, Iceland.
[4]TMO University, St. Petersburg 197101, Russia.
[5]Physics and Astronomy School, University of Southampton, Highfield Campus, Southampton SO171BJ, UK.
[6]School for Engineering of Matter, Transport, and Energy, Arizona State University, Tempe, AZ 85287, USA.
[7]SPIN-CNR, Viale del Politecnico 1, 00133 Rome, Italy.
[8]Spin Optics Laboratory, St-Petersburg State University, 1, Ulianovskaya 194021, Russia.
[9]SUPA, School of Physics and Astronomy, University of St. Andrews, St. Andrews KY16 9SS, UK
**e-mail: elena.ostrovskaya@anu.edu.au*

We present the design and realization of a hybrid monolayer $MoSe_2$-GaAs microcavity operating in the strong coupling regime (Fig1a)). This device combines the unique physics inherent to two-dimensional materials with the mature device platform in III–V optoelectronics and polaritonics. It was designed using transfer matrix calculations where the plasmon-polariton resonance was tuned to match the A-exciton resonance of the $MoSe_2$ monolayer and the exciton resonance of the GaAs quantum wells. We observe the three characteristic hybrid polariton resonances using temperature-dependent angle-resolved photoluminescence and reflection measurements (Fig1b), and explain their occupation by a thermodynamic model [1].
Furthermore, we observe bosonic condensation (Fig1c) in this hybrid device driven by excitons hosted in the atomically thin layer of $MoSe_2$ [2]. Our work paves the way towards highly efficient, ultra-compact polariton-based light sources and valleytronic devices based on bosonic quantum fluids hosted in atomically thin materials, which ultimately can be operated at room temperature.

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Anisotropic Kerr Nonlinearity of lithium hydride intercalated black phosphorus

Yang T[1*], Abdelwahab I[2,3], Lin H[1], Bao Y[2], Tan S[2,3], Fraser S[1], Loh KP[2,4] and Jia B[1]

[1]Centre for Micro-Photonics, Faculty of Science, Engineering and Technology, Swinburne University of Technology, PO Box 218, Hawthorn, VIC 3122, Australia
[2]Department of Chemistry, National University of Singapore, Singapore 117543, Singapore
[3]NUS Graduate School for Integrative Sciences and Engineering, Centre for Life Sciences, National University of Singapore, #05-01, 28 Medical Drive, Singapore 117456, Singapore
[4]Centre for Advanced 2D Materials and Graphene Research Centre, National University of Singapore, Singapore
**e-mail: tyang@swin.edu.au*

Black phosphorus (BP) is a promising material for broad near- and mid-infrared photonics and optoelectronics applications, such as transistors, lasers and photodetectors [1]. However, the rapid degradation of BP under ambient conditions limits its practical applications. Several approaches to passivate the surface and stabilize BP have been reported recently, which include coating Al_2O_3 using atomic layer deposition, encapsulation by hexagonal boron nitride (h-BN), oxygen plasma etching followed by Al_2O_3 coating and covalent functionalization. These procedures have been found to introduce irreversible and undesirable defects and modifications to BP, resulting in degraded device performance. In this context, Sherman *et al.* recently reported alkali-metal intercalated air-stable BP that was suitable for electronic and optoelectronic applications [2], where lithium was intercalated into BP in ultra-high vacuum followed by *in-situ* hydrogenation (abbreviated as LiH-BP); this approach effectively solved the stability in BP. However, the nonlinear response of LiH-BP has not been studied.

Herein, the nonlinear properties of single crystals of LiH-BP (thickness: 15 nm), in particular the polarization-dependent third-order nonlinearity, was recorded using a customized microscopic Z-scan setup having both spatial and polarization resolving abilities. The measured nonlinear absorption coefficient and nonlinear refractive index of LiH-BP are both higher than those of BP, indicating that Li intercalation efficiently enhances the nonlinear optical responses of pristine BP. We attribute this enhancement to the efficient photo-induced energy and charge (electron) transfer between the Li atoms (donor) and phosphorus atoms (acceptor). The strong nonlinear and anisotropic optical responses of LiH-BP indicate great potential of this material in integrated nonlinear photonics device applications.

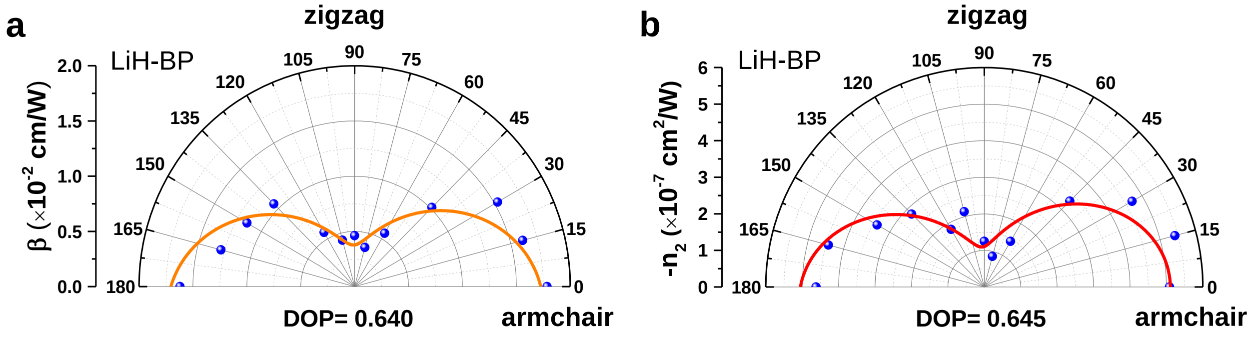

Fig. 1. Anisotropic nonlinear optical responses of LiH-BP flakes. (a) Dependence of nonlinear absorption coefficient of LiH-BP on the incident polarization. (b) Dependence of nonlinear refractive index of LiH-BP on the incident polarization.

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UNCONVENTIONAL SURFACE SPIN TEXTURES ON A 3D TOPOLOGICAL METAL

Yin, Yuefeng[1,2,3], Fuhrer, Michael S.[1,2], Medhekar, Nikhil V.[1,3*]

[1] ARC Center of Excellence in Future Low-Energy Electronics Technologies, Monash University, Clayton, VIC 3800, Australia
[2]School of Physics & Astronomy, Monash University, Clayton, Victoria 3800, Australia
[3]Department of Materials Science and Engineering, Monash University, Clayton, Victoria 3800, Australia
**e-mail: Nikhil.medhekar@monash.edu*

Understanding spin textures of the surface states of topologically nontrivial materials are essential for realizing their potentials in applications such as spintronics. Here we propose the existence of symmetry-protected direction-dependent surface spin textures on the surfaces of 3D materials using first principles calculations. We demonstrated these low-energy surface states are resulted from heavy spin-orbit coupling effects, accompanied by a phase transition from the band insulating state to the nontrivial state. The unconventional spin textures of these surface states feature an in-plane to out-of-plane spin polarization transition in the momentum space. Moreover, we have observed three-dimensional nodal lines in the crystal surviving the spin-orbit coupling effects. These symmetry-demanded nodal lines add more complicated electronic features such as drumhead surface states on the surface. These results highlight the importance of predicting new topological state by using the knowledge of crystalline symmetry. Our findings are expected to provide new insights for experimentalists to design new spin-based devices.

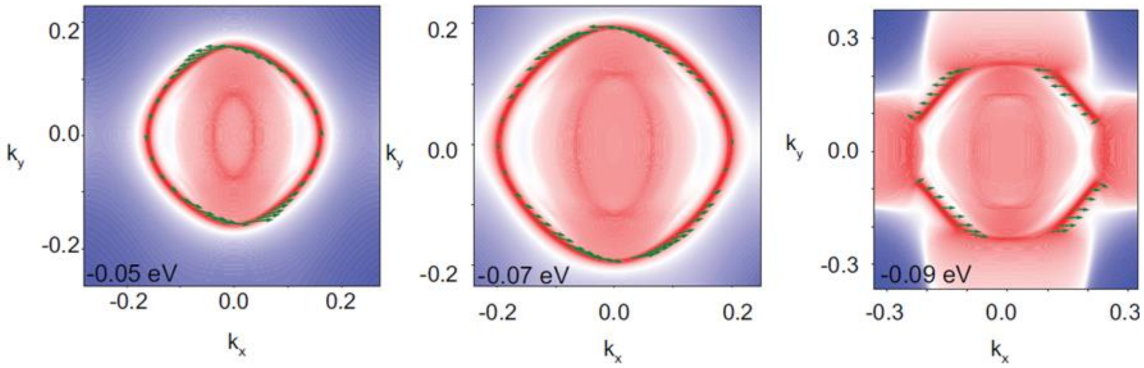

Fig. 1. Evolution of spin polarization on the surface band of a 3D topological metal.

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Contact-Engineered Electrical Properties of Monlayer MoS_2 Field-Effect Transistors via sulfur vacancy engineering

Jiankun, Xiao[1], Prof. Zheng Zhang[1], Prof. Yue, Zhang[1,*]
[1]*School of Materials Science and Engineering, University of Science and Technology Beijing, Beijing 100083, People's Republic of China*
**e-mail: yuezhang@ustb.edu.cn · zhangzheng@ustb.edu.cn*

Two dimensional transition metal chalcogenides (TMDCs), such as molybdenum disulfide, offer promise as next-generation electronic materials due to their direct band gap and atomically thin geometry. However, the large contact resistance at the metal–TMDCs interface is still a fundamental challenge in achieving practical TMDCs devices with good performance. To overcome this challenge, defect engineering and many doping profiles have been performed. Intrinsic defects in MoS_2 flakes can exhibit both n-type and p-type conduction in sulfur-deficient and sulfur-rich regions on a same sample, respectively.[1] Recently, studies examining anion (Se) vacancies by using a mild H_2 plasma treatment at the metal-WSe_2 contact regions can reduce the contact resistance to WSe_2.[2]

In our work, we report defect engineering by using a mild Ar plasma treatment to achieve low contact resistance to monolayer CVD grown MoS_2. It is confirmed that a large number of Ar plasma induced S vacancies by X-ray photoelectron spectroscopy (XPS), Raman spectra and Scanning transmission electron microscopy (STEM). The Ar plasma treatment is applied to fabricate MoS_2 field effect transistors at the metal-MoS_2 contact regions. The Ar-plasma-treated devices possess 100× improvement in ON current and a field effect Mobility of 132cm^2/(V·s) at room temperature due to lowering the metal-MoS_2 contact resistance.

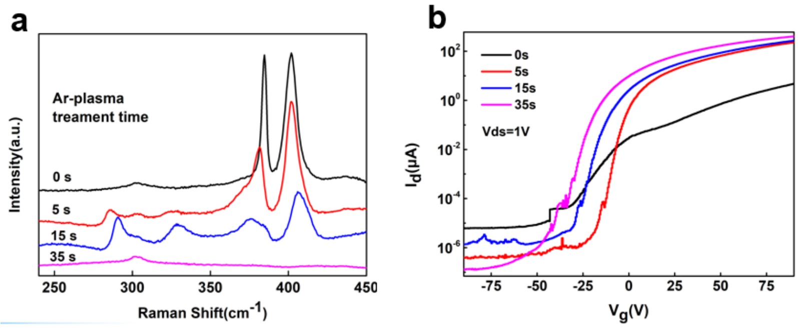

Fig1. a) Raman spectra measured before and after Ar_2 plasma on the same monolayer MoS_2 b). Transfer characteristics of no plasma treatment and Ar-plasma-treated MoS_2 FETs at V_{DS} = 1 V .

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Monosulfur vacancies control via moderate chemical process for properties regulation of monolayer MoS_2

Li, Gao[1,2], Prof. Zheng Zhang[1], Prof. Qing liang, Liao[1], Prof. Yue, Zhang[2,*]

[1]*School of Materials Science and Engineering, University of Science and Technology Beijing, Beijing 100083, People's Republic of China*
**e-mail: yuezhang@ustb.edu.cn, zhangzheng@ustb.edu.cn*

Due to atomic-level thickness, free dangling bonds and direct band gap, two-dimensional molybdenum disulfide have aroused great concern in research of the next generation electronic and photoelectric devices. However, structural defects inevitably occurring in MoS_2 affected their physicochemical performances at random due to the uncontrollable defects types.[1] Comparing with intrinsic defects, the artificial structural defects, either detrimental or beneficial, play more important role in regulating properties. Therefore, To find a facile and effective defect control strategy is significative. However, traditional strategies, including electron irradiation, ion excitation, plasma treatment and so on, most are physical strategies which usually performed poor controllability for types of defects and even destructived to the materials.[2]

Here, we presented a facile, effective and moderate chemical strategy to precisely control monosulfur vacancies in monolayer MoS_2 by using H_2O_2. The production of monosulfur vacancy attributed to the reactive energy matching between electronegativity of O ion in H_2O_2 and formation energy of V_S. These monosulfur vacancies precisely and effectively regulate electronic properties due to the trap states. By partially defect control in an individual MoS_2, a monolayer MoS_2 homojunction with good rectify behaviour has been designed as logic inverter with 0.34 voltage gain at V_{DD}=5V. We provide a facile and moderate strategy for precise control of structural defects in monolayer MoS_2, and explores an effective electronic regulation method for the construction of large area integrated MoS_2 electronic devices.

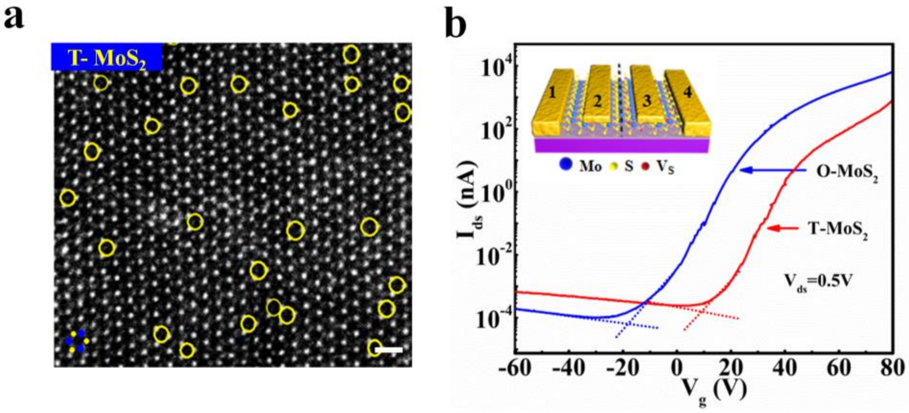

Fig1. a) STEM image of monolayer MoS_2 treated using H_2O_2, scale bar 1nm. b) the homojunction logic conversion characteristic using monosulfur vacancies regulation.

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NanoFrazor Lithography for 2D Materials

Zheng, Xiaorui[1], Calò, Annalisa[1,2], Albisetti, Edoardo[1,2,3], Liu, Xiangyu[1,2], Riedo, Elisa[1,2*]

[1]Advanced Science Research Center (ASRC), CUNY Graduate Center, New York NY 10031, USA
[2]Tandon School of Engineering, New York University, New York NY 11201, USA
[3]Dipartimento di Fisica, Politecnico di Milano, Milano 20133, Italy
**e-mail: elisa.riedo@nyu.edu*

Progress in nanotechnology depends on the capability to fabricate, position and interconnect nanometre-scale structures. However, the existing conventional lithography techniques pose limitations and challenges related to resolution, operational costs, and more importantly, the lack of flexibility to pattern novel materials such as graphene and transition-metal dichalcogenides [1,2].

Since the first patterning experiments performed with a scanning probe microscope in the late 1980s, scanning probe lithography has emerged as an alternative type of lithography for academic research that has provided striking capabilities to pattern three-dimensional relief structures with nanoscale features, the fabrication of the smallest field-effect transistor, or the patterning of proteins with 10-nm feature size. In this presentation, I will introduce the innovative NanoFrazor (Fig.1 left), the first commercialized scanning probe lithography facility, and focus on its great potential in the emerging two-dimensional materials. As an example, we have shown an innovative strategy based on thermal scanning probe lithography, which goes beyond conventional lithography, to fabricate with high reproducibility exceptional quality metal contacts on 2D materials (Fig.1 right).

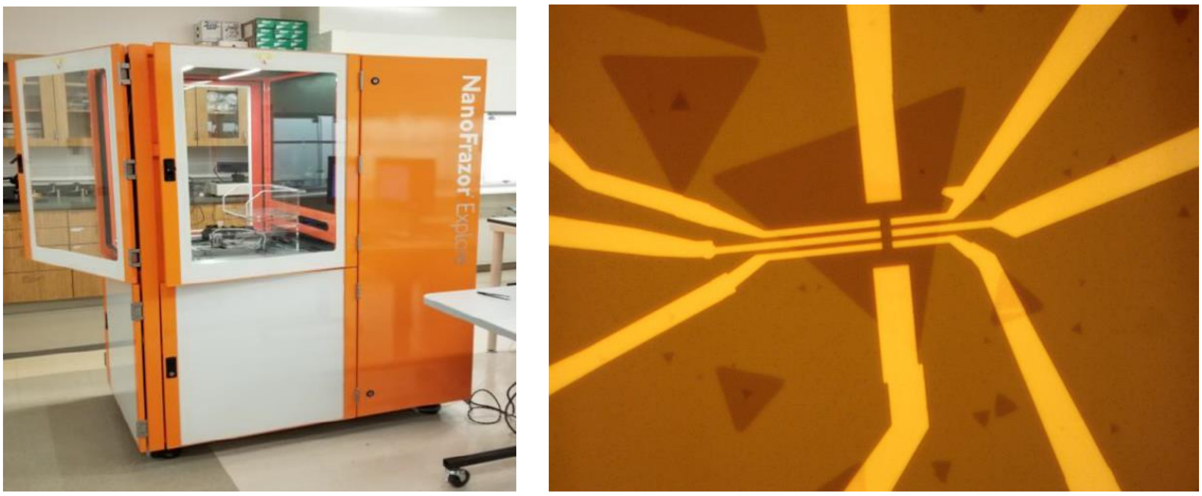

Fig. 1. Left: The photo of the NanoFrazor system based on scanning probe lithography. Right: The high quality metal contacts on monolayer MoS_2 flake fabricated by NanoFrazor.

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LIGHT-TUNABLE 1T TANTALUM DISULFIDE CHARGE-DENSITY-WAVE OSCILLATORS

Zhu, Chao[1], Chen, Yu[2], Liu, Fucai[1,3], Zheng, Shoujun[2,4], Li, Xiaobao[5], Chaturvedi, Apoorva[1], Fan, Hong Jin[2,4], Zhang, Hua[1], Yu, Ting[2], Liu, Zheng[1,6,7,*]

[1]Center for Programmable Materials, School of Materials Science and Engineering, Nanyang Technological University, Singapore 639798, Singapore.
[2]Division of Physics and Applied Physics, School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore 637371, Singapore.
[3]School of Optoelectronic Science and Engineering, University of Electronic Science and Technology of China, Chengdu, 610054, China.
[4]Centre for Disruptive Photonic Technologies, School of Physics and Mathematics Sciences, Nanyang Technological University, Singapore 637371, Singapore.
[5]School of Civil Engineering, Hefei University of Technology, Hefei, China.
[6]NOVITAS, Nanoelectronics Centre of Excellence, School of Electrical and Electronic Engineering, Nanyang Technological University, Singapore 639798, Singapore.
[7]CINTRA CNRS/NTU/THALES, UMI 3288, Research Techno Plaza, Singapore 637553, Singapore.
**e-mail: z.liu@ntu.edu.sg (Z.L.)*

External-stimuli-controlled phase transitions are essential for fundamental physics and design of novel functional devices. Charge density wave (CDW) is a metastable collective electronic phase featured by the periodic lattice distortion. Due to the enriched CDW phases in the 1T-TaS_2, much attention has been attracted to study the external control of these CDW phases. Although much work has been done in the electric-field-induced CDW transition, direct evidence from in-situ characterizations is still insufficient. Here, using the Raman spectroscopy, the electric-field-driven phase transition is in-situ observed in the ultrathin 1T-TaS_2, giving the direct evidence of the phase transition between nearly commensurate CDW and incommensurate CDW. More importantly, we show that light illumination can modulate the CDW phase at the room temperature. By integrating the light illumination with the ultrathin 1T-TaS_2 based oscillator, we realize the light control of the oscillator. The oscillation frequency can be tuned up to 30 % under the light illumination. The oscillation waveform can be tuned as well. This light tunability of the CDW phase transition adds more possibilities for its applications in compact on-chip oscillators as well as multifunctional electronic devices.

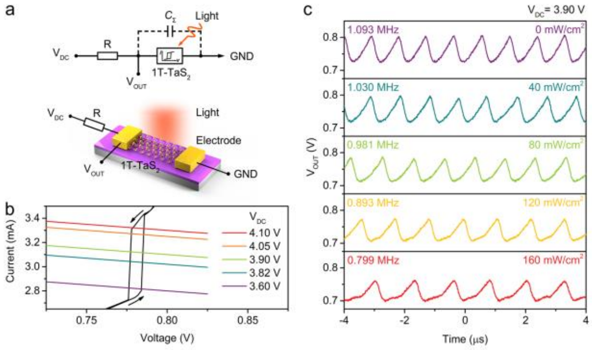

Fig. 1. Light-tunable 1T-TaS_2 based oscillator. (a) Diagram of the setup. (b) I-V characteristics of 1T-TaS_2 with the load lines under different VDC. (c) The oscillation of output voltage under different light intensities.

High-Efficiency Monolayer Molybdenum Ditelluride Light Emitting Diode and Photodetector

Yi Zhu,[1,2] Ziyuan Li,[2] Jiong Yang,[1] Linglong Zhang,[1] Zhenqing Luo,[1] Jianzheng Long,[1] Lan Fu[2*] and Yuerui Lu[1]*
[1]Research School of Engineering, College of Engineering and Computer Science, the Australian National University, Canberra, ACT, 2601, Australia

[2] Department of Electronic Materials Engineering, Research School of Physics and Engineering, the Australian National University, Canberra, ACT 2601, Australia

* To whom correspondence should be addressed: Yuerui Lu (yuerui.lu@anu.edu.au) and Lan Fu (lan.fu@anu.edu.au)

Silicon-based nanophotonic devices have attracted considerable interest because of their broad applications, including waveguides, couplers, modulators, and energy harvesting devices[1-2], which could be easily integrated onto silicon-based micro/nano industry platform. However, high-efficiency light sources, especially in the range of emission wavelength transparent to silicon, are still underexplored. Traditional off-chip or wafer-bonded III-V semiconductor light sources can be one option, but the complicated fabrication process and high-cost hindered their developments. The emerging monolayer transition-metal dichalcogenides (TMDs) become potential optical gain materials to bypass those obstacles due to their strong exciton emissions. Monolayer molybdenum ditelluride ($MoTe_2$) with an infrared emission transparent to silicon comes up to be a promising candidate for on-chip silicon-based nanophotonic applications. Here we demonstrate the monolayer $MoTe_2$ light emitting diode (LED) by taking advantage of the quantum tunneling effect. The device has a very high external quantum efficiency (EQE) of 9.5% at 83 K, which is so far the highest EQE obtained from LED devices fabricated from monolayer TMDs.

Measuring Electron Inelastic Mean Free Path in Epitaxial Graphene on SiC: Comparing Free-Standing-Graphene to the Buffer Layer

Amjadipour, Mojtaba[1,2*], MacLeod, Jennifer[1], Lipton-Duffin, Josh[1], Tadich, Anton[3], Boeckl, John[4], Iacopi, Francesca[2], Motta, Nunzio[1].

[1]*School of Chemistry, Physics and Mechanical Engineering, Science and Engineering Faculty, Queensland University of Technology, QLD, Australia.*
[2]*School of Electrical and Data Engineering, Faculty of Engineering and Information Technology, University of Technology Sydney, NSW, Australia.*
[3]*Australian Synchrotron, 800 Blackburn Road, Clayton, 3168 VIC, Australia.*
[4]*Air Force Research Laboratories, Wright-Patterson AFB, United States of America.*
**e-mail: mojtaba.amjadipour@uts.edu.au*

Thermal decomposition of SiC has proven to be a promising method to grow transfer-free wafer-scale graphene [1]. Epitaxial graphene has been the subject of many electron-collection-based measurements such as photoelectron spectroscopy and Auger electron spectroscopy. Having a precise understanding about electron inelastic mean free path (IMFP) in graphene is crucial for data interpretation using such measurements. A direct measurement of electron IMFP in epitaxial graphene fabricated on SiC is presented, indicating unexpected variations with respect to theoretical calculations and experimental data for graphite. The results indicate that the existing models for estimating IMFP in bulk materials (graphite) may not adequately show the electron interactions in 2D materials (graphene).

Epitaxial graphene growth leads to creation of a carbon rich layer at the interface between graphene and SiC substrate, commonly called the *buffer* layer. This interface layer is partially bonded to the SiC substrate adversely affecting graphene properties. Hydrogen intercalation is employed to eliminate the buffer layer and fabricate free-standing graphene on SiC [2]. Electron IMFP in free-standing graphene on SiC is compared to the buffer layer showing about 40% decrease for the buffer layer. This significant decrease in IMFP is most likely due to presence of sp^3 bonding between the buffer layer and SiC substrate causing more electron scattering.

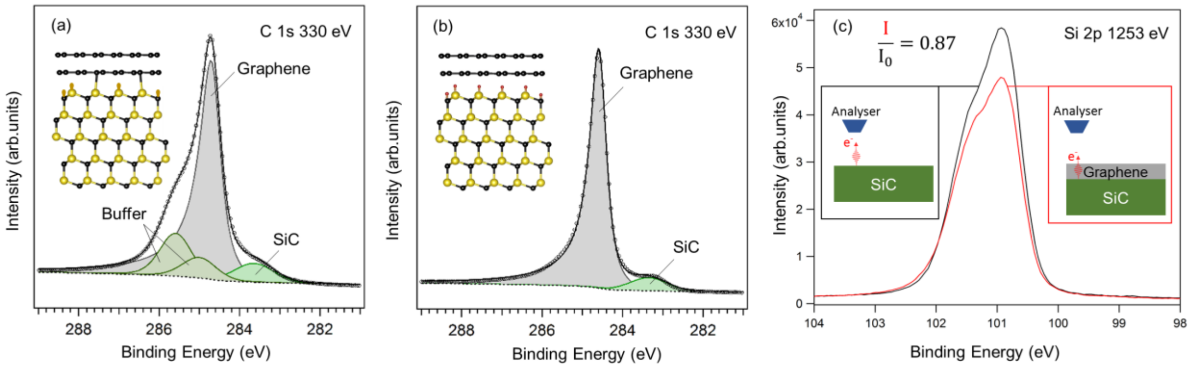

Fig. 1. (a) XPS spectrum of graphene sample with the buffer layer, (b) after 30 minutes hydrogen intercalation. (c) Intensity change due to having the graphene layer on SiC used for IMFP calculations.

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Photoinduced charge density wave phase transition in two-dimensional 1T-TaS_2

Chunhe, Dang, Wen, Wen, Liming, Xie*

[1] *National Center for Nanoscience and Technology (NCNST), Chinese Academy of Sciences*
**e-mail: xielm@nanoctr.cn*

Charge-density-wave (CDW) phase is a very intriguing property in quasi-1D or layered 2D metallic crystals. It is a complex quantum state consisting of a periodic modulation of the electronic charge density accompanied by a periodic atomic lattice distortion. For example, some layered transition metal dichalcogenides like tantalum disulfide (1T-TaS_2) exhibit different CDW symmetry-reducing phases by lowering the temperature. It is confirmed that the transitions can be affected not only by the temperature but also the applied electric field, pressure and laser. We have investigated the CDW transition from the nearly commensurate to the incommensurate CDW phases by applying electric field and light simultaneously. The factors on the phase transition, such as voltage, light power, light wavelength, have been investigated.

Liquid metal prepared oxide films as dielectrics for graphene devices

Gebert, Matthew[1*], Bhattacharyya, Semonti[1], Zavabeti, Ali[3], Atkin, Paul[3], Torben Daeneke[3,4], Kourosh Kalantar-zadeh[3,4,5], Fuhrer, Michael S.[1,2]

[1]*School of Physics and Astronomy, Monash University, Melbourne, Australia*
[2]*ARC Centre of Excellence in Future Low-Energy Electronics Technologies, Monash University, Melbourne, Australia*
[3]*School of Engineering, RMIT University, Melbourne, Australia.*
[4]*ARC Centre of Excellence in Future Low-Energy Electronics Technologies, RMIT University, Melbourne, Australia.*
[5]*School of Chemical Engineering and ARC Centre of Excellence in Future Low-Energy Electronics Technologies, University of New South Wales, Sydney, Australia*
**e-mail: mgeb1@student.monash.edu*

A novel liquid metal printing technique [1] allows the deposition of large area thin layer oxides such as Al_2O_3, Gd_2O_3 and HfO_2. This approach provides a new avenue to layering thin oxides, reducing the disorder at the interface to other materials often associated with thin film growth techniques.

Flat materials can be layered together to form heterostructures with unique and novel properties. We intend to study the effect of adding high-κ dielectric oxides to the surface of graphene and their influence on electronic properties. One expected consequence of introducing an oxide is an increase in charge carrier mobility due to the improved screening of Coulomb scattering. On the other hand, introducing an oxide layer may add charged impurities and degrade the performance, and remote scattering by oxide polar optical phonons may also reduce the mobility in graphene at elevated temperature.

We have both exfoliated single layer graphene, as well as transferred commercially-obtained single-layer graphene (grown by chemical vapour deposition on copper), to SiO_2 on Si substrates. Graphene films have been characterised by optical microscopy, atomic force microscopy, and Raman spectroscopy. Electrodes have been fabricated using optical lithography techniques and electrical measurements carried out at temperatures from 77 – 400 K.

We plan to transfer ultrathin oxides to graphene transistors and characterise the changes in temperature-dependent mobility due to changes in dielectric environment, charged impurities, and remote optical phonon scattering. We will present the latest results from this study at the conference.

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Electronic structure of WS_2 model devices and the influence the underlying substrate

Grubisic-Cabo, Antonija[1,*], Bhattacharyya, Semonti[1] , Kolesnichenko, Pavel[2], Zhang, Qianhui[3] , Wu,Tianhai[1,4], Kotsakidis, Jimmy C.[1], Volckaert, Klara [5] , Bianchi, Marco[5], Hofmann, Philip[5], Zheng, Changxi[1], Davis, Jeffrey[2], Fuhrer, Michael S.[1]

[1]School of Physics and Astronomy, Monash University, Melbourne, Australia.
[2]Centre for Quantum and Optical Science, Swinburne University of Technology, Melbourne, Australia.
[3]Department of Civil Engineering, Monash University, Melbourne, Australia.
[4]School of Physics, Peking University, Aarhus, Denmark.
[5]School of Physics and Astronomy, Aarhus University, Aarhus, Denmark.

**e-mail: Antonija.grubisic-cabo@monash.edu*

Two-dimensional transition metal dichalcogenides (TMDCs) have generated significant interest in the scientific community due to their remarkable optical and electronic properties [1]. Tungsten disulfide, WS_2, is of particular interest as it can be used in new kinds of electronics that rely on the spin and valley properties of electrons [2], called spintronics and valleytronics. Because of atomic thickness, the dielectric properties of TMDCs are known to be extremely sensitive to the properties of the supporting substrate [3], and therefore the optoelectronic properties of the material can be changed depending on the substrate in use and the environment around the TMDC, which has implications for device design and also offers opportunities for sensing. In order to measure the effect of substrate properties on electronic structure, we have prepared WS_2 on hexagonal boron nitride (h-BN), a common insulating substrate used in TMDC devices. We vary the thickness of h-BN by using substrates of few-layer hexagon boron nitride on copper and nickel, and thick h-BN on SiO_2/Si. We will report our results from photoluminescence measurements to determine the excitonic bandgap on these WS_2/h-BN devices and progress on angle-resolved photoemission spectroscopy (ARPES) measurements that can be used to measure the electronic structure.

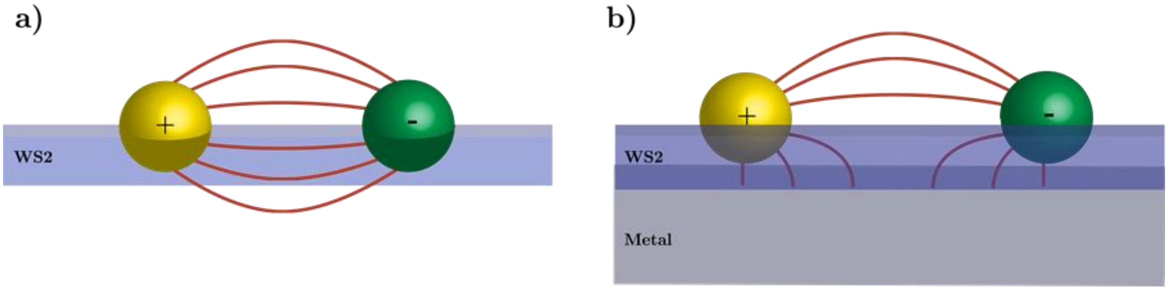

Fig. 1.

Changes in the Coulomb interaction of exciton - bound electron (green) and hole (yellow) in a 2D material in a) vacuum (low dielectric screening) and b) placed on a metallic substrate (high dielectric screening).

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Fundamental exciton linewidth in monolayer TMDs

Gupta, Garima[1], Majumdar, Kausik[1,*]

[1]*Department of Electrical Communication Engineering, Indian Institute of Science, Bangalore, India.*
**e-mail: kausikm@iisc.ac.in*

Sub-nanometre thick monolayer Transition Metal Di-chalcogenides (TMDs) are highly luminescent due to the ultra-short (~0.1 ps) radiative recombination lifetime of the strongly bound two-dimensional excitons [1]. Due to energy and momentum conservation, the spontaneous light emission from such radiative recombination is possible only for excitons lying within the light cone (Fig. 1a). A photoluminescence (PL) spectrum of monolayer $MoSe_2$ obtained at T = 3.2 K shows a total FWHM of 5.47 meV (Fig. 1b), of which the deconvoluted homogeneous linewidth is found to be 1.92 meV. This is two orders of magnitude larger than the light cone energy spread (□E~4 μeV).

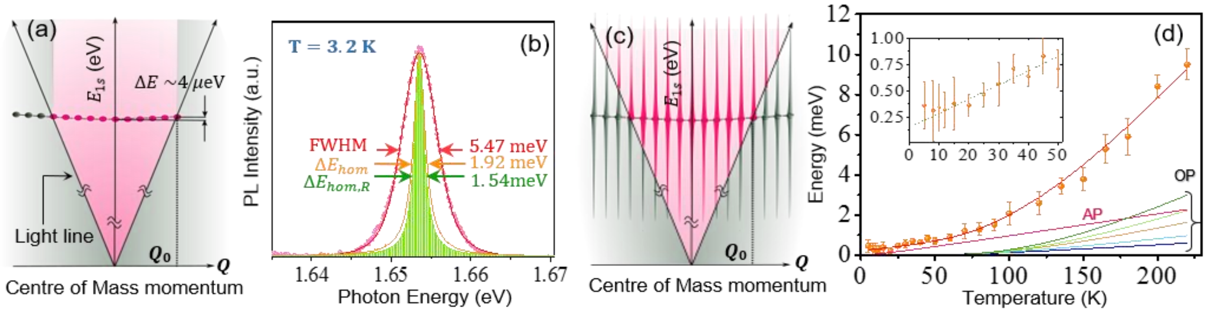

Fig. 1:(a) Conventional light cone. (b) $MoSe_2$ PL intensity (symbols), Lorentzian component of the fitted Voigt function, linewidth due to fundamental radiative limit. (c) Generalized light cone. (d) Non-radiative half-linewidth vs T, with contribution from acoustic and optical phonons shown separately.

In the wake of this huge mismatch, we present a generalized light cone picture which includes the large broadening in the excitonic states due to the short radiative lifetime (Fig. 1c). The light line (ħcQ) places a lower bound on the energy of excitons recombining radiatively. We propose a novel self-consistent methodology for calculating the exciton radiative lifetime, which efficiently segregates the radiative and the non-radiative components of the linewidth broadening. Using this approach, we estimate a fundamental lower limit of the spontaneous emission linewidth of 1.54±0.17 meV in monolayer $MoSe_2$, owing to purely exciton radiative lifetime in the absence of non-radiative dephasing processes (green line in Fig. 1b). However, this radiative limit is experimentally unattainable due to the additional non-radiative broadening resulting from zero-point energy of phonons [2]. To estimate the same, we plot the temperature dependent non-radiative half-linewidth in Fig. 1d under low excitation density which avoids excitation induced dephasing. The data fits well with exciton-phonon scattering induced broadening. An extrapolated half-linewidth of 150 μeV at T = 0 K (inset) quantifies the fundamental non-radiative linewidth broadening of 300 μeV in monolayer $MoSe_2$.

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When graphene meets electrolyte: how does graphene sense proton (H+)?

Jia, Xiaoyu1,2, Liu, Zhaoyang1, Chen, Zongping1,3, Narita, Akimitsu1, Müllen, Klaus1, Tielrooij, Klaas-Jan4, Bonn, Mischa1, I. Wang, Hai1,*

1Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany
2Graduate School Material Science in Mainz, University of Mainz, Staudingerweg 9, 55128 Mainz, Germany
3School of Materials Science and Engineering, Zhejiang University, 310027, Hangzhou, China
4ICFO - Institut de Ciències Fotòniques, The Barcelona Institute of Science and Technology, Castelldefels, Barcelona 08860, Spain
**e-mail: wanghai@mpip-mainz.mpg.de*

Graphene has been extensively used as electrodes in various electrochemical applications, including lithium ion batteries [1], dye sensitized solar cells [2] and super-capacitors [3]. Despite its relevance for these various applications of graphene, the effect of electrolyte solutions on the electronic properties, specifically conductivity, of graphene remains poorly understood. In the few available studies using graphene field effect transistors (FETs) for ionic sensing, conflicting results have been reported, for instance, on the mechanism and sensitivity of pH sensing using graphene FETs [4,5]. One major challenge is to separate contributions to the overall FET conductance from bulk electrolyte conductivity and from graphene itself, as the FET contacts are typically also exposed to the electrolyte.

Here we introduce THz spectroscopy as a contact-free, all optical means to track the intrinsic carrier conductivity of silica-graphene in contact with protons (H+) in water. While ions in the solution, as charge scattering centers, are generally expected to reduce the conductivity in graphene [6], we have observed that H+ substantially enhances the conductivity of graphene. Our result can be rationalized by noting that, proton has been widely reported to be able to go through graphene membrane [7,8], and stay between graphene and substrates. We suggest that these interfacial protons screen the surface charges or/and charge impurities in substrates, thereby enhancing the graphene conductivity. Our report provides new insight on the graphene's proton sensing mechanism, and highlights the importance and impact of proton transfer though graphene and interfacial charge screening on the graphene conductivity enhancement.

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Suppression of magnetic ordering for XXZ-type $NiPS_3$ in 2-dimension limit studied by Raman spectrascopy

Kim, Kangwon[1], Lim, Soo Yeon[1], Lee, Jae-Ung[1], Lee, Sungmin[2,3], Kim, Tae Yun[2,4], Park, Kisoo[2,3], Jeon, Gun Sang[5], Park, Cheol-Hwan[2,4], Park, Je-Geun[2,3], Cheong, Hyeonsik[1,*]

[1]*Department of Physics, Sogang University, Seoul 04107, South Korea*
[2]*Department of Physics and Astronomy, Seoul National University, Seoul 08826, South Korea*
[3]*Center for Correlated Electron Systems, Institute for Basic Science, Seoul 08826, South Korea*
[4]*Center for Theoretical Physics, Seoul National University, Seoul 08826, South Korea*
[5]*Department of Physics, Ewha Womans University, Seoul 03760, South Korea*
**e-mail: hcheong@sogang.ac.kr*

Transition metal phosphorus trisulfides ($TMPS_3$) are new class of magnetic van der Waals materials. Although all compounds are isostructural, they show different magnetic ground states depending on the TM element: $FePS_3$ [1], $NiPS_3$, and $MnPS_3$ have Ising-, XXZ-, and Heisenberg-type antiferromagnetic ordering, respectively. Since $TMPS_3$ can be exfoliated into atomically thin films, they are suitable for studying magnetism in the 2-dimensional (2D) limit. It is well known that there is no magnetic order at finite temperature for 1-dimension or 2D for isotropic Heisenberg systems [2]. We investigated XXZ-type antiferromagnetic $NiPS_3$ in the 2D limit by Raman spectroscopy. Raman spectroscopy is a powerful technique for studying 2D magnetic materials, as it can investigate phonon scattering as well as magnetic scattering. Below the Néel temperature, several Raman signatures due to antiferromagnetic phase transition are observed in the Raman spectrum of bulk $NiPS_3$: 2-magnon scattering, Fano resonance [3], suppression of the quasi-elastic scattering, and splitting of a phonon mode. The Néel temperature of $NiPS_3$ can be estimated by analyzing the temperature dependence of these signatures. We synthesized bulk single-crystal $NiPS_3$ by the vapour transport method and prepared atomically thin samples down to the monolayer by using mechanical exfoliation. We measured temperature dependent Raman spectra of few-layer $NiPS_3$ samples and found that the Néel temperature is similar for the thickness down to bilayer, but seems to be suppressed significantly for monolayer.

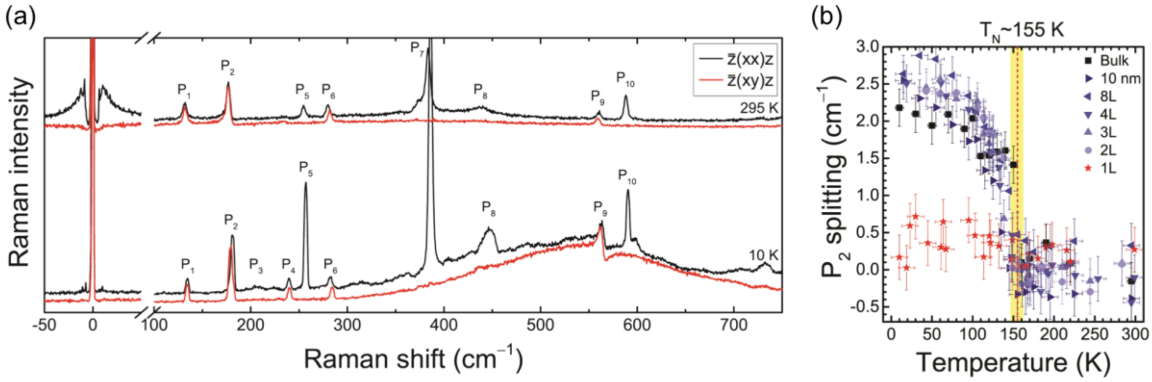

Fig. 1. (a) Polarized Raman spectra of bulk $NiPS_3$ at T=10 and 295 K. (b) Temperature dependence of P_2 splitting for various thicknesses of $NiPS_3$.

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Photoluminescence and differential reflectance microspectroscopy of tungsten disulphide monolayers

Kolesnichenko, Pavel[1,2], Zhang, Qianhui[3], Zheng, Changxi[3,4], Fuhrer, Michael[3,4], Davis, Jeffrey[1,2*]

[1]*ARC Centre of Excellence in Quantum and Optical Science, Swinburne University of Technology, Melbourne, Victoria 3122, Australia*
[2]*ARC Centre of Excellence in Future Low-Energy Electronics Technologies, Swinburne University of Technology, Melbourne, Victoria 3122, Australia*
[3]*Monash University, Melbourne, Victoria 3800, Australia*
[4]*ARC Centre of Excellence in Future Low-Energy Electronics Technologies, Monash University, Victoria, 3800 Australia*
**e-mail: jdavis@swin.edu.au*

Amongst other materials in the family of 2D transition metal dichalcogenides (TMDCs), monolayers of tungsten disulphides (WS_2) exhibit the highest photoluminescence (PL) quantum yield [1], which makes them promising candidates for realization of optoelectronic devices. However, the controllable growth of the materials has not yet been achieved: CVD-grown monolayers manifest a great deal of variation in size, shapes and quality, preventing them from massive industrialization. We will report correlated PL and differential reflectance maps, which provide complementary information on optical properties of the monolayers. In the presence of significant sample variation, our measurements show that B-excitons establish themselves as more robust and less sensitive to defects, stresses and strains than A-excitons (Fig. 1).

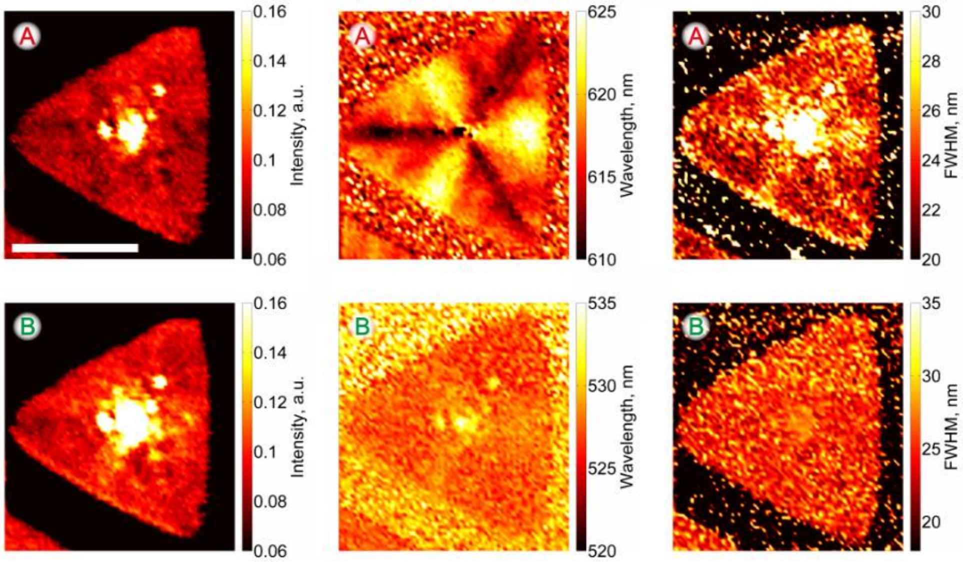

Fig. 1. Differential reflectance microspectroscopy images of WS_2 monolayers: mapping of the (left) intensity, (middle) wavelength and (right) width of (top row) A-exciton and (bottom row) B-exciton spectral features. The length of the scale bar is 10 um.

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Photoluminescence induced oxidation of monolayer WS_2

Kotsakidis, Jimmy C.[1], Zhang, Qianhui[2], Vazquez de Parga, Amadeo L.[3,4], Zheng, Changxi[2], Currie, Marc[5], Helmerson, Kristian[1], Gaskill, Kurt D.[5], Fuhrer, Michael S.[1*]

[1]School of Physics and Astronomy, Monash University, Victoria 3800, Australia.
[2]Department of Civil Engineering, Monash University, Victoria 3800, Australia.
[3]Dep. Física de la Materia Condensada and Condensed Matter Physcis Center (IFIMAC), Universidad Autónoma de Madrid, Cantoblanco 28049, Madrid, Spain.
[4]IMDEA Nanociencia, Cantoblanco 28049, Madrid, Spain.
[5]U.S. Naval Research Laboratory, Washington D.C. 20375, USA.

**e-mail: Michael.Fuhrer@monash.edu*

Monolayer semiconducting transition metal dichalcogenides (S-TMDs) exhibit exceptional optical and electronic properties, largely due to their bandstructure, which includes spin splitting due to large spin-orbit coupling and a large direct optical bandgap.

However, S-TMDs have been observed to oxidize in ambient conditions, which can degrade their optical and electrical performance. Therefore, understanding the oxidation mechanism of S-TMDs in ambient conditions is crucial for continued basic research efforts and incorporation of S-TMDs into future electronic and opto-electronic applications.

In this work, we reveal that oxidation of the S-TMD, WS_2, in ambient, is driven by bandgap photoexcitation and we describe a possible chemical reaction pathway.

Through a series of controlled experiments, WS_2 monolayer crystals grown via chemical vapor deposition (CVD) were exposed to low power light with wavelengths of 532nm, 650nm and 760nm for one week.

It was found that the WS_2 oxidised only when exposed to light with enough energy to excite an optical bandgap transition and that the WS_2 remained un-oxidised two weeks after growth in the absence of light.

Furthermore, we find that even for limited exposure to above-bandgap illumination in ambient – at levels routine for photoluminescence (PL) or Raman spectroscopy characterization – causes significant degradation of WS_2 via oxidation.

These findings suggest that researchers must be extremely careful when handling S-TMDs in order to prevent their oxidation, and has far-reaching consequences to past, present and future studies.

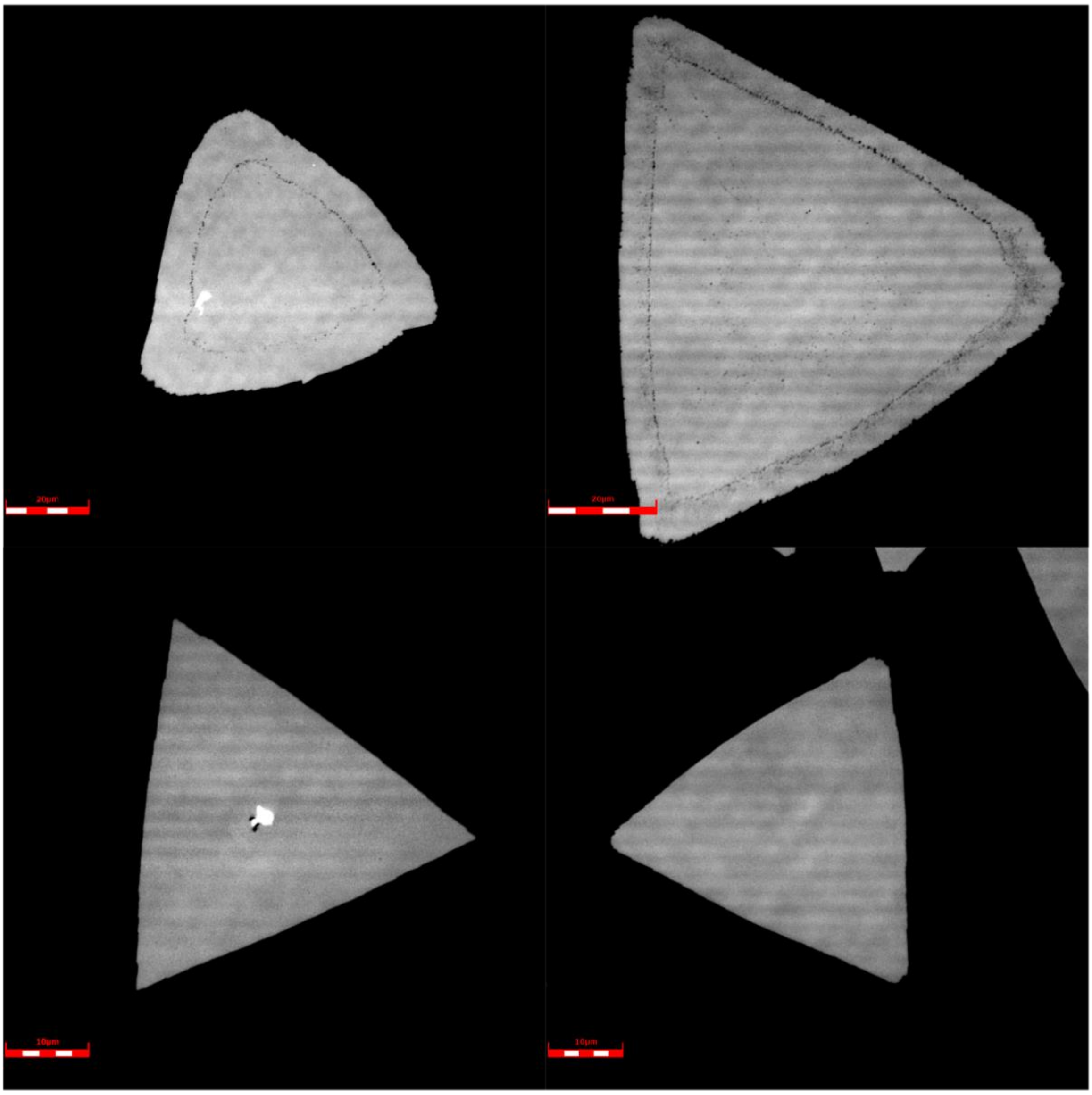

Fig. 1. Confocal micrographs of low-power laser experiments, all samples exposed to light for seven days in ambient conditions. **A)** 532nm experiment showing monolayer WS2 oxidation. Scale bar = 20µm. **B)** 650nm experiment showing oxidation. Scale bar = 20µm.**C)** 760nm light experiment, no obvious signs of oxidation. Scale bar = 10µm **D)** Control sample kept in darkness 2 weeks after growth. Scale bar = 10µm.

Transport properties of two-dimensional electron gas with Rashba and Zeeman effects

Lee, Yik[1,*], Smith, Jackson[1,**], Cole, Jared[1,***]

[1]*Chemical and Quantum Physics, School of Science, RMIT University, Melbourne, Australia*
**e-mail: yik.kheng.lee@student.rmit.edu.au*
*** e-mail: jackson.smith@rmit.edu.au*
****e-mail: jared.cole@rmit.edu.au*

Given current power consumption trends, improvements in the energy efficiency of modern electronic devices are sorely needed [1]. Spintronics, where spin manipulation replaces charge manipulation, is a promising way to achieve this. However, it is difficult to design such nanoscale devices as electrical transport properties change at these length scales because quantum effects come into play.

One example of a nanoscale device is the two-dimensional electron gas (2DEG). In such a system, spin-orbit coupling (for example via the Rashba effect) leads to a coupling between the spin and momentum of conduction electrons. Furthermore, if an external magnetic field is applied, the Zeeman effect results in a coupling between the spin of the electrons and the external magnetic field. The interaction of these two effects leads to interesting topological phenomena such as the anomalous Hall effect and edge states [2,3].

We investigate how the transport properties of two-dimensional materials are affected by the interplay of the Zeeman and Rashba effects in nanoscale devices. Using the non-equilibrium Green's functions (NEGF) method, combined with a tight-binding model of a 2DEG, we model different device geometries. In doing so we analyze the effects of varying different factors such as spin-orbit coupling strength, magnetic field, device geometry, and disorder.

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Anomalous polarized Raman response of ReSe$_2$

Lim, Soo Yeon[1], Kim, Keunui[1], Kim, Jung Hwa[2], Lee, Zonghoon[2], Cheong, Hyeonsik[1,*]

[1]Department of Physics, Sogang University, Seoul, South Korea
[2]Department of Materials science and engineering, UNIST, Ulsan, South Korea
**e-mail: hcheong@sogang.ac.kr*

ReSe$_2$ is a van der Waals layered semiconductor with an indirect bandgap of ~ 1.3 eV. ReSe$_2$ has a distorted octahedral structure (1T′) with in-plane anisotropy unlike other hexagonal transition metal dichalcogenides (TMDs) such as MoSe$_2$ and WSe$_2$. Since rhenium (Re) atom has an additional electron compared to other group-Ⅵ TMDs, diamond shaped rhenium chains are formed. Due to the structural in-plane anisotropy resulting in an optical and electrical anisotropy, ReSe$_2$ can be used as polarization sensitive optoelectronic devices [1].

We performed polarized Raman spectroscopy of ReSe$_2$ with the 1.96 eV-excitation and identified two sides of ReSe$_2$ by comparing opposite Raman responses in terms of polarization dependence shown in Fig. 1. We re-confirmed the non-equivalent polarization dependences of two sides of the ReSe$_2$ by flipping the same sample on transparent substrates. Additionally, we determined the direction of the rhenium chains with a mode at ~ 160 cm^{-1} by using the 1.96 eV-excitation and confirmed it with HR-STEM measurements. We studied polarization dependence of Raman response with different excitation energies. The polarization dependence patterns vary dramatically with different excitation energies.

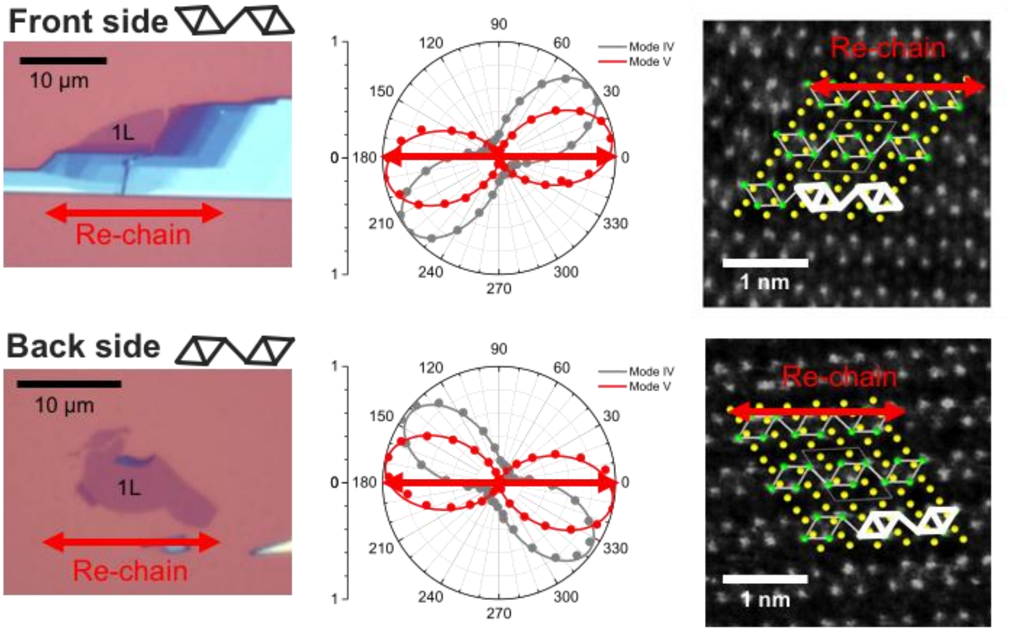

Fig. 1. Identification of two sides of monolayer ReSe$_2$

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Moire phonos in twisted bilayer MoS2

Lin, Miao-Ling[1,2], Tan, Qing-Hai[1,2], Wu, Jiang-Bin[1], Chen, Xiao-Shuang[3], Wang, Jin-Huan[4], Pan, Yu-Hao[5], Zhang, Xin[1], Cong, Xin[1,2], Zhang, Jun[1,2], Ji, Wei[5], Hu, Ping-An[3], Liu, Kai-Hui[4], Tan, Ping-Heng[1,2]*

1 State Key Laboratory of Superlattices and Microstructures, Institute of Semiconductors, Chinese Academy of Sciences, Beijing 100083, China
2 CAS Center of Excellence in Topological Quantum Computation, and College of Materials Science and Opto-Electronic Technology, University of Chinese Academy of Sciences, Beijing 101408, China,
3 Key Laboratory of Micro-systems and Micro-structures, Manufacturing of Ministry of Education, Harbin Institute of Technology, Harbin 150080 , China
4 State Key Laboratory of Mesoscopic Physics, School of physics and Collaborative Innovation Center Quantum Matter, Peking University, Beijing 100871. China
5 Department of Physics, Renmin University of China, Beijing 100872, China
**e-mail: phtan@semi.ac.cn*

Compared to conventional semiconductor heterostructures, van der Waals heterostructures (vdWHs) based on two-dimensional materials (2DMs) are readily fabricated by direct chemical-vapor-deposition growth or wet/dry transfer. Those vdWHs have ultraclean and atomically sharp interfaces, providing a versatile platform for studying interface physics. Also, the material choice of the components, layer thickness and interlayer twist angle θ widely enrich the vdWHs and provide additional degrees of freedom to engineer their optical and electronic properties. The Moiré patterns in vdWHs create a periodic potential for electrons, excitons and phonons to yield many interesting phenomena, such as Hofstadter butterfly spectrum and Moiré excitons. Here, in the twisted bilayer MoS2 (tBLM), one of the simplest prototype of vdWHs, we show how the periodic potentials of Moiré patterns induce different phonon modes and relate those to the lattice dynamics from its constituent, monolayer MoS2. We report the observation of new Raman modes related to Moiré phonons in as-grown/transferred tBLMs with different twist angles, which are folded from the off-center phonons in monolayer MoS2. However, the folded phonons related to crystallographic superlattices are not observed in the Raman spectra.[1] By varying the twist angle, the Moiré phonons of tBLM can be used to map the phonon dispersion of the constituent layers (Fig.1). 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 intensity related to Moiré phonons in all tBLMs are strongly enhanced when the excitation energy approaches the C exciton energy. This study can be extended to investigate Raman spectra in various vdWHs to deeply understand their Moiré phonons, lattice dynamics, excitonic effects and interlayer coupling.

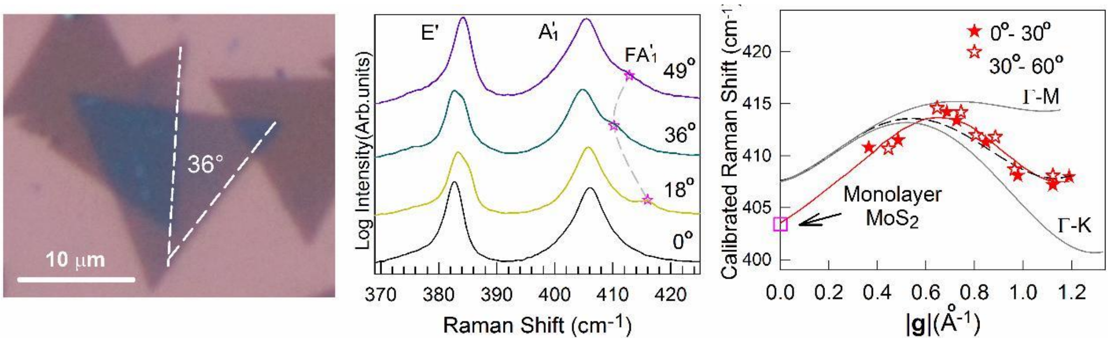

Fig. 1 The optical images and Raman spectra of tBLM in the A'1 spectral regiion by varying the twist angle. The wavevector-dependent frequencies of Moiré phonon related to mode are summarized, along with the theoretical phonon dispersion of A'1 mode along the Γ-K and Γ-M directions are shown.

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Functional 2D boron nitride nanosheets and their applications in energy and environment

Dan Liu presenting, Weiwei Lei
[1]Institute for Frontier Materials, Deakin University, Waurn Ponds, Victoria 3216, Australia
**e-mail: dan.liu@deakin.edu.au;weiwei.lei@deakin.edu.au*

BN nanosheets, also called “white graphene”, consist of a few layers of alternating boron and nitrogen atoms in a hexagonal arrangement. The polarity of BN bonds and the high surface area of h-BN-related nanostructures provide good adsorption properties of various substances ranging from organic pollutants to hydrogen.[1-4]

In addition, recently, significant efforts have been focused on the isolation and functionalization of BN nanosheets to achieve better dispersion, which would enable applications in optical devices, biological systems and composites. However, the concentration of the h-BN dispersions was typically below 2 mg mL^{-1}, even after long periods of intense ultrasonication. Therefore, the development of a practical high-yield process to achieve highly water-soluble BN nanomaterials remains a challenge. And, it is very difficult to achieve aqueous dispersion of h-BN using conventional routes.

Here, we present a simple and efficient one-step method for the preparation and functionalization of few-layer BN by solid state ball milling of commercially available h-BN and urea powder.[5] The colloidal solutions of multi-layer h-BN can have unprecedentedly high concentrations, up to 30 mg/mL, and are stable for up to several months. They can be used to produce freestanding membranes simply by filtration. The functional BN nanosheets membranes exhibit good applications in super-thermal conductivity composites, nanofluidic device, energy generator, molecular separation and Li-S batteries as a separator (in Figure 1).[6-9]

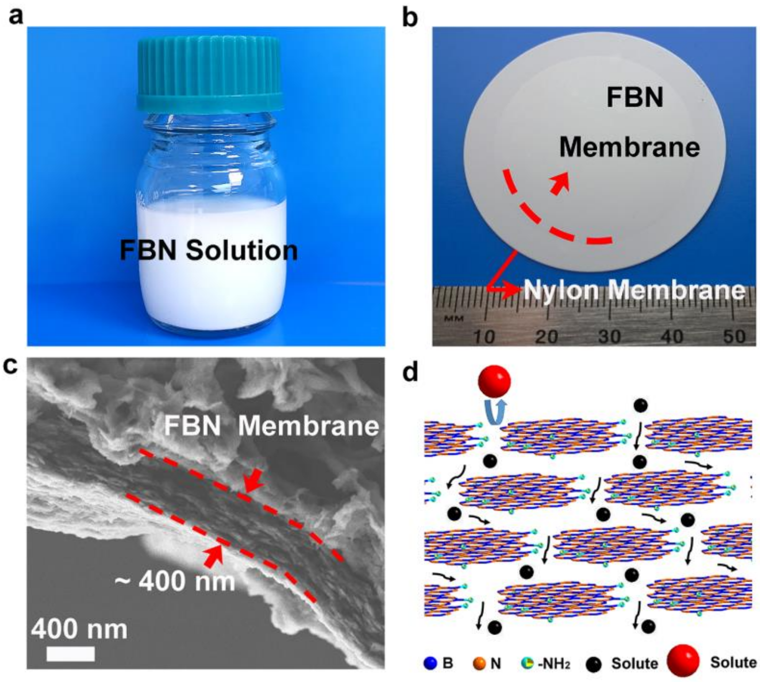

Fig. 1 The preparation of the functionalized boron nitride (FBN) membrane and solute separation mechanism.

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Air-Stable Passivation of Topological Dirac Semimetal Na_3Bi Thin Films

Liu, Chang[1,2,*], Collins, James[1,2], Hellerstedt, Jack[3,4], Edmonds, Mark[1,2], Fuhrer, Michael[1,2]

[1] *School of Physics and Astronomy, Monash University, Clayton, Victoria 3800, Australia*
[2] *ARC Centre of Excellence in Future Low-Energy Electronics Technologies, Monash University, Clayton, Victoria 3800, Australia*
[3] *Institute of Physics of the Czech Academy of Sciences, v.v.i., Cukrovarnicka 10, 162 00 Praha 6, Czech Republic*
[4] *Regional Centre of Advanced Technologies and Materials, Palacky University, Slechtitelu27, 78371 Olomouc, Czech Republic*
**e-mail: chang.liu2@monash.edu*

Na_3Bi is a 3-dimensional topological Dirac semimetal, possessing a band structure with linear band dispersion along all three directions in momentum space [1]. Thin films possess mobility in excess of 7000 cm^2/Vs, and doping comparable to bulk crystals [2], as well as ultra-low potential fluctuations comparable to graphene on h-BN [3]. In addition, ultra-thin Na_3Bi has been isolated and demonstrated as a large bandgap quantum spin Hall insulator with electric field-tuned topological phase transition [4]. This makes Na_3Bi a promising candidate for low-energy electronic devices and switches. However, Na_3Bi is highly reactive in air limiting measurements to ultra-high vacuum conditions until a suitable air-stable capping layer is found.

Here, we report on the utilization of magnesium difluoride (MgF_2) to passivate the Na_3Bi surface and protect it upon exposure to ambient conditions. We demonstrate that MgF_2 does not chemically react with the Na_3Bi surface, and has minimal influence on its electronic properties. The left panel of Figure 1 shows that Na_3Bi thin films capped with MgF_2 remain stable in air and remain metallic for hours. This allows samples to be transported to low temperature cryostats, in order to study the electronic properties at high magnetic field and wide temperature range as shown in the right panel of Figure 1.

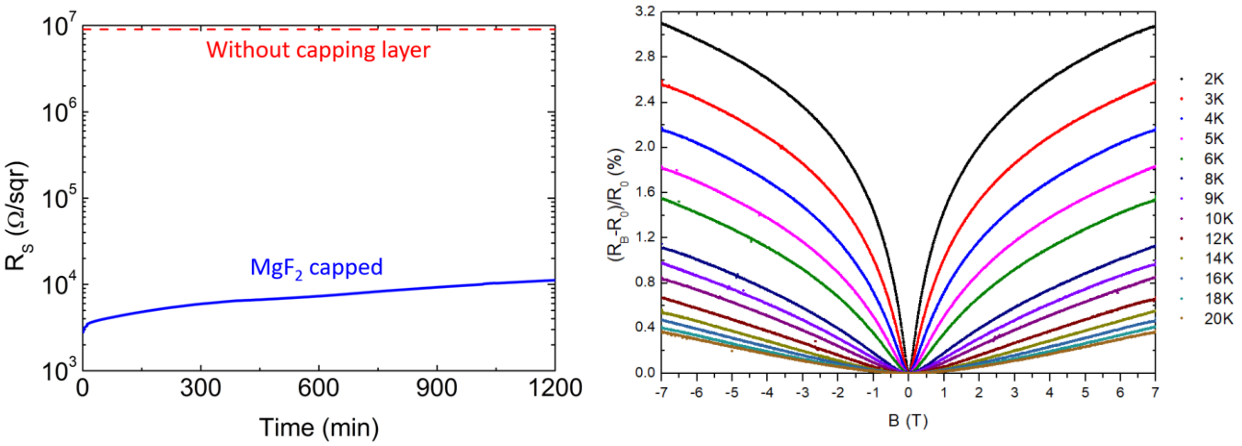

Fig. 1. Left: Sheet resistance of 20 nm Na_3Bi film with/without MgF_2 capping layer upon air exposure. Right: Temperature dependent magnetoresistance, demonstrating strong weak anti-localization.

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Electrochemically exfoliated black phosphorous nanosheets for nanoelectronic device applications

Pawar, Mahendra1, Late, Dattatray1,*

1Physical and Materials Chemistry Division, CSIR-National Chemical Laboratory, Pune - 411008, India
**e-mail: datta099@gmail.com*

Since last decade, two dimensional (2D) layered materials such as graphene, transition metal dichalcogenides (TMDC's), hexagonal boron nitride (hBN) have attracted a great deal of attention in various fields. The electronic and optical properties of 2D materials displayed significant interest in numerous nanoelectronic device applications. Recently, as a promising candidate to 2D materials, atomically thin Black Phosphorous (BP) nanosheets have been effectively exfoliated from bulk crystals and utilized in different studies such as field effect transistor, gas sensor, energy storage applications. It is still not clear if the ultrathin BP sheet is an ideal structure for the enhanced gas-solid interactions due to its large surface area. To further investigate this concern, we have synthesized few layer nanosheets of BP using an electrochemical exfoliation method. The surface morphology and thickness of the nanosheets were identified using Atomic Force Microscopy (AFM), Transmission Electron Microscopy (TEM), and Raman spectroscopy. The BP nanosheets thick film sensor showed increase in the conductance and excellent sensitivity with increase in relative humidity. Further, the few layer BP nanosheets based transistor showed good mobility (7.3 cm2/Vs) and on/off ratio of 104. The UV light irradiation on the BP nanosheets exhibits good response and recovery time. The overall results shed light on important electronic and optical properties of ultrathin sheets of BP material, which can be utilized in future device applications.

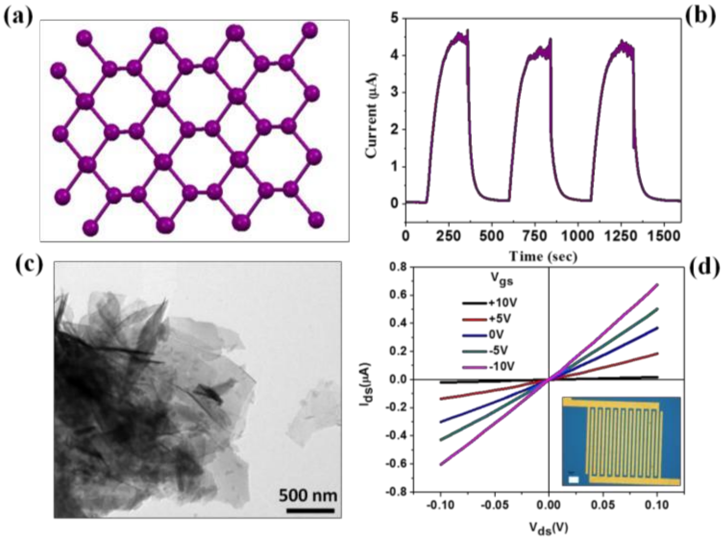

Fig. 1. (a) Top view of single layer BP, (b) Humidity sensor (response and recovery time) study, (c) TEM image of few layer BP nanosheets and (d) Output characteristics of the transistor device (inset is the interdigited electrodes fabricated on SiO2/Si substrate with scale bar 20 µm).

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Energy dispersion and magnetoresistance of graphene in the presence of topological defect

Roshanzamir, Mohammad*

Division of Elementary Particles and Field Theory, Department of Physics, Faculty of Basic Sciences
Shahrekord University, Shahrekord, Iran
**e-mail: m.roshanzamir@sku.ac.ir*

The relativistic quantum dynamics of massless fermions in a curved space-time is studied and the effects of geometric theory on the landau levels and also magnetoresistance in the atomic disclinated graphene lattice are investigated in the presence of magnetic flux and external nonuniform magnetic field. It can be shown within the analysis of the behavior of the above physical quantities as a function of magnetic flux that the presence of topological defect reduces the degeneracy of energy levels, Fig. 1 and the curvature of the conical surface affects the pattern of oscillations of magnetoresistance, Fig. 2.

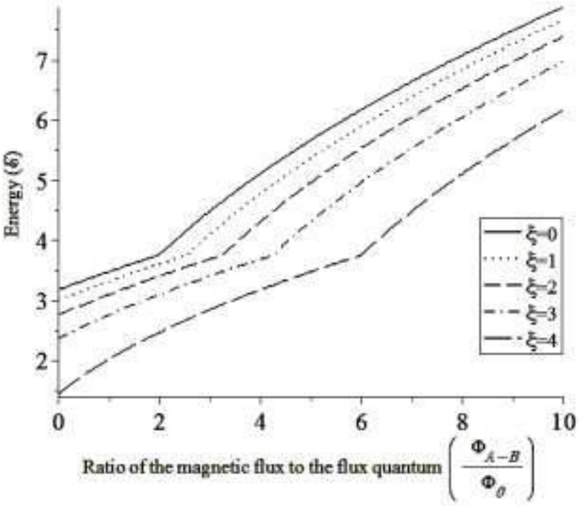

Fig. 1. Energy versus Aharonov-Bohm flux parameter with $(n,k,a,b)=(2,1,0.2,4)$ for $\xi=0,1,\ldots,4$.

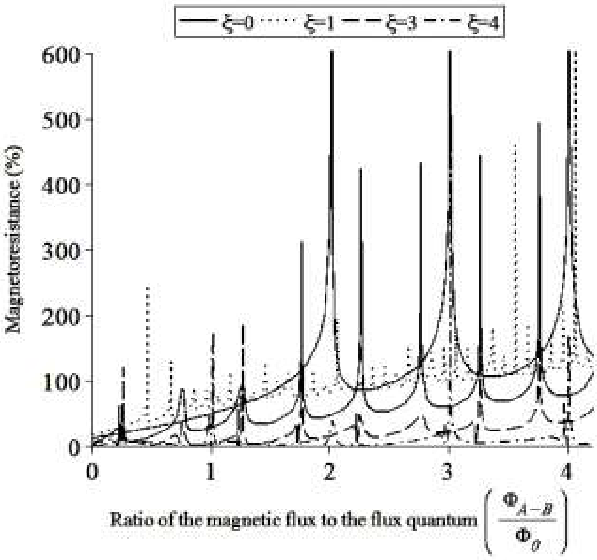

Fig. 2. Magnetoresistance as a function of Aharonov-Bohm flux with $(k,a,b)=(1,0.2,\pm4)$ for summation of $1\leq n\leq 7$ and $-7\leq \ell \leq 7$ with $k=\pm1$ related to $\varsigma=-1$ for $\xi=0,1,\ldots,4$.

Anisotropic $SnSe_{(1-x)}S_x$ alloys studied by using polarized Raman spectroscopy

Sriv, Tharith[1], Nguyen, Thi Minh Hai[2], Nguyen, Van Quang[2], Cho, Sunglae[2], Cheong, Hyeonsik[1,*]

[1]Department of Physics, Sogang University, Seoul 04107, Korea
[2]Department of Physics, University of Ulsan, Nam-gu, Ulsan 44610, Korea
**e-mail: hcheong@sogang.ac.kr*

Tin compounds such as SnS and SnSe have orthorhombic crystal structure that belong to the D_{2h}^{16} (Pnma) space group. These materials have promising semiconducting properties, which are useful in thermoelectric devices and photovoltaic applications [1-2]. The different perspective views of these materials along the *a-, b-* and *c*-axial directions lead to interesting anisotropic nature [3]. Polarized Raman spectroscopy has been used effectively to study the anisotropic properties of thin materials such as black phosphorous [4], SnS flakes synthesized by physical vapor deposition (PVD) [5], SnSe nanoplates that were grown using PVD [6]. More interestingly, the Raman studies on $SnS_{(2-x)}Se_x$ alloys have been done [7-8]. However, to the best of our knowledge, no Raman investigation on $SnSe_{(1-x)}S_x$ monochalcogenide alloys has been conducted. In this study, we performed the low-frequency Raman spectroscopy of the $SnSe_{(1-x)}S_x$ (x=0.2, 0.4, 0.5, 0.6, and 0.8) crystals that were synthesized by using temperature gradient method (Fig. 1). We also measured the polarization dependence of the Raman spectra of these crystals and compared the results with those of SnS and SnSe. The results of the measurements show interesting anisotropic properties, which are useful for further understanding of these alloys.

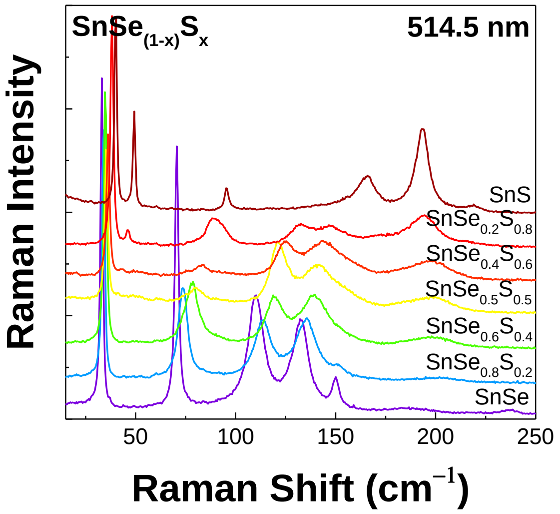

Fig. 1. Raman spectra of $SnSe_{(1-x)}S_x$ alloys measured by using 514.5 nm excitation wavelength laser

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Low-temperature scanning tunnelling microscopy of topological semimetals

Wei Tao and Bent Weber
Nanyang Technological University Singapore

Monolayers of the transition metal dichalcogenides WTe_2- a type-II Weyl semimetal candidate in the bulk - are predicted to be a quantum spin Hall (QSH) insulator in its monolayer form. Here, we present successful van-der-Waals epitaxy of monolayer 1T’-WTe_2 and its atomic-scale electrical characterization using low-temperature (4.5K) scanning tunnelling microscopy (STM). Atomic-resolution STM visualizes the 1T’ lattice, with boundary states visible, whilst local probe spectroscopy confirms a bulk gap (~50meV) and a strongly enhanced density of states at the QSH edge.

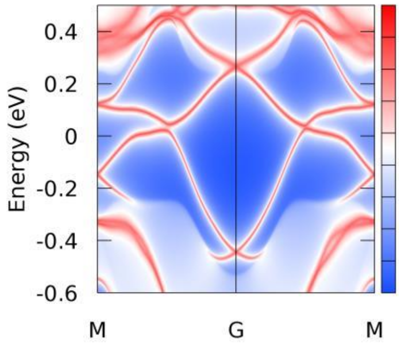
Robust topological edge states in 2D TCIs on substrates

Wang, Chutian[1,3], Yin, Yuefeng[1,2,3], Fuhrer, Michael[2,3], Medhekar, Nikhil[1,3*]

1Deptment of Materials Science and Engineering, Monash University, Clayton Victoria 3800 Australia
2School of Physics and Astronomy, Monash University, Clayton Victoria 3800 Australia
3ARC Centre of Excellence in Future Low Energy Electronics Technologies, Monash University, Clayton Victoria 3800 Australia

**e-mail:*
nikhil.medhekar@monash.edu

Two-dimensional quantum spin Hall insulators are promising candidates to realise dissipationless electron transport, because the ballistic edge states are topologically protected. One of the key challenges in topological materials device design is to conveniently turn the edge states on and off. Two-dimensional topological crystalline insulators (TCI) are promising in this regard, as turning on/off edge states can be easily achieved by adding an electrical field that breaks the mirror symmetry. However, 2D TCI phases are yet to be demonstrated experimentally due to difficulties in synthesis of these materials and in ensuring the stability of their topologically protected edge states. As several previous studies have shown, the edge states can no longer be topologically protected when the materials are placed on mirror symmetry breaking substrates. In this study, using planar bismuthene as a representative example, we show that TCI phases can indeed be maintained on some substrates. The results suggest that when there is a weak interaction between the ultrathin film and substrates, the ballistic edge states can be preserved. This research provides guidelines for selection of appropriate substrates for the experimental realisation of topological edge states.



(a) (b) (c)

Fig. 1. (a) Freestanding planar bismuthene edge states. (b) Planar bismuthene on substrate without breaking the edge states. (c) Planar bismuthene where edge states are broken by substrate.

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The phonon confinement effect in two-dimensional nanocrystals of black phosphorus with anisotropic phonon dispersions

Xin, Cong[1,*], Ping-Heng, Tan[1]

[1]State Key Laboratory of Superlattices and Microstructures, Institute of Semiconductors, Chinese Academy of Sciences, Beijing 100083, China.
**e-mail: congxin@semi.ac.cn*

To understand the Raman spectra of nanocrystals(NCs), Richter, Wang and Ley proposed a widely phonon confinement model, referred as RWL model. This model has been extensively used to understand the Raman spectra of two-dimensional NCs, such as graphene and MoS_2. In order to simplify the calculations in the RWL model, the phonon dispersion relations are approximately considered to be isotropic in the Brillouin zone (BZ), and only phonon dispersions along the high symmetry axes in the BZ are involved. However, this simplified approximation may yield distorted results in some systems whose phonon dispersion curves are anisotropic along the different high symmetry directions. Here, to examine this issue, we investigate RWL model in black phosphorus (BP), a typical anisotropic two-dimensional crystal exhibiting pronounced anisotropy in phonon dispersions. A detailed study is performed on the Raman spectra of BP NCs prepared by the ion implantation technique. With decreasing NC size, the peak positions of the three characteristic Raman modes, , and modes, remain almost unchanged, while the line shapes of and modes exhibit significant asymmetrical broadening tails towards higher- and lower-frequency sides, respectively. It is found that the RWL model based on one- dimensional phonon dispersion along Γ–Y and Γ–X axes in the BZ cannot interpret the unusual frequency invariance and inhomogeneous line shape broadening of these three modes. However, after considering the contribution of two-dimensional anisotropic phonon dispersions from the whole BZ, the frequency and asymmetrical broadening of the and modes can be well reproduced. This study demonstrates that the RWL model is applicable for crystals with anisotropic phonon dispersions once the phonons in the whole two-dimensional or three-dimensional BZ are properly taken into account, and provides a physically sound route into understanding the phonon confinement effect for anisotropic systems. [1].

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Towards Understanding and Engineering the Properties of Perovskites for LED and Solar Cell Applications

Tingting, YIN[1], Jiaxu, Yan[2], Ze Xiang, Shen[1,2,*]

[1]Division of Physics and Applied Physics, School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore 637371, Singapore
[2]Centre for Disruptive Photonic Technologies, School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore 637371, Singapore
**e-mail: zexiang@ntu.edu.sg*

Abstract

Hybrid organic-inorganic perovskites (bulk and quantum dots) are of great interest as promising materials for potential applications in solar cells and LEDs, due to their high carrier mobility, tunable spectral absorption range and easy processing. New crystal structures and physical properties of this class materials can be readily developed under high pressure [1] and low temperature [2], providing significant insights into pressure-induced structural mechanism and engineering.

In first part of this presentation, the novel optical properties of bulk $CH_3NH_3PbBr_3$ single crystals under high pressure will be discussed. At ~ 2.3 GPa, photoluminescence intensity is enhanced by ~ 400 times, and broad emission appear at 4.2 GPa. In second part, the pressure-induced sintering of $CH_3NH_3PbBr_3$ quantum dots (QDs) of 10 nm into nanocrystals of 100 nm will be reported. After release, the nanocrystals present new optical behaviors [2]. In third part, high-pressure study of ultra-thin flakes (50 nm) of $(C_4H_9NH_3)_2PbI_4$ 2D perovskite will be presented. Extensive characterization techniques, including time-resolved spectroscopy, Raman spectroscopy, photoluminescence and absorption spectroscopy, in-situ X-ray diffraction (XRD) and transmission electron microscopy (TEM) as well as ab initio calculation, are introduced to study the pressure-induced structural evolution and physical properties change from hybrid perovskites.

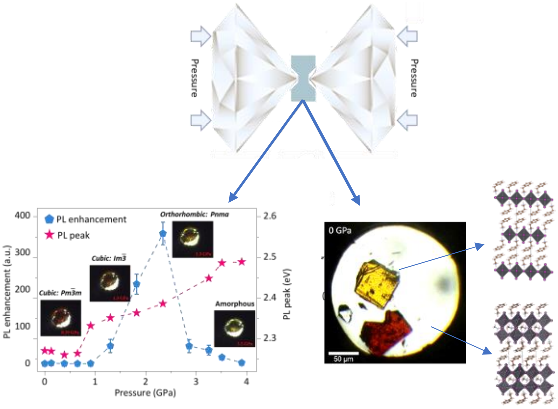

Fig. 1. Optical-property variations of perovskites under high pressure.

Our results can guide the understanding and engineering the optoelectronic properties of perovskites for LED and solar cell applications.

Keywords: Perovskites, Phase transition, photoluminescence, absorption, time-resolved, ab initio calculation.

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