

# Controlled Growth and Device Application of Two-Dimensional Ferro-Semiconductors

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Keywords: Ferroelectricity $\square$ In<sub>2</sub>Se<sub>3</sub>; spin glass; Cr<sub>2</sub>Se<sub>3</sub> $\square$ chemical vapor deposition;

The controllable preparation of high-quality, low-dimensional ferroelectric and ferromagnetic materials is the foundation for the development of functionalized, miniaturized, and integrated ferroelectric information components. Stable ferroelectric polarization and ferromagnetic properties are difficult to exist under two-dimensional limit conditions, which limits the discovery and further application of low dimensional ferromagnetic materials. Therefore, exploring new low dimensional ferromagnetic materials with good stability and simple and efficient material preparation is currently a highly challenging research topic in the field of nano information functional devices.

We develop the controlled growth method of  $\alpha$ -In<sub>2</sub>Se<sub>3</sub> with accurately understanding its atomic structure layout and symmetry breaking for the first time. Piezoelectric microscope and second harmonic spectrum were used to prove its out of plane ferroelectricity. Based on the coupling characteristics of ferroelectricity and semiconductor, highly sensitive flexible electromechanical functional devices were developed, in which relevant work was published in Nano Letters 2017, 17, 5508. Implemented the  $\alpha$ -In<sub>2</sub>Se<sub>3</sub> and other two-dimensional sulfides have prepared high-quality, large-area, and thickness controllable fixed-point oriented single crystal array growth, which has developed the ultra-high photoelectric sensitivity and high uniformity photodetector array of In<sub>2</sub>Se<sub>3</sub> was published in Nature Communications 2015, 6, 697.

We also realized the large area preparation of chalcogenide ferroelectric ferromagnetic semiconductor materials with low Gibbs free energy earlier, and characterized the thermal conductivity of polycrystalline WTe<sub>2</sub> as low as 0.8 W m<sup>-1</sup> K<sup>-1</sup> by time-domain thermal reflection spectrum, which is close to the theoretical extremely low value of disordered lattice vibration; We also developed the phase controlled growth of Cr based non layered materials, revealing the spin glass properties of crystalline Cr<sub>2</sub>Se<sub>3</sub>. The related results were published in Advanced Functional Materials 2017,85928; Journal of Materials Chemistry, 2019,7,10598 $\square$ Chemistry of Materials 2021, 33, 10, 3851-3858.

# Atomic structure-properties study of defects in emerging 2D materials

by Junhao Lin | Southern University of Science and Technology

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Keywords: 2D materials, defect, ferroelectricity, ferromagnetism, structure-property relation

Two-dimensional (2D) materials are considered to be the candidates for future nano-electronic, optoelectronic and spintronics applications. It is well known that defects are determinant to the properties of materials, thus understanding defects in 2D materials serves as the key step for functionality engineering and improved performance in devices.

In this talk, I will first show the atomic scale structure-properties correlation studies of various defect structures in emerging 2D materials, by quantitative intensity analysis in a low-voltage scanning transmission electron microscope (STEM). Secondly, I will introduce the universal strategy to overcome the structural degradation problem of air-sensitive 2D materials. We develop a home-built interconnected inert gas protection system compatible with atomic STEM imaging, and I will show the recent breakthroughs in structure-properties correlation of various air-sensitive 2D materials. Examples including but not limit to: monolayer amorphous carbon where the high-density distorted defect network contribute to its ultrahigh mechanical toughness; intrinsic defect structures in air-sensitive  $\text{WTe}_2/\text{MoTe}_2$  monolayer and their heterostructures with resonating phonon vibrations; superlattice reconstruction in dative epitaxial heterostructure and self-intercalated 2D magnetic heterojunction with exotic magnetic responses, etc.

# Effect of a seed layer on the properties of CdZnTe thick films prepared by close-spaced sublimation method

by Jian Huang | Ke Xu | Ke Tang | Linjun Wang | Shanghai University | Shanghai University | Shanghai University | Shanghai University

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*Keywords: CdZnTe, Close-spaced sublimation, seed layer*

CdZnTe (CZT) is an II-VI direct band gap compound semiconductor with excellent performance which has a wide range of applications in solar cells, radiation detectors and other fields. Close-spaced sublimation (CSS) method is one of the best methods to prepare high-quality CZT thick films, but the preparation of CZT thick films by this method generally requires a higher substrate temperature, which limits the application of CZT thick films in flexible devices, integrated circuits and other fields. Therefore, how to prepare high-quality CZT thick films at lower temperature has become one of the research hotspots.

In this work, a homo-seed layer is first introduced on the substrate by magnetron sputtering, and then a CZT thick film is prepared on the seed crystal layer by CSS method. The effects of seed layers and deposition temperature on the properties of CZT thick films were investigated in detail. The experimental results show that the addition of the seed layer can effectively improve the performance of CZT thick films under the condition of lower deposition temperature. This provides an effective method for the application of CZT thick films in flexible devices and integrated circuits and other fields.

# Fabrication of high-performance thermally conductive phase change material composites with 2D boron nitride based porous ceramic network for efficient thermal management

by Jooheon Kim | Chung-ang university

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Keywords: Polymer-matrix composites; phase change materials; thermal conductivity; 2D material; heat management

The phase change material (PCM) has a great potential for heat energy storage and efficient heat management. However, achieving high performance PCM composites is still challenging because of its low thermal conductivity and weak mechanical properties. In this study, a novel PCM consisting of erythritol-grafted bisphenol A (ETBPA) was fabricated and filled with porous BN filler network consisting of carbonized cellulose nanofiber (CNF). Based continuous filler network formed by arrangement of 2D BN, the composite exhibited an ultra-high thermal conductivity (13.09 W/mK) along through plane direction, 300% increased tensile strength, and a latent heat of 98.4 J/g. The fabricated ETBPA/BNCNF/BN composites enabled efficient thermal management performance via the combination of heat absorption and heat dissipation properties by their high thermal conductivity and large latent heat. The fabricated PCM composites has potential to contribute to the research of thermal management systems.

# Highly thermally conductive and insulating composites fabricated through the hot-pressing of hollow h-BN/rGO/epoxy structure

by Jangwoo Cho | Minsu Kim | Jooheon Kim | School of Chemical Engineering and Materials Science, Chung-Ang University, Seoul 06974, Republic of Korea | School of Chemical Engineering and Materials Science, Chung-Ang University, Seoul 06974, Republic of Korea | Department of Intelligent Energy and Industry, Graduate School, Chung-Ang University, Seoul 06974, Republic of Korea

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Keywords: Hexagonal boron nitride; reduced graphene oxide; thermal conductivity; hybrid filler; volume resistivity

Polymer composites come with several benefits such as cost-effectiveness, simple processing, and a wide range of uses. In our research, we created hexagonal boron nitride (h-BN)/epoxy spheres using NaCl and then removed the NaCl with water to form h-BN/epoxy hollow structures. We then coated these structures with reduced graphene oxide (r-GO) to produce h-BN/r-GO/epoxy hollow structures. These structures were converted into composites using a high-pressure, high-heat hot pressing method, which resulted in a vertical alignment of the h-BN components to create a heat transfer path, with r-GO evenly distributed throughout. The thermal conductivity of the h-BN/r-GO/epoxy composite was found to be 4.12 W/m·K, a 2060% increase compared to that of pure epoxy. Despite the inclusion of electrically conductive r-GO, the h-BN/r-GO/epoxy composite retained its insulating properties, which is attributed to the even distribution of insulating h-BN within the h-BN/r-GO/epoxy hollow structures.

# Iron oxide/magnesium oxide nanoparticles/graphene oxide, and cellulose composites synthesized with a Polydopamine linker exhibit excellent thermal conductivity, EMI shielding, and electrical insulation properties

by Jihoon Kim | Wondu Lee | Jooheon Kim | Chung-Ang University | Chung-Ang University | Chung-Ang University

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Symposium: 1. 2D Materials (2DM)

Keywords: Thermal conductivity; Electromagnetic interference shielding effectiveness; Nanoparticle; Chemical linking

The rapid progression of electronic devices has hastened the need for efficient heat regulation. Simultaneously, the widespread adoption of wireless communication has heightened concerns surrounding electromagnetic interference (EMI) shielding. Both excessive heat and EMI represent significant risks to both electronic device functionality and human well-being. To address these challenges, there is a demand for materials offering exceptional thermal conductivity and high EMI shielding effectiveness (EMI SE). In this study, we systematically modified graphene oxide (GO) sheets with polydopamine (PDG). Additionally, we surface-treated iron oxide (IO) and magnesium oxide (MO) nanoparticles with polydopamine, respectively. Through covalent bonding, IO and MO nanoparticles were attached to GO sheets alongside polydopamine (PDG/IO/MO), ensuring uniform dispersion across the PDG sheets. This unique PDG/IO/MO hybrid filler exhibited strong compatibility with a polydopamine-treated cellulose matrix, creating dual heat transfer pathways due to the strategic placement of IO and MO fillers on the PDG sheets. Consequently, the resulting cellulose/PDG/IO/MO composites demonstrated exceptional electrical insulation (surpassing  $109 \Omega \cdot \text{cm}$ ), EMI SE (65.29 dB), through-plane thermal conductivity ( $5.83 \text{ W/m} \cdot \text{K}$ ), and tensile strength (155.49 MPa).

# Photovoltaic effect in low-dimensional vdW structures and its application

by Xiaolong Chen | Southern University of Science and Technology

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*Keywords: 2D materials, photovoltaic effect, vdW materials*

Photovoltaic effect is the key mechanism of various optoelectronic devices, including solar cells and photodectors. Here, I will introduce recent studies on bulk/intrinsic photovoltaic effect, a nonlinear optical effect arising from the broken inversion symmetry of materials which is considered as a promising mechanism to overcome the Shockley-Queisser limit, in low-dimensional vdW structures, including one-dimensional vdW edges and grain boundaries. Then, electrical-tunable photovoltaic effect in vdW structures and its applications in constructing miniaturized spectrometers will be introduced.

# Room-temperature spin injection in van der Waals layered semiconductors

by Xu Li | Xiamen University

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Keywords: GeSe, Spin injection, Spin transport

The emerging spintronic devices are developed through manipulating, transmitting, and detecting the spin degree of freedom in electrons. The van der Waals (vdw) layered crystals are considered a promising candidate for future electronic devices due to their intriguing features, including thin thickness, no dangling bonds, high mechanical flexibility, and atomic-level flatness. Nonetheless, the electrical spin injection in vdw crystals remain challenging. In this work, highly efficient spin injection and transport are achieved in GeSe through engineering the tunneling barrier structure. A CoFeB/MgO tunnel spin injector yields a moderate spin polarization of 4.96%. By introducing the vdw hexagonal-BN tunnel barrier, a high spin polarization of 5.71% is achieved. The spin polarization is further elevated to as high as 18.31% by applying a larger bias current of 500 nA. Such a voltage dependence represents a spin injection mechanism of hopping conduction. **This work is the first report on the effective spin injection in an air-stable vdw semiconductor at room temperature.** The high spin polarization exceeding that of graphene and BP also demonstrates the high potential of GeSe in semiconductor spintronic devices.



# Single-atom sites confined in 2D layered double hydroxide material design based on electrostatic repulsion principle

by Zhao Cai | China University of Geosciences

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*Keywords: electrostatic repulsion, energy efficiency., layered double hydroxide, single atom catalyst, water splitting*

Electrolysis of water to produce hydrogen is a key technology facing the global energy crisis and environmental issues. The rational design and controllable preparation of advanced 2D catalytic materials with regulated active sites are of utmost importance in reducing the overpotential of electrochemical reactions and improving energy conversion efficiency. We put forward to introduce single atom active sites to layered double hydroxide water splitting electrocatalysts based on electrostatic repulsion manipulation. Such structural control of electrocatalytic materials at the atomic scale significantly improved the energy conversion efficiency of hydrogen/oxygen evolution reactions. These findings provide new opportunities for the development of advanced 2D electrocatalyst materials with favorable atomic arrangement.

# Plasmon-engineered low-power optoelectronic synaptic devices based on 2D materials

by Ziwei Li | Ming Huang | Hunan University | Hunan University

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Keywords: 2D material, MoS<sub>2</sub>, optoelectronic synapse, photodetector

Abstract. Flexible wearable systems represent the future frontier of intelligent perception and display technology, necessitating devices that possess high-performance capabilities, low power consumption, and biocompatibility. Optoelectronic synaptic devices, leveraging 2D materials, exhibit brain-like neural network computing power and retina-like "sensing memory computing integration," thereby transcending the confines of traditional von Neumann computing architecture. This study primarily focuses on low-power optoelectronic synaptic devices modulated by plasmons. It introduces a novel approach utilizing metal nanostructure templates to induce the growth of monolayer molybdenum disulfide, facilitating controlled growth of two-dimensional semiconductor materials at predetermined locations. Moreover, this work proposes mechanisms for regulating light-matter interactions, including plasmon-induced enhancement of near-field electromagnetic fields and doping with hot electrons, thereby significantly augmenting the material's light absorption capacity and photoelectric conversion efficiency. By harnessing the information processing capabilities of "sensing memory computing," the photoelectric synaptic device showcases a photosensitive response of 6000 A/W, temporary information storage capacity exceeding 2000 s, and a remarkably low power consumption of 20-40 pJ per stimulus. Furthermore, through neural network learning, this device exhibits brain-like associative memory capabilities, enabling the restoration and reconstruction of memory information for blurred images.

## References

- [1] M. Huang, W. Ali, J. Huang, L. Yang, R. Sun, Y. Xie, C. Zhu, C. Yao, Y. Tan, X. Liu, S. Li, Z. Li\* and A. Pan\*, *Adv. Sci.* 10, 2300120, 2023.
- [2] Z. Luo†, Y. Xie†, Z. Li\*†, Y. Wang, L. Li, Z. Luo, C. Zhu, X. Yang, M. Huang, J. Huang, D. Liang, X. Zhu, D. Li and A. Pan\*, *Nano Res.* 15, 3539-3547, 2022.
- [3] Z. Li\*, W. Yang, M. Huang, X. Yang, C. Zhu, C. He, L. Li, Y. Wang, Y. Xie, Z. Luo, D. Liang, J. Huang, X. Zhu, X. Zhuang, D. Li and A. Pan\*, *Opto-electron. Adv.* 4, 210017, 2021.

# Magnetic and topological properties of an Fe(biphenolate)<sub>3</sub> network

by Xiang-Long Yu | Southern University of Science and Technology

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Keywords: *first-principles calculations, magnetic insulator, quantum anomalous Hall effect, tight-binding model, two-dimensional metal-organic material*

Metal-organic materials, as an emerging quantum system, demonstrate distinctive properties and hold potential applications across various fields. In this work, we employ a combination of first-principles calculations and model analysis to systematically investigate a synthesized two-dimensional metal-organic material, an Fe(biphenolate)<sub>3</sub> network. Our results show that its ground state is an antiferromagnetic insulator with weak exchange couplings, primarily governed by a superexchange interaction. Furthermore, we find that the Fe(biphenolate)<sub>3</sub> network, when polarized in a ferromagnetic manner, can exhibit the intriguing behavior of a quantum anomalous Hall (QAH) insulator with three consecutive nontrivial bandgaps. Our subsequent study on substrate effect suggests that a hexagonal boron nitride substrate with a wide bandgap could potentially serve as an ideal candidate for producing the QAH effect.

# Realization of two-dimensional kagome lattice and its potential valleys confine effects

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Keywords: Kagome lattice; Ge; Scanning Tunneling Microscopy/Spectroscopy; DFT calculations

Kagome lattice is composed of corner-sharing triangular lattice with geometry frustration, topology, spin and correlation. However, current research focuses on two-dimensional surfaces of three-dimensional kagome crystal materials, which inevitably bring interlayer interactions and thus affect their intrinsic electronic structures. Due to the reduced interlayer interaction, the intrinsic electronic structure of the two-dimensional kagome lattice can be reflected, and the two-dimensional kagome lattice is only constructed in very few systems. In this study, two types of kagome lattice prepared by Au(111) surface epitaxy were studied using ultra-high vacuum low-temperature scanning tunneling microscopy combined with density functional theory calculations. In the Bi/Au system, two kinds of single atom germanium superlattices are constructed based on the template effect of electron cage lattice. The template effect of cage lattice is confirmed by first principles calculation and Mulliken population analysis [1]. In addition, in the Ge/Au system, the Dirac node-line semi-metal  $\text{Au}_2\text{Ge}$  protected by mirror inversion symmetry is prepared by epitaxy, and on this basis, the two-dimensional kagome lattice  $\text{Au}_5\text{Ge}$  is further studied to study the local doping characteristics of metal atoms [2-3].

## Reference

[1] Q. Tian et al. Two-dimensional artificial Ge superlattice confining in electronic kagome lattice potential valleys. *Nano Lett.*, 23, 21, 9851–9857 (2023)

[2] Q. Tian et al. Twist-Angle Tuning of Electronic Structure in Two-Dimensional Dirac Nodal Line Semimetal  $\text{Au}_2\text{Ge}$  on Au(111) *ACS Nano*, Revision

[3] Q. Tian et al. Two-dimensional kagome topological nodal line semimetal  $\text{Au}_5\text{Ge}$  with flat band. To be submitted to PRL.

# Strong Correlations in Rhombohedral Multilayer Graphene

by Shuigang Xu | Westlake University

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Keywords: flat band, graphene, moire superlattice, strong correlations

Monolayer graphene possesses unique Dirac band, which endows it abundant exotic properties including ultrahigh mobility, half-integer quantum Hall effect, and Klein tunnelling effect. However, the linear band makes graphene stay away from strong correlations. In multilayer graphene, there is a metastable allotrope named as rhombohedral graphene. In rhombohedral multilayer graphene, the low-energy electrons are concentrated on its two surfaces and can be approximated described by power-law dispersion relations. With increasing the layer number, the surface bands of rhombohedral multilayer graphene at low energy become extremely flat. Due to the instability to electronic interactions endowed by their large density of states, rhombohedral multilayer graphene hosts many strongly correlated states. Here, we experimentally show that the low-temperature electronic transport in rhombohedral multilayer graphene is dominated by surface states. The extreme flat surface band results in spontaneous gap opening, indicating the surface states are strong correlated. By further introducing moiré superlattice in rhombohedral multilayer graphene, the surface flat band can be isolated from highly dispersive high-energy bands by utilizing zone folding effect. As a result, we observe layer-polarized ferromagnetism by polarizing surface states using finite displacement field. Our work establishes rhombohedral multilayer graphene as a promising platform for exploring exotic electron correlations.

# Quantitative characterization of giant optical anisotropy in Ta<sub>2</sub>NiSe<sub>5</sub>

by QihangZhang | HonggangGu | ShiyuanLiu | State Key Laboratory of Intelligent Manufacturing Equipment and Technology, Huazhong University of Science and Technology, Wuhan, 430074, PR China | State Key Laboratory of Intelligent Manufacturing Equipment and Technology, Huazhong University of Science and Technology, Wuhan, 430074, PR China | State Key Laboratory of Intelligent Manufacturing Equipment and Technology, Huazhong University of Science and Technology, Wuhan, 430074, PR China

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Keywords: Mueller matrix spectroscopic ellipsometry, Ta<sub>2</sub>NiSe<sub>5</sub>, critical point analysis, optical anisotropy

Optical anisotropy provides an additional degree of freedom for property modulation and device design based on novel low-dimensional materials. Ta<sub>2</sub>NiSe<sub>5</sub>, as a typical low-symmetry material with giant optical anisotropy, has been widely investigated for photodetectors and lasers. We have successfully extracted the complete dielectric tensor of Ta<sub>2</sub>NiSe<sub>5</sub> in the wide spectral range of UV-visible-infrared (200 -1700 nm) using advanced Mueller matrix spectroscopic ellipsometry to quantitatively characterize its giant optical anisotropy. We have also deeply investigated the physical formation mechanism of this property by combining first principle calculations and critical point analysis. Its giant optical anisotropy is expected to be useful the design of novel optical devices, and the revelation of the physical mechanism facilitates the modulations of its optical properties.

# 2D Materials for High Performance Integrated Modulators and Photodetectors

by Junjia Wang | Southeast University

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Keywords: 2D materials, hybrid integration, modulators

Integrated optoelectronic devices can break through the bottleneck of conventional optical systems, and meet the requirements of super large capacity and super high-speed information systems and data centers. The demand for higher bandwidth, higher efficiency, and lower energy consumption is ever-increasing for optoelectronic devices. 2D materials have the potential to build high-performance optoelectronic devices due to their various electro-optic response, high theoretical mobility, and easy integration. In this regard, we demonstrated (1) a microscale graphene thermo-optic modulator with a compact area of  $7.54 \mu\text{m}^2$  and high heating performance of up to  $67.4 \text{ K } \mu\text{m}^3 \cdot \text{mW}^{-1}$ ; (2) a graphene electro-absorption modulator with a high modulation efficiency up to 5.3 dB/V and a high-speed data transmission rate up to 50 Gb/s; (3) a black phosphorus photodetector with responsivity more than 2 A/W. Our work enables the construction of high-performance integrated photonic circuits compatible with CMOS technology paves the way for low-power consumption optoelectronic devices.

# Ultrafast two-dimensional flash memory

*by Chunsen Liu | Fudan university*

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*Symposium: 1. 2D Materials (2DM)*

*Keywords: 2D materials; ultrafast flash memory*

Rapid digital advances have led to a huge increase in data-driven computing tasks, and ultrafast non-volatile memory is becoming increasingly important. Flash memory now dominates the non-volatile memory market due to its simple mechanism and ability to support low-cost, high-density integration. However, the relatively low speed of flash memory is its main drawback, limiting its performance in accelerating the computation of artificial intelligence applications. Two-dimensional (2D) materials have atomically flat interfaces and the ability to be stacked into suitable heterostructures. By introducing 2D materials as the thin-channel material of flash memory, its carriers are confined to an atomically thin channel, which will improve gate controllability and maximize tunneling efficiency. This report focuses on the breakthrough in the programming speed of 2D flash memory and the application of ultrafast flash memory in the in-memory computing.



# Physical property modulation in 2D homo- and hetero-structures via pressure engineering

by Juan Xia | University of Electronic Science and Technology of China

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Keywords: Two-dimensional materials, interlayer coupling, pressure engineering, spectroscopy, stacking order

Two-dimensional (2D) materials and their van der Waals heterostructures (vdWs HSs), exhibit attractive optical and optoelectronic properties thanks to the different band alignments and interlayer interactions. Further, their sensitivity to interlayer distance allows effective tuning of material properties through external modulation of lattice parameters. Therefore, it is of both fundamental and practical importance to explore interlayer coupling in 2D vdWs structures, especially their dynamic response and underlying mechanisms to different tuning techniques. So far, only limited changes in lattice parameters have been achieved (e.g., less than 2% volume change using strain engineering, or ~5% interlayer spacing using piston-cylinder setup), hampering effective tuning of physical properties in 2D structures.

In this talk, we demonstrate effective tuning of the interlayer interaction in 2D WS<sub>2</sub> by pressure engineering, and find that the pressure-triggered interlayer coupling exhibits prominent stacking dependence, which is experimentally observed for the first time in WS<sub>2</sub>. In addition, we experimentally explore the interplay of stacking and pressure degrees of freedom in revealing unique phase transitions in bilayer MoS<sub>2</sub>, towards a phase diagram in the stacking-pressure space. In AA MoS<sub>2</sub>, interlayer sliding and asymmetric intralayer compressing precede intralayer rotation, while in AB MoS<sub>2</sub>, asymmetric intralayer compressing and intralayer distortion occur simultaneously. This may unleash the stacking degree of freedom in designing 2D devices with tailored properties correlated to interlayer coupling.

# Collective modulation of solution-processed molybdenum disulfide for tunable electronics and optics

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Keywords: 2D materials thin-films, electronics, optics, solution-processing

Molybdenum disulfide ( $\text{MoS}_2$ ), with the electronic wavefunctions confined in a two dimension configuration, allows a convenient modulation of the electronic structures with the external fields. Its solution-processed counterpart holds promise towards scalable tunable electronics and optics fabrication, given the cost-effectiveness and mass production of the solution-processing. The state-of-art reports, however, show inferior device performance as a result of the discrete nature of the solution-processed nanoflake thin-films. In this work, we present collective modulation of the macroscopic electronic properties of solution-processed  $\text{MoS}_2$  thin-films with the local electrostatic fields and explore its applications in tunable electronics and optics.

Through theoretical studies with density-functional theory calculations, we show that the local electrostatic fields can redistribute the charges in solution-processed  $\text{MoS}_2$  nanoflakes, leading to a collective modulation of the macroscopic electronic properties of the nanoflake thin-films. Using our purposed modulation mechanism, we fabricate nonlinear semiconductor-ferroelectric junctions and ferroelectric transistor memory, based on solution-processed  $\text{MoS}_2$  thin-films and ferroelectrics as electric field mediums. Beyond  $\text{MoS}_2$ , we show the modulation approach is applicable to the other solution-processed 2D materials, such as the other transition metal dichalcogenides (e.g.  $\text{MoTe}_2$ ) and bismuth telluride ( $\text{Bi}_2\text{Te}_3$ ). Besides electronic properties, we show that the modulation mechanism can alter the optical properties and demonstrate electro-optical modulator fabrication from the solution-processed  $\text{MoS}_2$  thin-films.

Given the scalability of solution-processing, as well as its adaptability to the CMOS processes and the emerging printing techniques for scalable device fabrication, this modulation approach and the enabled devices hold the potential to practical scalable device applications. To explore the potential application scenarios of our devices, we simulate a reservoir computing hardware based on the characteristics of our device. The device-parameterized reservoir computing model successfully replicates patterns of dynamical

systems (e.g. Lorentz-63, Mackey-Glass, et al.), showing the capability to unveil chaotic time-series signal patterns of, for instance, IoT sensors and brain-computer interfaces.

# Ultrafast Photoresponse in 2D van der Waals Materials and Heterostructures

by Xiao Wang | Hunan University

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Keywords: 2D Materials, Ultrafast Photoresponse, van der Waals Heterostructures

Understanding the fundamental charge carrier dynamics is of great significance for photodetection with both high speed and high responsivity. By time-resolved photocurrent (TRPC) measurements, we showed that 2D van der Waals materials can exhibit picosecond photoresponse speed with atomically thin thickness. However, when increasing thickness to gain higher responsivity, the response time of single 2D materials usually slows to nanoseconds, limiting their photodetection performance. We demonstrated that van der Waals heterojunctions can realize a much fast photoresponse time owing to the reduced average photocurrent drift time, while preserving a high responsivity. We further constructed van der Waals heterostructure photodetectors based on p-n and n-n junctions and manipulated the picosecond photoresponse by combining photovoltaic (PV) and photothermoelectric (PTE) effects. In addition, constructing heterostructure with different rotation symmetries can generate spontaneous polarization, which leads to the bulk photovoltaic effect. In this regard, we demonstrated ultrafast bulk photovoltaic response in symmetry engineered van der Waals heterostructures.

# Flexo-photovoltaic effect in MoS<sub>2</sub>

by Jie Jiang | Zhejiang University

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Keywords: Bulk-photoelectric effect; Strain gradient engineering; 2D/3D hybrid system; MoS<sub>2</sub>

The theoretical Shockley-Queisser limit of photon-electricity conversion in conventional  $p$ - $n$  junction could be potentially overcome by the bulk photovoltaic effect that uniquely occurs in non-centrosymmetric materials. Using strain gradient engineering, the flexo-photovoltaic effect, i.e., strain gradient-induced bulk photovoltaic effect, can be activated in centrosymmetric semiconductors significantly expanding material choices for future sensing and energy applications. Here, we propose a strain gradient engineering approach based on the structural inhomogeneity and phase transition of a two-dimensional/three-dimensional (2D/3D) hybrid system. We report an experimental demonstration of the flexo-photovoltaic effect in an archetypal 2D material MoS<sub>2</sub> transferred on a VO<sub>2</sub> microbeam. The experimental bulk photovoltaic coefficient in MoS<sub>2</sub> is orders of magnitude higher than that in most non-centrosymmetric materials. Our findings unveil the fundamental relation between the flexo-photovoltaic effect and a strain gradient in low-dimensional materials, which could potentially inspire the exploration of novel optoelectronic phenomena in strain gradient-engineered materials. The MoS<sub>2</sub>/VO<sub>2</sub> hybrid structure sheds light on emerging phenomena and brings new opportunity in 2D/3D interfaces.

# Exploration towards a new phase diagram for bilayer MoS<sub>2</sub> with both stacking and pressure degrees of freedom

by Chenyin Jiao | University of Electronic Science and Technology of China

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Keywords: 2D materials; phase diagram; phase transition; stacking order; Raman spectroscopy

The phase diagram serves as a blueprint for designing the structure of a material, offering a comprehensive representation of its different phases under specific conditions, such as pressure ( $P$ ) and temperature ( $T$ ). Beyond the traditional  $P$  and  $T$  axes, additional axes can be involved in the study of phase diagrams for 3D materials, such as composition, magnetic field, and doping. This expansion of degrees of freedom allows the phase diagram to serve as a roadmap for material design, providing an initial reference for manipulating processing variables and thus achieving desired microstructures.

Despite having one less dimension compared with 3D materials, two-dimensional (2D) van der Waals materials possess an additional degree of freedom: stacking. The stacking order can play a crucial role in controlling and inducing phase transitions in 2D materials. However, in studying phase diagrams for 2D materials, the exploration of stacking degree of freedom has largely been overlooked, limiting our understanding and hindering future applications.

Here, we experimentally explore the interplay of stacking and pressure degrees of freedom in revealing unique phase transitions in bilayer MoS<sub>2</sub>, towards a phase diagram in the stacking-pressure space. Our findings reveal that the bilayer system experiences phase transitions with strong stacking dependence: In AA stacking, interlayer sliding and asymmetric intralayer compressing precede intralayer rotation, while in AB stacking, asymmetric intralayer compressing and intralayer distortion occur simultaneously. Under further elevated pressure, the bilayer system transitions into 1T' phase before amorphization. Our findings offer valuable insights for creating comprehensive phase diagrams and exploring exotic phases and phase transitions of 2D materials in a broader parameter space.

# Two-Dimensional Materials Based Artificial Synapse for Neuromorphic Visual Perception

by Yuan Li | Huazhong University of Science and Technology

Abstract ID: 10474

: ThinFilms2024

Symposium: 1. 2D Materials (2DM)

Keywords: 2D materials, artificial synapse, heterostructures, neuromorphic device, visual perception

Artificial synapse that mimics the biological neuron functions are basic building blocks for the emergent neuromorphic devices with high computing speed and low power consumption, holding great potential to overcome the traditional von Neumann bottleneck and create a new paradigm for various complex artificial systems such as vision perception, pattern recognition, and image classification. However, bulk materials with uncontrollable surface defects and dangling bonds which inevitably create strong charge scattering are not desirable to realize the synaptic functionalities of neuromorphic devices. Therefore, two-dimensional (2D) materials with atomically thin dangling-bond-free surfaces and excellent physical/chemical properties have emerged as promising candidates for neuromorphic hardware. Here we report our recent progress in the development of novel 2D neuromorphic materials and their integration in artificial visual perception systems. We have designed and prepared a series of 2D materials and heterostructures to realize the synaptic functions based on innovative mechanism such as intrinsic defect capture, plasmonic enhancement, and anisotropic polarization, enabling the successful development of neuromorphic visual imaging and recognition devices with integrated sensing, memory, and computing functionalities. Our research represents a critical step forward in the field of neuromorphic computing, offering promising avenues for the realization of advanced artificial intelligence systems capable of sophisticated visual processing tasks.

# Phase-controlled growth of non-layered two-dimensional materials

by Xilong Zhou | School of Physics, Central South of University

Abstract ID: 10374

: ThinFilms2024

Symposium: 1. 2D Materials (2DM)

Keywords: 2D materials; non-layered materials; phase control; cobalt sulfide

2D transition metal chalcogenides (TMCs) have attracted broad interests due to their unique physical and chemical properties and potential applications in the fields of electronics, optoelectronics and catalysis. Many TMCs have different structural phases, which often exhibit significantly different properties. Utilizing phase control can further expand the application field of the TMCs. Non-layered materials have a large number of unsaturated atoms on their surfaces, making them more competitive than layered materials in catalysis, carrier transport, and other fields. Although non-layered materials are widely used, there are still many difficulties in their preparation. Additionally, there are few researches on the phase control of non-layered materials.

In this study, we prepared cobalt sulfide in two different new phase states by chemical vapor deposition, using temperature changes to control the phase state. We studied the structural differences between these two phases and fabricated devices to test the performance their differences. There is an approximately 80-fold difference in the carrier mobility of cobalt sulfide between the two phases. Additionally, we explain the mechanism of phase control through temperature changes and successfully achieved experimental lithography on non-layered materials such as CoSe and In<sub>2</sub>S<sub>3</sub>.



# Synthesis of twisted bilayer MoS<sub>2</sub> with a wide range of twist angles by airflow perturbation

by Cheng Li | School of Physics, Central South University

Abstract ID: 10375

: ThinFilms2024

Symposium: 1. 2D Materials (2DM)

Keywords: twist bilayer MoS<sub>2</sub>; chemical vapor deposition; strong interlayer coupling

Twist bilayer transition metal dichalcogenides (TMDs), including MoS<sub>2</sub>, have attracted significant interest due to their unique moiré superlattice induced electronic flat bands. The synthesis of high-quality twisted bilayer TMDs with uniform moiré potentials is crucial for exploring strong correlation effects, unconventional superconductivity, and the quantum anomalous Hall effect. However, the synthesis of large-area and high-quality twist bilayer MoS<sub>2</sub> (tBMoS<sub>2</sub>) with wide twist angles would be significant for exploring twist angle-dependent physics and applications. However, synthesis tBMoS<sub>2</sub> using chemical vapor deposition (CVD) is still difficult, which needs to overcome the formation energy barrier for nonstable twist bilayer.

Here, we propose a regulation of dynamics to change the growth primitive step during synthesis and disrupt the steady growth process observed in traditional MoS<sub>2</sub> bilayer materials. This method reduces the proportion of thermodynamically stable stacking modes. By employing CVD with instantaneous airflow perturbation, we directly synthesize tBMoS<sub>2</sub> with twist angles from 0° to 60°. Transmission electron microscopy clearly reveals uniformly periodic moiré patterns without reconstruction, while electron diffraction in the bilayer region consistently confirms in-plane epitaxial growth. Additionally, ultra-low-frequency Raman spectra demonstrate strong interlayer coupling and exhibit a clear angle-dependent relationship. Our study paves the way for controllable growth of tBMoS<sub>2</sub> for both fundamental research and practical applications.

# A Comprehensive Exploration of PPS/MgO@MoS<sub>2</sub> Core-Shell Composites for Enhanced Thermal and Mechanical Performance

by Minsu Kim | Jooheon kim | Chung-ang University | Chung-ang University

Abstract ID: 10396

: ThinFilms2024

Symposium: 1. 2D Materials (2DM)

Keywords: Polyphenylene sulfide; Magnesium Oxide; Molybdenum sulfide; Core-shell structure; Thermal conductivity

The growing worldwide energy crisis and environmental issues have prompted the exploration of sustainable alternatives across different sectors, such as the automotive realm. Electric vehicles (EVs) have surfaced as a practical substitute for traditional fossil fuel-driven vehicles, with their efficacy being contingent upon the weight of the vehicle. In this investigation, we present polyphenylene sulfide (PPS) as an advanced engineering plastic, boasting exceptional resistance to high temperatures and chemical stability. Its versatility makes it suitable for a range of applications within the automotive industry. However, the thermal conductivity of PPS is lower than those of other engineering plastics. Therefore, a novel core-shell structure comprising magnesium oxide (MgO) and molybdenum sulfide (MoS<sub>2</sub>) was fabricated to enhance the thermal and mechanical properties. The core-shell structure was elucidated via a comprehensive analysis using various techniques. Furthermore, the PPS/MgO@MoS<sub>2</sub>/PA composites were synthesized to address the challenges associated with high filler ratios. Tensile strength evaluations and thermal conductivity assessments confirmed the effectiveness of the proposed materials for diverse engineering applications, particularly in EVs. Additionally, surface treatments with polyformaldehyde and (3-aminopropyl)triethoxysilane (PA) improved the adhesion with the PPS matrix, which enhanced the mechanical tensile strength to 90 MPa. As the filler ratio increased, the MgO@MoS<sub>2</sub> core-shell achieved a high through-plane heat conductivity of 4.07 W/m·K, which is 22 times compared to pristine PPS. Hence, this study provides valuable insights into the ongoing pursuit of sustainable automotive solutions by addressing the critical issues of energy efficiency, environmental impact, and materials science.

# Phase-controlled synthesis and element doping engineering of 2D nonlayered Cr-based semiconductors

by Xiulian Fan | School of Physics, Central South University

Abstract ID: 10403

: ThinFilms2024

Symposium: 1. 2D Materials (2DM)

Keywords: chromium sulfide, heteroatom doping, phase control, surface passivation

Nonlayered two-dimensional (2D) materials have been extensively investigated for their ferromagnetic, ferroelectric, spin glass state, and high carrier mobility properties, leading to significant advancements in electronic and optoelectronic devices. However, nonlayered materials encounter challenges associated with the presence of high-density dangling bonds, diverse phase states, and obstacles in achieving extensive growth over large areas. To address the aforementioned challenges, it is imperative to develop a scalable and efficient phase-controlled growth method, achieve heteroatom doping, and explore both the growth mechanism and physical properties of 2D Cr-based chalcogenides for their potential applications.

Herein, we report the exploration for a stable synthesis strategy of phosphorous doping in the nonlayered  $\text{Cr}_2\text{S}_3$  nanoflakes via atmospheric chemical vapor deposition (APCVD). Our study highlights the utilization of phosphorous doping in nonlayered  $\text{Cr}_2\text{S}_3$  to finely tune its electronic structure, thereby achieving enhanced intrinsic resistive properties. Additionally, we implemented a modified ultralow gas flow CVD growth strategy, for tuning the mass transport across the boundary layer to change the reaction dynamics, thus achieving large area trigonal 2D nonlayered  $\text{Cr}_2\text{S}_3$  continuous thin films. The proposed method not only enables precise phase control of  $\text{Cr}_2\text{S}_3$ , but also presents a novel avenue for the fabrication of large-area films composed of non-layered materials.

# Broadband miniaturized spectrometers based on 2D materials.

by *Andreas Liapis | Faisal Ahmed | Hoon Hahn Yoon | Yawei Dai | Md Gius Uddin | Xiaoqi Cui | Fedor Nigmatulin | Zhipei Sun* | Department of Electronics and Nanoengineering, Aalto University, Finland. | Department of Electronics and Nanoengineering, Aalto University, Finland. | School of Electrical Engineering and Computer Science, Gwangju Institute of Science and Technology, Korea. | Department of Electronics and Nanoengineering, Aalto University, Finland. | Department of Electronics and Nanoengineering, Aalto University, Finland. | Department of Electronics and Nanoengineering, Aalto University, Finland. | Department of Electronics and Nanoengineering, Aalto University, Finland.

Abstract ID: 10414

: ThinFilms2024

Symposium: 1. 2D Materials (2DM)

Keywords: miniaturization, spectroscopy, vdW heterostructures

Conventional spectrometers rely on bulk optical components such as gratings or filters to separate colors from one another, and therefore cannot be miniaturized without sacrificing either their spectral resolution or their operating bandwidth. Ultra-miniaturized reconstructive spectrometers overcome this limitation by not requiring that colors be separated before detection. In this work, we combine the electrically-modulated spectral response of 2D material heterostructures with a reconstruction algorithm to extract spectral information with resolution equivalent to that of a table-top spectrometer, even though the total device footprint is on the order of a few tens of micrometers.

Here, we will present a high-performance broadband spectrometer based on a single van der Waals heterostructure diode that can achieve nanometer-level accuracy spanning both the visible and NIR wavelength ranges.

M.G. Uddin, *et al.* *Nat Commun* **15**, 571 (2024).

# Temperature Dependent Dielectric Function of NiI<sub>2</sub>

by Tae Jung Kim | Xuan Au Nguyen | Youjin Lee | Je-Geun Park<sup>2</sup> | Young Dong Kim | Kyung Hee University | Kyung Hee University | Seoul National University | Seoul National University | Kyung Hee University

Abstract ID: 10438

: ThinFilms2024

Symposium: 1. 2D Materials (2DM)

Keywords: Critical point, Dielectric function, Ellipsometry, NiI<sub>2</sub>

Nickel iodide (NiI<sub>2</sub>) has garnered attention in the field of van der Waals materials for its promising characteristics, which suggest its potential applications in next-generation optoelectronic devices. As a layered material, NiI<sub>2</sub> exhibits intriguing physical properties such as antiferromagnetism and ferroelectricity, which are hypothesized to persist even in ultrathin dimensions. For the device application of NiI<sub>2</sub>, knowledge of its optical properties, such as the dielectric function, is necessary. Although there are a few studies on the dielectric functions, systematic study on temperature dependence of critical points (CPs) of NiI<sub>2</sub> has not been reported, yet. In this work, we report the dielectric function of NiI<sub>2</sub> from 0.74 to 6.42 eV at temperatures from 30 to 300 K using dual rotating compensators ellipsometry. The CP energies were determined by standard lineshape analysis of numerically calculated second derivatives of  $\epsilon$  with respect to energy. Several CPs are distinguished at low temperature where the CPs are blue shifted and sharpened as a result of the reduced lattice constant and electron-phonon interaction. These results will be useful for physical understanding and application for the device based on NiI<sub>2</sub>.

# Bringing 2D FETs from research labs to mass production: the gap to bridge

by Yury Illarionov | Southern University of Science and Technology, Shenzhen, China

*Abstract ID: 10445*

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*Symposium: 1. 2D Materials (2DM)*

*Keywords: 2D materials, LAB research, field-effect transistors, mass production*

Recent research advances at fabricating FETs with 2D semiconductors have inspired the industry to begin with integration of these new technologies into FAB process flows. For instance, Intel already has 300mm FAB process for MoS<sub>2</sub>, WS<sub>2</sub>, WSe<sub>2</sub> and MoSe<sub>2</sub> at CMOS compatible temperatures, Imec has also demonstrated functional MoS<sub>2</sub> and WS<sub>2</sub> FETs produced using their 300mm FAB lines, and TSMC is currently working on gate-all-around (GAA) 2D FETs and stacking of multiple channels. Furthermore, all these key players have already demonstrated trial complementary integration of 2D FETs.

However, the transition of new 2D technologies from LAB research to FAB process lines is still very challenging due to a number of open questions, such as the need to satisfy CMOS thermal budget below 450C, top-gate integration by growing 3D oxides on 2D channels and reliability limitations due to charge trapping near the channel/oxide interfaces. Furthermore, the industry is currently focused only on transition metal dichalcogenide channels and 3D oxide insulators, while being unable to use alternative technologies such as Bi<sub>2</sub>O<sub>2</sub>Se/Bi<sub>2</sub>SeO<sub>5</sub> which have already resulted in the first 2D FinFETs in LAB research.

In this talk I will summarize recent progress made by the industry at integrating 2D FETs into FAB lines and discuss the main challenges which arise on this way. I will also give some futuristic view on the possible development of FAB integration of 2D FETs in the coming years.

# Electrical properties and evaluation of band tail states in Mg doped p-type hBN multilayer films

by Niall Tumilty | National Yang Ming Chiao Tung University

Abstract ID: 10446

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Symposium: 1. 2D Materials (2DM)

Keywords: CVD, Fermi level, XRD, p-type hBN, precursor temperature

A series of Mg doped p-type multi-layered hBN films were prepared by atmospheric pressure chemical vapor deposition (APCVD) at different dopant precursor temperatures. Temperature dependent conductivity measurements were performed from 0.1 Hz to 10 MHz to analyze the characteristics of band tail states close to the valence band edge. Johnscher's universal power law ( $A\omega^s$ ) is successfully applied to understand localized charge carrier transport through these states, where 'S' increases from 0.8 to 1.39, indicating that non-overlapping small polaron hopping (NSPT) conduction mechanism dominates up to 300C. Polaron binding energies and tunneling distances of 0.2 - 0.5 eV and 30 - 40 Å are calculated. The density of states  $N(E(F))$  was extracted from a fit to the AC conductivity data yielding values of  $1E22 - 3E23/cm^3$  eV, confirming the conductive nature of our samples. Fermi level position is observed through UPS whereby  $E(F)$  moves towards the valence band edge ( $E(F)-E(V)$ ) as dopant precursor temperature increases from 750C to 950C yielding values of 1.8 eV and 0.5eV, respectively, correlating with a reduction in sample resistance by a factor of  $10^8$  compared to undoped hBN. Overall, we show that AC conductivity is an effective method to evaluate mid gap states in 2D materials. Hole concentrations of the order of  $10^{17}/cm^3$ , mobility between 30 - 60 $cm^2/Vs$  and an acceptor level is measured at 40meV.

# Multifunctional Programmable Soft Actuator Based on 2D Materials

by Xiuju Song | Zhejiang University

Abstract ID: 10478

: ThinFilms2024

Symposium: 1. 2D Materials (2DM)

Keywords: 2D Materials, MXene, graphene, programmable, soft actuator

Stimuli-responsive actuators are considered as intelligent devices due to their ability to convert various environmental stimuli into mechanical motion through rapid and reversible deformation. These devices have shown significant potential applications in fields such as soft robots, micro electro mechanical systems (MEMS), and other forefront areas. To date, numerous functional materials have been utilized in the preparation of stimulus-responsive actuators, including hydrogel, magnetic materials, liquid crystal elastomers, shape memory alloys, and carbon materials. Among these materials, two-dimensional materials stand out as being especially important for the development of stimuli-responsive actuators due to their unique physical and chemical properties.

In this work, we propose a novel design for soft actuators that uses two-dimensional materials and polymers to construct Janus structured bilayer membranes. Inspired by various plants in nature, we design the graphene oxide/ polyethylene actuator and graphene@PDMS/PVDF actuator. These actuators have excellent performance, characterized by large deformations, rapid response (up to 90.5°/s), and reversible actuation. These actuators are able to support various programmable movements and engineering applications, such as indicating water pollution, convertible mountain and valley fold, and performing the Five-animal Exercise. It is indicated that the enormous application potential of the bilayer actuator is in the fields of bioengineering, origami technology, soft robotics, and beyond.



# On-chip electrocatalytic investigation of 2D Molybdenum phosphides

by Qiyuan He | City University of Hong Kong

Abstract ID: 10483

: ThinFilms2024

Symposium: 1. 2D Materials (2DM)

Keywords: Molybdenum diphosphide, Molybdenum phosphides, On-chip electrocatalytic microdevice, hydrogen evolution reaction, tellurene

On-chip electrocatalytic microdevice (OCEM) is an emerging platform for investigating microscopic nanocatalysts, offering precise electrochemical measurements and unique perspectives inaccessible in conventional electrochemical methods. Owing to strong adaptability, OCEMs are becoming increasingly capable in measuring the electrocatalytic performance of nanomaterials, identification of active sites, *in-situ* transport measurement, field-effect modulation of catalysts, and incorporation of *in-situ* characterization. In this talk, I will give a general introduction to the OCEM platform, review its development, and showcase its capability in developing novel electrocatalysts and explore exotic catalytic mechanisms. Recently, by taking advantage of the high space resolution in OCEM measurement, we have interrogated the electrocatalytic active sites of phosphorus-doped MoS<sub>2</sub> (P-MoS<sub>2</sub>) at individual nanosheet levels and found significantly enhanced edge-oriented HER activity. By further increasing the P doping, we can synthesize nonlayered 2D Molybdenum phosphide (MoP) and Molybdenum diphosphide (MoP<sub>2</sub>), via a unique surface-confined atomic substitution in gas phase. Moreover, OCEM measurements conclusively demonstrated that nonlayered 2D MoP and MoP<sub>2</sub> nanosheets exhibit excellent electrocatalytic HER in acidic and neutral electrolyte, respectively. Lastly, the surfactant-free solution synthesis of single-crystalline 2D tellurene is demonstrated with record high hole mobility and high stability in iontronic applications. In conclusion, we showcase our continuous effort in the gas-solid synthesis of 2D thin films and adaptability of OCEM methodology in exploring their electrochemical properties.

# Electronics and Optoelectronics Based on 2D Tellurium

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Abstract ID: 10488

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Symposium: 1. 2D Materials (2DM)

Keywords: 2D tellurium, electronics, heterostructures., memory devices, photodetectors

Tellurium (Te) is semiconductor with truly one-dimensional crystal structure, where single helical molecular chains are stacked together via vdW interactions. The naturally terminated surfaces except for the two ends endow Te with advantages over conventional three-dimensional materials, thus making it very promising for fabrication of electronic and optoelectronic devices. In this talk I will present our recent works on electronics and optoelectronics based on 2D tellurium. First, I will present the fabrication of high-performance short-wave infrared (SWIR) photodetectors and focal plane arrays based on Te nanoflakes and evaporated  $\text{Se}_x\text{Te}_{1-x}$  thin films with tunable bandgaps. Then, I will present the fabrication of high-performance transistors, logic gates and circuits based on evaporated Te thin films and Te nanobelts grown h-BN. Finally, I will present the fabrication of electronic/optoelectronic memory devices based on 2D tellurium-based vdW heterostructures for reservoir computing.

# Two-dimensional electronic devices towards intelligent vision sensors

by Zhenxing Wang | National Center for Nanoscience and Technology, Beijing, China

Abstract ID: 10492

: ThinFilms2024

Symposium: 1. 2D Materials (2DM)

Keywords: Ferroelectric semiconductor, Memristor, computing in sensor, neuromorphic device

Artificial intelligence technology has become the core driving force for the new round of technological and industrial revolutions in the information age. After more than 70 years of development, the performance potential given by the von Neumann architecture has almost reached its limit. Exploring new computing architectures and intelligent electronic devices has become the focus of attention.

Due to the weak van der Waals force between the adjacent layers, the heterostructure based on two-dimensional materials is not limited by the interface lattice, polarity, thermal expansion coefficient and other physical mismatches. It can realize the heterostructure construction of any kind of materials, different stacking sequences, different stacking angles and thicknesses, showing unique physical properties and potential in building new structural devices.

In this talk, I would report our research progress on two-dimensional electronic devices towards intelligent vision sensors. These kinds of devices employ the neuromorphic computation and own a computation-in-sensor architecture. They show the great application potential in intelligent machine vision system in the future.

## Reference

- Wang, and Z. Wang\* *et al*, *Nano Lett.* 2023, 23, 4524
- Cai, Z. Wang\* *et al*, *Adv. Funct. Mater.* 2023, 33, 2212917.
- Jiang, J. He\* and Z. Wang\*, *et al*, *Adv. Mater.* 2023, 35, 2211701.
- Wang, Z. Wang\* and J. Shi\*, *et al*, *Adv. Mater.* 2023, 35, 2209465.
- Li\* and Z. Wang\* *et al*, *Adv. Mater.* 2023, 2301472.
- Wu, F. Wang\* and Z. Wang\* *et al*, *Nano Lett.* 2022, 22, 7094.
- Yang, F. Wang\*, Z. Cheng, Z\*. Wang\* *et al*, *Adv. Funct. Mater.* 2022, 2205468.
- Wang, F. Wang, Z. Wang\*, and J. He\* *et al*, *Science Bulletin* 2021, 2288
- Wang, Z. Wang\*, and J. He\* *et al*, *Science Bulletin* 2020, 65, 1444-1450.
- Yin, Z. Wang\*, and J. He\* *et al*, *Nano Lett.* 2020, 20, 4144-4152.
- Wang\*, Z. Wang\*, and X. Sun\* *et al*, *Angew. Chem. Int. Ed.* 2024, e20242033.

# Mixed-dimensional van der Waals heterostructures for novel optoelectronic devices

by Qisheng Wang | Nanchang University, China

Abstract ID: 10506

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Symposium: 1. 2D Materials (2DM)

Keywords: , 2D materials, optoelectronic devices, traditional materials, van der Waals heterostructures

Photoelectric detection and imaging devices based on Si, PbS,  $\text{Hg}_x\text{Cd}_{1-x}\text{Te}$ , GaAs/ $\text{Al}_{1-x}\text{Ga}_x\text{As}$  quantum Wells and InAs/ $\text{Ga}_{1-x}\text{In}_x\text{Sb}$  superlattices and other materials have been widely used in defense and aviation, industrial automation, optical fiber communication, astronomical exploration, health care, security monitoring and environmental monitoring industries. However, limited by devices performance and functions, the traditional optoelectronic materials cannot meet the requirements for rapid developing optoelectronic information technology. This report proposes a new materials system of two-dimensional (2D)/three-dimensional (3D) semiconductor heterojunctions (1) which couples the emerging 2D materials with traditional semiconductors, giving rise to a series of interesting optoelectronics properties. We first report a large-area growth of 2D materials ( $\text{MoS}_2$ ,  $\text{WS}_2$ ,  $\text{WSe}_2$ ) array with excellent electrical properties. Then we will show several types of 2D/3D heterojunctions ( $\text{MoS}_2/\text{PbS}$ , graphene/ $\text{PbS}$ ) (2-9) with novel optoelectronic phenomenon of photo-gating effect, non-volatile infrared memory. At the end of the report, a silicon-compatible growth of large-area graphene/ $\text{PbS}$  heterostructure thin film will be presented. Our work provides a new class of high-performance optoelectronic devices based on mixed-dimensional van der Waals heterostructures with novel technology of optical information recording and processing.

## References

- (1) Nanotechnology 32 (2021) 505610
- (2) J. Phys. D: Appl. Phys. 53 (7), 075108, 2019
- (3) Sci. Adv. 2018, 4:eaap7916
- (4) Adv. Mater. 2016, 28, 6497
- (5) Nano Lett. 2015, 15, 1183
- (6) ACS Nano 2014, 8, 7497
- (7) Adv. Mater. 2016, 28, 8051

(8) Adv. Mater. 2016, 28, 3596

(9) Small 2015, 11, 5388

# In-memory sensing and computing based on ferroelectric materials

by Bobo Tian | East China Normal University

*Abstract ID: 10527*

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*Symposium: 1. 2D Materials (2DM)*

*Keywords: ferroelectric, in-memory computing, in-memory sensing and computing, in-sensor computing*

Rapid developments in Internet of Things (IoT) and Artificial Intelligence (AI) trigger higher requirements for image perception and learning of external environments through visual systems. However, limited by von Neumann bottleneck, the physical separation of sensing, memory, and processing units in a conventional personal computer (PC) based vision system tend to consume significant energy consumption, time latency and additional hardware costs. The emerging bio-inspired neuromorphic visual systems, by integrating sensing, memory and computational tasks of multiple functionalities into one single namely retinomorph device, provide an opportunity to overcome these limitations. An architecture for the in-memory sensing and computing (IMSC) paradigm that combines all three modules has been developed based on ferroelectrics. Here I give a summary on ferroelectric retinomorph devices for in-sensor memory and computing.

# In Situ Dual-Interface Passivation Strategy Enables the Efficiency of Formamidinium Perovskite Solar Cells over 25%

by yuchuan shao | shanghai institute of optics and fine mechanics

Abstract ID: 10528

: ThinFilms2024

Symposium: 1. 2D Materials (2DM)

Keywords: buried interface, in situ passivation, perovskite, solar cell, top interface

Perovskite solar cells (PSCs) are promising candidates for next-generation photovoltaics owing to their unparalleled power conversion efficiencies (PCEs). Currently, approaches to further improve device efficiencies tend to focus on the passivation of interfacial defects. Although various strategies have been developed to mitigate these defects, many involve complex and time-consuming post-treatment processes, thereby hindering their widespread adoption in commercial applications. In this work, we develop a concise but efficient in situ dual-interface passivation strategy wherein 1-butyl-3-methylimidazolium methanesulfonate (MS) is employed as a precursor additive. During perovskite crystallization, MS can either be enriched downward through precipitation with  $\text{SnO}_2$ , or can be aggregated upward through lattice extrusion. These self-assembled MS species play a significant role in passivating the defect interfaces, thereby reducing non-radiative recombination losses, and promoting more efficient charge extraction. As a result, a PCE >25% (certified PCE of 24.84%) was achieved with substantially improved long-term storage and photo-thermal stabilities. This strategy provides valuable insights into interfacial passivation and holds promise for the industrialization of PSCs

# Optoelectronic Property Tuning in Molybdenum Ditelluride via Lattice Structure Manipulation

by Ya-Qing Bie | Sun Yat-sen University

Abstract ID: 10543

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Symposium: 1. 2D Materials (2DM)

Keywords: exciton emission, molybdenum ditelluride, phase transition, twist-bilayer

Layered 2H-MoTe<sub>2</sub> has emerged as a promising near-infrared material with notable optical activity, making it ideal for hybrid integration with silicon photonics in optical communications. Its polymorphic nature, a characteristic of van der Waals materials, suggests that its optoelectronic properties can be finely adjusted through phase transitions and controlled stacking, presenting a rich set of properties alongside challenges in robustness. Understanding the distinct phases and lattice structure manipulation mechanisms is therefore essential. Our studies explore two methods of lattice structure manipulation. In the first approach, we detail the transition of monolayer MoTe<sub>2</sub> from the 2H to the 1T' phase, achieved using field-enhanced terahertz pulses rather than visible light. This method limits structural damage by high energy photons thanks to the lower energy of terahertz photons. We introduce a single-shot terahertz-pump-second-harmonic-probe technique, revealing a phase transition out of the 2H phase within 10 ns post-photoexcitation. The second approach examines exciton emission in MoTe<sub>2</sub> homobilayers with controlled twist angles ranging from 0° to 60°, focusing on small-twist regions. Low-temperature photoluminescence measurements allowed us to track exciton emission evolution with increasing twist angles. We also detected neutral and charged excitons in a 1.4° twisted MoTe<sub>2</sub> bilayer using gate-dependent and field-dependent photoluminescence, offering insights into phase transition mechanisms and excitonic behavior in thin semiconductors based on twist angles. Our findings contribute vital experimental insights into phase transitions and excitonic dynamics in atomically thin semiconductors, paving the way for advanced optoelectronic applications.

## References

- [1] Nature Communications 14 (1), 5905, 2023
- [2] Advanced Optical Materials 11 (17), 2300424, 2023
- [3] Advanced Optical Materials 12 (5), 2301747, 2024
- [4] Nature Nanotechnology 12, 1124-1129, 2017



# Surface/interface-dominated growth dynamics of novel transition metal dichalcogenide monolayers

by Zhu Chao | Southeast University

Abstract ID: 10546

: ThinFilms2024

Symposium: 1. 2D Materials (2DM)

Keywords: growth mechanism, scanning transmission electron microscopy, transition metal dichalcogenides

The investigation of material growth and evolution mechanisms is of great importance for the controllable synthesis and property manipulation. In this talk, I will discuss our recent efforts in exploring the growth and evolution dynamics of novel transition metal dichalcogenide (TMD) monolayers using (scanning) transmission electron microscopy ((S)TEM) techniques, especially with the focus on the driven effect of surface/interface structures during these processes. We have demonstrated the synthesis of ultra-long MoS<sub>2</sub> nano-channels within MoSe<sub>2</sub> monolayers, based on intrinsic grain boundaries. A strain-driven growth mechanism is proposed that the strain fields near the grain boundaries not only lead to the preferred substitution of selenium by sulfur atoms but also drive the coherent extension and formation of MoS<sub>2</sub> channels. In addition, we have developed a co-deposition strategy to fabricate a wafer-scale network of platinum single-metal-atom-chains within monolayer MoS<sub>2</sub> film. The stable four-coordinated motifs at the zigzag edges of MoS<sub>2</sub> are uncovered to be responsible for the migration of platinum atoms along the growth direction, and the followed connection of inversely oriented MoS<sub>2</sub> domains, obeying a surf-zip dynamic mechanism. Besides, we also unraveled the surface-vacancy guided phase evolution mechanism of PtSe<sub>2</sub>, from crystalline structure to amorphous phase. During this process, the sequential generation of selenium vacancies give rise to the decrease of coordination number, the followed displacement of platinum atoms, and the finally complete amorphization of PtSe<sub>x</sub> monolayers.

# Reconfigurable photodetection from two-dimensional materials

by Jinshui Miao | Shanghai Institute of Technical Physics, Chinese Academy of Sciences

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Reconfigurable image sensors for the recognition and understanding of real-world objects are now becoming an essential part of machine vision technology. The neural network image sensor — which mimics neurobiological functions of the human retina — has recently been demonstrated to simultaneously sense and process optical images. However, highly tunable responsivity concurrently with non-volatile storage of image data in the neural network would allow a transformative leap in compactness and function of these artificial neural networks (ANNs) that truly function like a human retina. Here, we demonstrate a reconfigurable and non-volatile neuromorphic device based on two-dimensional (2D) semiconducting metal sulfides that is concurrently a photovoltaic detector. A convolutional neuromorphic network (CNN) is also designed for image process and object detection using the same device. The results demonstrated reconfigurable and non-volatile photodetectors can be used for future optoelectronics devices for neuromorphic computing.

# Cr<sub>2</sub>Te<sub>3</sub> Encapsulated Liquid Metal for Wearable Sensors

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Gallium (Ga) based liquid metal (LMs) has been widely used in human-machine interface electronics due to its non-toxicity, high conductivity, deformability and unique surface chemistry. Because of these properties, LMs have been integrated as device components in electrical conductors for a variety of flexible and stretchable electronic devices, including soft robots, actuators, and sensors. Liquid metal-based electronic devices have been manufactured in various forms, including injection into microchannels, fiber or porous structures, and mixing with other soft/elastic materials or dispersing in mechanically flexible composite electrodes. However, the exposed liquid metal tends to form an oxide layer, which causes the viscosity of the droplet surface and prevents it from deforming and moving precisely.

Here, we proposed a magnetic liquid metal droplet coated by two-dimensional transition-metal dichalcogenides (TMDs). Cr<sub>2</sub>Te<sub>3</sub> nanoflake was chosen as a material for encapsulating liquid metals because of its intrinsic magnetic properties while having good mechanical frictional properties. Under a magnetic field, the droplet can be driven to produce accurate deformation due to the magnetic response of the surface Cr<sub>2</sub>Te<sub>3</sub> layer. The droplet was tested to prove it has a mechanical strength and can maintain its structure and inherent properties under 5000 cycles of rolling. These characteristics enable the droplet to be used in deformable, mobile, high mechanical strength and magnetic field-driven floating electrode designs. Based on the above work, we designed a memory array that can be written by magnetic tracks. The array consisted of droplet-based memory elements, each of which can store a specified number of potentials and switch potentials by changing magnetic fields. The memory array made of liquid drops showed accurate magnetic track path recognition, so that the magnetic field information could be perceived, stored and learned. The stored electrical signal had a large signal-to-noise ratio, which ensures the accurate reading of the stored data.