AVS Taiwan Chapter: Emergent phenomena and related physics in novel van der Waals heterostructures

Time: 24/January/2019 Location: Tin Ka Ping Photonic Building (EO-103)
Chair: Prof. Po-Wen Chiu, NTHU

13:00~13:05
Speaker: Vice president Jinn P. Chu, NTUST
Title: Opening

13:05~13:35
Speaker: Prof. C. K. Shih, The University of Texas at Austin, USA
Title: Probing and Tuning Interlayer Interactions to Control Electronic and Photonic Properties of 2D Heterostructures

13:35~14:05
Speaker: Dr. Chia-Hao Chen, NSRRC
Title: A Multiferroic Supported Monolayer WSe_2 P-N Homojunction

14:05~14:35
Speaker: Prof. Shuyun Zhou, Tsinghua University, China
Title: Band Structure Engineering of Monochalcogenides and van der Waals Heterostructures

14:35-15:05
Speaker: Prof. Tay-Rong Chang, NCKU
Title: Electronic Structures of Topological Quantum Thin-Film

15:05-15:30 Coffee Break

15:30-16:00
Speaker: Prof. M. Batzill, University of South Florida, USA
Title: Lattice Imperfections in van der Waals Materials for Introducing Functionalities

16:00-16:30
Speaker: Prof. Yi-Hsien Lee, NTHU
Title: Optics of Two-Dimensional Monolayer Semiconductors

16:30-17:00
Speaker: Dr. K. Tsukagoshi, NIMS, Japan
Title: Heterojunction Based on Atomically Thin Semiconductor and its Application

17:00-17:30
Speaker: Prof. Y. H. Chu, NCTU
Title: van der Waals Heteroepitaxy on Muscovite

17:30-17:45
Speaker: AVS Title: AVS publication

Probing and Tuning Interlayer Interactions to Control Electronic and Photonic Properties of 2D Heterostructures

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Atomically thin, single crystalline 2D electronic materials have recently emerged, offering a remarkably wide range of building blocks of nanostructures, ranging from metals (e.g. graphene), large gap insulators (BN), to semiconductors (transition metal dichalcogenides and black phosphorous). One key advantage of these van der Waals materials lies in the flexibility of stacking different types of materials to form heterostructures, providing a design platform for achieving novel device functionality. In vdW hetero-bilayers, the interface encompasses the whole heterostructure and interlalyer interactions become the controlling parameter for the electronic structure.

In this talk I will first discuss directly probing the inter-layer interactions through the “lens” of moiré patterns using scanning tunneling microscopy and spectroscopy (STM/S). I will show that the interlayer coupling is strongly dependent on the inter-atomic alignment of the constituent layers. Moreover, as a consequence of moiré pattern formation, the energy band structure of the hetero-bilayer also shows lateral modulation, forming a 2D electronic superlattice. The moiré pattern “lens” also provides us with a means to measure the 2D strain tensor with high precision and high spatial resolution. In addition, the strain profile shows a direct correlation with the band gap modification.

As the periodic potential modulation also provides lateral confinement for excitons, an intriguing scenario occurs – the 2D lateral superlattices also form 2D exciton quantum dot arrays. Recent reports of ultra-sharp atomic like spectra provide a direct confirmation of such a scenario. Finally, I will add another control knob and show evidence for valley spin mediated interlayer couplings, and their effect on excitonic states of the hetero-bilayer.

A Multiferroic Supported Monolayer WSe_2 P-N Homojunction

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Multiferroic materials possess the ability to control both their magnetic and ferroelectric characteristics. This ability is highly sensitive to the stimulus of electric, magnetic, or optical fields. In this regard, this category of multifunctional materials is an ideal substrate to functionalize the ultra-thin monolayer two-dimensional (2D) materials.

The electronic properties of the 2D materials span from insulator, semiconductor, semimetal, metal, to superconductor and topological insulator. Joining with multiferroic materials, the heterostructures of the wide variety of material combinations will definitely open a new route for the development of emergent functional systems.

In this presentation, we will show the results of our first effort to bringing multiferroic and 2D materials together. We manipulated the carrier concentration of semiconducting monolayer WSe_2 into a p-n homojunction by locally reversed the ferroelectric polarization of the supporting $BiFeO_3$ substrate [1]. The stable WSe_2 p-n homojunction is demonstrated with optical and scanning probe methods, synchrotron radiation based scanning photoelectron spectromicroscopy, and transport measurement. This work provides a non-volatile control of WSe_2 doping and a promising way to produce a p-n homojunction as a future building block of 2D device applications.

Reference:

[1] Jhih-Wei Chen et al., Nature Comm. 9(2018)3143.

Band Structure Engineering of Monochalcogenides and van der Waals Heterostructures

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Two-dimensional (2D) materials provide an important playground for exploring fundamental physics and potential applications. In this talk, I will present our recent process on the band structure structure of 2D materials and heterostructures. In particular, I will present our recent work on the electronic structure of a few transition metal monochalcogenides - thermoelectric SnSe [1] and charge density wave material CuTe [2]. I will also present our recent progress on the band structure engineering of two prototypical examples of van der Waals heterostructures, a commensurate graphene/BN heterostructure with Moire pattern [3], and an incommensurate 30° twisted bilayer graphene which shows symmetries similar to a quasicrystal [4].

References:

[1] Kenan Zhang et al., “Widely tunable band gap in a multivalley thermoelectric semiconductor SnSe by potassium doping”, Phys. Rev. Materials **2**, 054603 (2018).

[2] Kenan Zhang et al., “Experimental evidence for charge density wave in the layered copper chalcogenide CuTe”, PRL 121, 206402 (2018).

[3] Eryin Wang et al., “Gaps induced by inversion symmetry breaking and second-generation Dirac cones in graphene/hexagonal boron nitride”, Nat. Phys. **12**, 1111-1115 (2016).

[4] Wei Yao et al., “Quasicrystalline 30° twisted bilayer graphene as an incommensurate superlattice with strong interlayer coupling”, PNAS **115**, 6928 (2018).

Electronic Structures of Topological Quantum Thin-Film

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The topological insulator (TI) is a newly discovered phase in condensed matter systems. The TI is featured by a bulk energy gap originating from spin-orbit coupling and time-reversal symmetry protected gapless surface states, which is distinct from the conventional band insulator. In the past decade, the three-dimensional topological insulating phase has been proposed and realized in many compounds, whereas the two-dimensional topological quantum thin-film that exhibits exotic surface and/or interface physics has remained elusive. In this talk, we will review the electronic structures of metal/TI heterostructure [1,2], WTe_2 thin-film [3,4], type-II nodal line [5], and new type of topological crystalline insulator [6] by using first-principles calculations, and discuss various exotic phenomena observed experimentally in these compounds.

References:

[1] Ching-Hao Chang et al., Newtype large Rashba-splitting in quantum-well-state induced by spin-chirality in metal/topological-insulator, NPG Asia Materials 8, e332 (2016).

[2] Shu Hsuan Su et al., Selective hydrogen etching leads to 2D Bi (111) bilayers on Bi2Se3: Large Rashba splitting in topological insulator heterostructure, Chemistry of Materials 29, 8992 (2017).

[3] Su-Yang Xu et al., Electrically switchable Berry curvature dipole in the monolayer topological insulator WTe_2, Nature Physics 14, 900(2018).

[4] Qiong Ma et al., Observation of the nonlinear Hall effect under time reversal symmetric conditions, Nature, in press (2018).

[5] Tay-Rong Chang et al., Realization of a Type-II Nodal-Line Semimetal in Mg_3Bi_2, Advanced Science, 1800897 (2018).

[6] Xiaoting Zhou et al., Topological crystalline insulator states in the Ca_2As family, Phys. Rev. B (Rapid communication), in press (2018).

Lattice Imperfections in van der Waals Materials for Introducing Functionalities

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Edges, defects, and dopants in 2D transition metal dichalcogenides have been shown to give rise to chemical, electronic, and magnetic properties in these materials. To utilize the potential of these modifications a detailed understanding of their controlled formation and atomic scale properties is needed. In our group we aim at synthesizing 2D materials by molecular beam epitaxy and study approaches for controlled modifications by alloying, doping, one-dimensional modifications (edges or grain boundaries) or interfacing with dissimilar materials. In this talk we present our studies on the controlled formation of metallic mirror twin grain boundaries in $MoSe_2$ [1] or $MoTe_2$ [2] by incorporation of excess Mo into the lattice. Very high density of MTB networks can be obtained in $MoTe_2$ that effectively metallizes the material and thus may act as a metallic contact patch [3]. Such line defects may also increase electrocatalytic properties for hydrogen evolution reactions [4]. On a more fundamental level, we show that these 1D metallic grain boundaries host one dimensional electron gas and we present the first angle resolved photoemission (ARPES) studies of such line defects. These studies show evidence for the presence of Tomonaga-Luttinger Liquid behavior of 1D electron systems [5]. Finally, we show that other transition metals may also be incorporated into $MoTe_2$ and the incorporation of vanadium induces room temperature ferromagnetic ordering and thus is an example of a 2D dilute ferromagnetic semiconductor.

References:

[1] Y Ma, S Kolekar, H Coy Diaz, J Aprojanz, I Miccoli, C Tegenkamp, M Batzill. Metallic Twin Grain Boundaries Embedded in $MoSe_2$ Monolayers Grown by Molecular Beam Epitaxy. ACS Nano 11, 5130-5139 (2017).

[2] HC Diaz, Y Ma, R Chaghi, M Batzill. High density of (pseudo) periodic twin-grain boundaries in molecular beam epitaxy-grown van der Waals heterostructure: $MoTe_2/MoS_2$. Appl. Phys. Lett. 108, 191606 (2016).

[3] PM Coelho, HP Komsa, H Coy Diaz, Y Ma, AV Krasheninnikov, M Batzill. Post-Synthesis Modifications of Two-Dimensional MoSe2 or MoTe2 by Incorporation of Excess Metal Atoms into the Crystal Structure. ACS Nano 12, 3975-3984 (2018).

[4] T Kosmala, H Coy Diaz, HP Komsa, Y Ma, AV Krasheninnikov, M Batzill, S Agnoli. Metallic Twin Boundaries Boost the Hydrogen Evolution Reaction on the Basal Plane of Molybdenum Selenotellurides. Adv. Energy Mat., 1800031 (2018).

[5] Y Ma, et al. Angle resolved photoemission spectroscopy reveals spin charge separation in metallic MoSe2 grain boundary. Nature Commun. 8, 14231 (2017).

Optics of Two-Dimensional Monolayer Semiconductors

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Monolayers of transition metal dichalcogenides (TMDs) exhibits strong spin-orbital coupling with unique band structures, which enables valleytronics and nonlinearity of the are ideal for the explore many body effects and.[1-4] Here, micro-cavity are designed and fabricated to integrate the CVD-grown TMD monolayers for the study of light-matter interactions and polariton physics. Some interesting observations and potential applications of the integrated 2D systems will be discussed.[5,6]

References:

[1] E.J. Sie et al, Nature Materials, 14, p.290–294 (2015).

[2] E.J. Sie et al, Science 355 (6329), 1066-1069, (2017).

[3] Xiaoze Liu et al, Nature Photonics, 9, p.30–34 (2015).

[4] Liang Guo et al, Nature Phys., (just accept).

[5] Jinwei Shi et al, Nature Comm. 8, 35 (2017).

[6] C. Yang et al, VLSI (2016).

Heterojunction Based on Atomically Thin Semiconductor and Its Application

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Growth of a uniform oxide film with a tunable thickness on two-dimensional transition metal dichalcogenides is of great importance for electronic and optoelectronic applications in next generation atomically-controlled hetero semiconducting structure. Here we demonstrate homogeneous surface oxidation of atomically thin WSe_2 with a self-limiting thickness from single- to trilayers.

Exposure to ozone (O_3) below 100 °C leads to the lateral growth of tungsten oxide selectively along selenium zigzag-edge orientations on WSe_2. With further O_3 exposure, the oxide regions coalesce and oxidation terminates leaving a uniform thickness oxide film on top of unoxidized WSe_2. At higher temperatures, oxidation evolves in the layer-by-layer regime up to trilayers. The oxide films formed on WSe_2 are nearly atomically flat. Using photoluminescence and Raman spectroscopy, we find that the underlying single-layer WSe_2 is decoupled from the top oxide but hole-doped.

The hole-doping by the under-stoichiometric tungsten oxides (WOx with x < 3) grown on WSe_2 can be used as both controlled charge transfer dopants and low-barrier contacts for p-type WSe_2 transistors. WO_x-covered WSe_2 is highly hole-doped due to surface electron transfer from the underlying WSe_2 to the high electron affinity WO_x. The dopant concentration can be reduced by suppressing the electron affinity of WO_x by air exposure, but exposure to O_3 at room temperature leads to the recovery of the electron affinity. Hence, surface transfer doping with WOx is virtually controllable. Transistors based on WSe_2 covered with WO_x show only p-type conductions with orders of magnitude better on-current, on-off current ratio, and carrier mobility than without WO_x, suggesting that the surface WO_x serves as a p-type contact with a low hole Schottky barrier.

As a function of the above heterostructure of WSe_2 wiht WO_x, photocurrent generation was observed. The he responsivity of the oxide-covered WSe_2 transistor is observed to exceed 3000 A/W, suggesting the effectiveness of surface oxidation in facilitating the photogating effect in 2D semiconductors.

Further thin-film function, which will be developed in the atomically-thin film herostructures, will be introduced.

References:

[1] Self-limiting surface oxidation of atomically thin WSe_2, M.Yamamoto, S.Dutta, K. Wakabayashi, M. S. Fuhrer, K.Ueno, K.Tsukagoshi, Nano Letters 15, 2067–2073 (2015).

[2] Surface Oxides on Single- and Few-layer WSe_2 as Controlled Dopants and Low-Barrier Contacts, M.Yamamoto, S.Nakaharai, K.Ueno, K.Tsukagoshi, Nano Letters, 16, 2720–2727 (2016).

[3] Pronounced photogating effect in atomically thin WSe_2 with a self-limiting surface oxide layer, M.Yamamoto, K.Ueno, K.Tsukagoshi, Applied Physics Letters 112, (18) 181902/1-6 (2018).