Workshop on
Quantum Materials for the Post-Si Era
2023 7/31~8/2, Pohang

Institute for Basic Science (POSTECH campus), Auditorium 104

Invited Speakers:

Prof. Wei Ruan (Fudan university)
Prof. Gil Young Cho (POSTECH)
Prof. Yan Zhang (Peking University)
Dr. Jhinhwan Lee (IBS CALDES)
Prof. Zheng Liu (Tsinghua University)
Dr. Jae Whan Park (IBS CALDES)
Prof. Wenyu He (ShanghaiTech University)
Prof. Wei Jiang (BIT)
Prof. Huaqing Huang (Peking University)
Dr. Yinong Zhou (UC Irvine)
Prof. Feng Liu (University of Utah)
Dr. Gurjyot Sethi (University of Utah)
Prof. Minghu Pan (SNNU)
Prof. Miao Zhou (Beihang University)
Prof. Yunhao Lu (Zhejiang University)
Prof. Chen Si (Beihang University)
Prof. Xiaoming Zhang (OUC)
Dr. Xiaoyin Li (Universiy of Utah)
Dr. Young-Jae Choi (IBS CALDES)
Prof. Raj Ganesh S Pala (IIT at Kanpur)

Organizers:

Prof. Han Woong Yeom (Institute for Basic Science)
Prof. Feng Liu (University of Utah)
Prof. Zheng Liu (Tsinghua University)
Dr. Kyung-Hwan Jin (Institute for Basic Science)

Center for Artificial Low D Electronic Systems

THE UNIVERSITY OF UTAH

2023 WQMPE program

time	7/31 (Mon.)	time	8/1 (Tue.)	time	8/2 (Wed.)
8:50~9:10	Registration				
9:10~9:20	**Opening**		Prof. Zheng Liu		Dr. Jhinhwan Lee
	Prof. Han Woong Yeom	9:00~9:35	Prof. Wei Jiang*	9:00~9:35	Prof. Chen Si*
9:20~9:55	Prof. Wei Ruan*	9:35~10:10	Prof. Huaqing Huang*	9:35~10:10	Prof. Xiaoming Zhang*
9:55~10:30	Prof. Gil Young Cho*	10:10~10:30	Dr. Yinong Zhou#	10:10~10:30	Break (20 min)
10:30~10:50	Break (20 min)				Prof. Feng Liu
	Prof. Gil Young Cho		Prof. Wei Jiang	10:30~10:50	Dr. Xiaoyin Li#
10:50~11:25	Prof. Yan Zhang*	10:50~11:05 11:05~11:25	Prof. Feng Liu (BS) Dr. Gurjyot Sethi#	10:50~11:10	Dr. Young-Jae Choi#
				11:10~11:45	Prof. Raj Pala*
11:25~12:00	Dr. Jhinhwan Lee*	11:25~12:00	Prof. Minghu Pan*	11:45~12:00	**Closing**
12:00~14:00	Lunch				
	Prof. Miao Zhou		Prof. Huaqing Huang		
14:00~14:35	Prof. Zheng Liu*	14:00~14:35	Prof. Miao Zhou*		
14:35~15:10	Dr. Jae Whan Park*	14:35~15:10	Prof. Yunhao Lu*		
15:10~15:45	Prof. Wenyu He*	15:10~18:00	Discussion and Excursion (Bulguksa)		
15:45~18:00	Discussion and Excursion (Youngildae)				
18:00~20:00	Dinner				

*35 min talk (30 min talk, 5 min Q&A)
#20 min talk (17 min talk, 3 min Q&A)
Brainstorming Session (BS)

The schedule is provided in Korean Standard Time (KST).

2023 WQMPE Schedule

7/31 (Mon.)

Session 1 (Chair: Prof. Han Woong Yeom)

9:20~9:55 Prof. Wei Ruan (Fudan University)
Strong correlation effects in the triangular-lattice charge-density-wave material 1T-$TaSe_2$

9:55~10:30 Prof. Gil Young Cho (POSTECH)
Correlated States of Inverted David Starts in 1T-Transition Metal Dichalcogenides

Session 2 (Chair: Prof. Gil Young Cho)

10:50~11:25 Prof. Yan Zhang (Peking University) - Online -
Exotic correlated phenomena in transition-metal dichalcogenides

11:25~12:00 Dr. Jhinhwan Lee (IBS CALDES)
Spin-polarized STM Study of 1T-TaS_2 Domains and Domain Walls

Session 3 (Chair: Prof. Miao Zhou)

2:00~2:35 Prof. Zheng Liu (Tsinghua University)
Toward a better understanding on 1T-TaS2 - the first-principles perspective

2:35~3:10 Dr. Jae Whan Park (IBS CALDES)
Electronic properties of diverse domain wall configurations in 1T-TaS_2

3:10~3:45 Prof. Wen-Yu He (ShanghaiTech University) - Online -
Quantum Spin Liquid Physics in 1T-TaS_2/$TaSe_2$

8/1 (Tue.)

Session 1 (Chair: Prof. Zheng Liu)

9:00~9:35 Prof. Wei Jiang (Beijing Institute of Technology)
Enhancement of Intrinsic Spin Hall Effect in Chiral Topological Semimetals

9:35~10:10 Prof. Huaqing Huang (Peking University)
Nonlinear Hall Detection of the N´eel Vector for Two-Dimensional Antiferromagnetic Spintronics

10:10~10:30 Dr. Yinong Zhou (University of California, Irvine) - Online -
Higher-dimensional spin selectivity in chiral crystals

Session 2 (Chair: Prof. Wei Jiang)

10:50~11:05 Prof. Feng Liu (University of Utah)
What's more on yin-yang flat bands

11:05~11:25 Dr. Gurjyot Sethi **(University of Utah)** **- Online -**
p+ip Excitonic Insulator in Flattened Dirac Bands of a Superatomic Graphene

11:25~12:00 Prof. Minghu Pan (Shaanxi Normal University) **- Online -**
Observation of FClat Band in Mesoscale Ordered 2D Hydrogen-Bond Organic Framework

Session 3 (Chair: Prof. Huaqing Huang)

2:00~2:35 Prof. Miao Zhou (Beihang University)
Orbital physics for the design of low-dimensional quantum materials on substrate

2:35~3:10 Prof. Yunhao Lu (Zhejiang University)
Topological and Ferroelectric properties of 2D puckered elemental layer

8/2 (Wed.)

Session 1 (Chair: Dr. Jhinhwan Lee)

9:00~9:35 Prof. Chen Si (Beihang University) **- Online -**
Emergent quantum states in two-dimensional charge density wave materials

9:35~10:10 Prof. Xiaoming Zhang (Ocean University of China)
Topological Superconductivity of Line Defects in Transition Metal Dichalcogenides

Session 2 (Chair: Prof. Feng Liu)

10:30 ~10:50 Dr. Xiaoyin Lin (University of Utah) **- Online -**
Higher-order Topological Point State

10:50~11:10 Dr. Young-Jae Choi (IBS CALDES)
Divergence of the phonon Edelstein effect

11:10~11:45 Prof. Raj Ganesh S Pala (Indian Institute of Technology at Kanpur) **- Online -**
Non-Native Structures: What, Why & How…?

Zoom links

Day 1, July 31 (Monday)
Zoom Link:
https://us06web.zoom.us/j/86020876619?pwd=a3NJYmczSGk5WHZRN2d6ajJ0bFl3dz09
Meeting ID: 860 2087 6619
Password: 132568

Day 2, August 1 (Tuesday)
Zoom Link:
https://us06web.zoom.us/j/81146187756?pwd=NzhiM1FBc2trTG9mYjlXK0J6K3FkUT09
Meeting ID: 811 4618 7756
Password: 987793

Day 3, August 2 (Wednesday)
Zoom Link:
https://us06web.zoom.us/j/85779808466?pwd=VWJoV2dFdDRSWThjOUZ3SmFSUjlIdz09
Meeting ID: 857 7980 8466
Password: 191488

Talk No. 1

Strong correlation effects in the triangular-lattice charge-density-wave material 1T-$TaSe_2$

Wei Ruan
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Abstract

At low temperatures the transition metal dichalcogenides 1T-TaX_2 (X = S, Se) possess charge density wave states that are arranged in triangular superlattices. Although both experiment and theory have shown evidence for strong correlation effects in such systems, there are still debates, especially regarding the insulating nature of a monolayer of 1T-$TaSe_2$. In this talk I will discuss our studies on 1T-$TaSe_2$ as its thickness is varied from single-layer to bulk. First I will present evidence for Mott insulating state in single-layer 1T-$TaSe_2$ by investigation of its electronic structure and identification of its localized magnetic moments. With increasing number of layers we observe a Mott-to-metal transition at 7 layers, accompanied by the emergence of a metallic band crossing the Fermi level beyond 7 layers. This observation resolves the mystery of 1T-$TaSe_2$ bulk metallicity and provides unequivocal evidence that few-layer 1T-$TaSe_2$ and bulk 1T-$TaSe_2$ surface are Mott insulators. Such a localized spin system in a frustrated triangular lattice were predicted to host quantum spin liquids (QSLs) with gapless spinons. At last I will present evidence for QSL behavior in single-layer 1T-$TaSe_2$ through two observations: a long-wavelength super-modulation that is explained quantitatively by a QSL-based spinon Fermi surface instability, and two in-gap resonance peaks that are explained by spinon Kondo screening and emergent gauge fluctuations.

Talk No. 2

Correlated States of Inverted David Starts in 1T-Transition Metal Dichalcogenides

Gil Young Cho
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Abstract

1T-transition metal dichalcogenides (1T-TMD) have been an interesting platform for exploring the intertwinement of emerging strong correlation phenomena and charge-density waves. For example, 1T-TaS_2 and $TaSe_2$ have been proposed to realize spin liquids and thus bringing a lot of attention from experimental and theoretical communities. The standard charge-density wave structure at the low temperatures for 1T-TMDs is the David stars, which nicely explains spectral Mott gaps observed in scanning tunneling probes. In this work, we will consider an alternative structure model, known as the inverted David star structure, and theoretically explore its emerging physics. The structure, in contrast to the David stars, explicitly breaks the inversion symmetry and it leads to a flat band with significant Rashba spin-orbit couplings. This leads to several interesting consequences including large spin Hall effect with room-temperature functionality, emerging Chern insulators, incommensurate magnetic orders and also spin liquids, which can either break the rotational or time-reversal symmetries.

Talk No. 3

Exotic correlated phenomena in transition-metal dichalcogenides

Yan Zhang
International Centre for Quantum Materials, School of Physics, Peking University, Beijing 100871, China
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Abstract

Transition metal chalcogenides are a series of materials that exhibit rich electronic phases. In this talk, I would like to focus on the correlated phenomena in transition metal chalcogenides. We used angle-resolved photoemission spectroscopy (ARPES) to characterized the energy scales of interactions in 1T-TaS_2. We found that the competition between U and $t_\perp$ is responsible for the complex electronic properties in 1T-TaS_2. Moreover, by using in-situ alkali-metal deposition method, we studied the phase diagram of 1T-TaS_2. We found that the balance between U and $t_\perp$ is sensitive to the sample temperature and carrier doping, which results in a complex phase competition of 1T-TaS_2 in a small temperature and doping region.

Talk No. 4

Spin-polarized STM Study of 1T-TaS_2 Domains and Domain Walls

Jhinhwan Lee, Hae-Ryong Park, Jae-Whan Park, Kyung-Hwan Jin, and Han-Woong Yeom
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Abstract

Quantum spin systems like a spin chain and a spin liquid have attracted great interest for their rich physics and potential uses in quantum spintronics. The strongly correlated charge density wave (CDW) state in a layered material 1T-TaS_2 is a candidate for quantum spin liquid with frustrated spins in a two-dimensional (2D) triangular lattice. However, its magnetic properties have been elusive and controversial. Here, we directly detect the spatially and energetically resolved magnetic response of the spins in the CDW domains and domain walls using spin-polarized scanning tunneling spectroscopy (SP-STS) under varied external magnetic fields and a combined theoretical simulation of density functional theory (DFT) and Landau-Lifshitz-Gilbert (LLG) method. We discover frustrated and paramagnetic spin polarized states for CDW domains due to antiferromagnetically coupled spins in the bilayers with excess net spin moment, indicative of 2D spin frustration in the triangular CDW superlattice. On the other hand, the domain walls between CDW domains exhibit ferrimagnetic spin orderings made of trimer spin chains. Our findings may offer a novel insight into spin frustration in layer materials and an intriguing material platform for quantum spin devices with 2D frustrated spin systems and coexisting quantum spin chains.

Talk No. 5

Toward a better understanding on 1T-TaS2 - the first-principles perspective

Zheng Liu
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Abstract

I will review a wide range of first-principles calculation results on 1T-TaS2 and discuss how these results help understand novel properties of this material.

Talk No. 6

Electronic properties of diverse domain wall configurations in 1T-TaS_2

Jae Whan Park[1], Qirong Yao[1], Jinwon Lee[1,2], and Han Woong Yeom[1,2]
[1]*Center for Artificial Low Dimensional Electronic Systems, Institute for Basic Science (IBS), Pohang 37673, Korea*
[2]*Department of Physics, Pohang University of Science and Technology, Pohang 37673, Korea*
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Abstract

Two-dimensional (2D) van der Waals material, 1T-TaS_2, has garnered significant attention for its intriguing properties rooted in Mott physics. Within the Mott gap, the discommensurate domain walls exhibit 1D in-gap states, leading to the noteworthy phenomena, such as metal-insulator transitions [1], emerging superconductivity [2,3], and the formation of various metastable states for device functionality [4-6]. In this study, we employ a combination of scanning tunneling spectroscopy and density functional theory calculations to examine the atomic and electronic properties of different type of domain walls, including the most common straight domain wall, as well as, zigzag domain walls, kink states, and domain wall engineering induced by adsorbates. For the kink states within the domain wall, we observe the mobile kinks and antikinks trapped by pinning defects using scanning tunneling microscopy. Additionally, we explore the influence of interlayer coupling on 1D domain wall states by employing bilayer structure.

Reference

[1] Wilson, J. A., Di Salvo, F. J. & Mahajan, S. Charge density waves and superlattices in metallic layered transition-metal dichalcogenides. Adv. Phys. **24**, 117 (1975).
[2] Sipos, B. et al. From Mott state to superconductivity in 1T-TaS_2. Nat. Mater. **7**, 960 (2008).
[3] Ang, R. et al. Real-space coexistence of the melted Mott state and superconductivity in Fe-substituted 1T-TaS_2. Phys. Rev. Lett. **109**, 176403 (2012).
[4] Stojchevska, L. et al. Ultrafast switching to a stable hidden quantum state in an electronic crystal. Science **344**, 177 (2014).
[5] Yoshida, M., Suzuki, R., Zhang, Y., Nkano, M. & Iwasa, Y. Memristive phase switching in two-dimensional 1T-TaS_2 crystals. Sci. Adv. **1**, e1500606 (2015).
[6] Vaskivskyi, I. et al. Controlling the metal-to-insulator relaxation of the metastable hidden quantum state in 1T-TaS_2. Sci. Adv. **1**, e1500168 (2015).

Talk No. 7

Quantum Spin Liquid Physics in 1T-TaS_2/$TaSe_2$

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Abstract

Quantum spin liquid phase has been a long sought exotic state of matter since 1980s. Recently, it was predicted that in the transition metal dichalcogenides 1T-TaS_2 [1], the ground state of its Mott insulating phase is a U(1) quantum spin liquid with spinon Fermi surface [2]. In this talk, I will briefly review how the 1T-TaS_2 was proposed as a quantum spin liquid candidate in 2017, and further introduce the recent studies on the related material: monolayer 1T-$TaSe_2$ [3,4]. I will talk about the recent tunneling spectroscopy measurements on the Co atom embedded on the monolayer 1T-$TaSe_2$ [5] and present our explanation to the pair of band edge resonance peaks observed in the experiment [6]. I will show that the spinon Kondo resonance on the magnetic impurity combined with the gauge field fluctuations in the spin liquid can give rise to a pair of band edge resonance peaks observed in the experiment. In the rest of my talk, I will further introduce our latest study of the magnetic field effects on the electronic density of states of a quantum spin liquid. I will talk about the Landau quantization signature of the spinon Fermi surface [7] and the anomalous Zeeman response [8] in the U(1) gapless quantum spin liquid. The connection between our theoretical simulations and a recent scanning tunneling spectroscopy measurement [9] will be presented.

[1] K. T. Law and P. A. Lee, Proc. Natl. Acad. Sci. (USA) **114**, 6996 (2017).
[2] W.-Y. He, X. Y. Xu, G. Chen, K. T. Law, and P. A. Lee, Phys. Rev. Lett. **121**, 046401 (2018).
[3] Y. Chen et al., Nat. Phys. **16**, 218 (2020).
[4] W. Ruan et al., Nat. Phys. **17**, 1154 (2021).
[5] Y. Chen*, W.-Y. He*, W. Ruan* et al., Nat. Phys. **18**, 1335 (2022).
[6] W.-Y. He and P. A. Lee, Phys. Rev. B **105**, 195156 (2022).
[7] W.-Y. He and P. A. Lee, Phys. Rev. B **107**, 195155 (2023). Editor's suggestion.
[8] W.-Y. He and P. A. Lee, Phys. Rev. B **107**, 195156 (2023). Editor's suggestion.
[9] C. J. Butler, M. Yoshida, T. Hanaguri, and Y. Iwasa, Phys. Rev. B **107**, L161107 (2023).

Talk No. 8

Enhancement of Intrinsic Spin Hall Effect in Chiral Topological Semimetals

Wei Jiang
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Abstract

The spin Hall effect (SHE), which transduces charge current into spin current, is one of the essential cornerstones of spintronics. Here we propose a new intrinsic SHE (ISHE) enhancement mechanism in topological semimetals with high Chern numbers, and present a series of promising material candidates with large intrinsic spin Hall conductivities (ISHC) and spin Hall angles (SHA) for potential spintronic applications. By way of model Hamiltonian calculations and statistical analysis of 260 non-magnetic semimetals with chiral crystal structure, we unravel a positive correlation between the maximum Chern number and the ISHE, i.e., the ISHC and, under specific conditions, the SHA. Such positive correlations in topological gapless systems represent a novel mechanism to enhance ISHE, distinct from the conventional spin-orbit induced anticrossing mechanism in gapped systems. Additionally, our first-principles calculations of 38 chiral topological semimetals from space group 198, which can support zero-dimensional nodes with the highest Chern number (C = 4), reveal multiple realistic materials with large ISHC and even larger SHAs than Pt. Our discovery not only enriches the fundamental understanding of SHE but also provides an ideal material system conducive to efficient charge-to-spin conversion applications.

Talk No. 9

Nonlinear Hall Detection of the N´eel Vector for Two-Dimensional Antiferromagnetic Spintronics

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Abstract

The respective unique merit of antiferromagnets and two-dimensional (2D) materials in spintronic applications inspire us to exploit 2D antiferromagnetic spintronics. However, the detection of the N´eel vector in 2D antiferromagnets remains a great challenge because the measured signals usually decrease significantly in the 2D limit. Here we propose that the N´eel vector of 2D antiferromagnets can be efficiently detected by the intrinsic nonlinear Hall (INH) effect which exhibits unexpected significant signals. As a specific example, we show that the INH conductivity of the monolayer manganese chalcogenides MnX (X=S, Se, Te) can reach the order of nm·mA/V2, which is orders of magnitude larger than experimental values of paradigmatic antiferromagnetic spintronic materials. The INH effect can be accurately controlled by shifting the chemical potential around the band edge, which is experimentally feasible via electric gating or charge doping. Moreover, we explicitly demonstrate its 2π-periodic dependence on the N´eel vector orientation based on an effective k.p model. Our findings enable flexible design schemes and promising material platforms for spintronic memory device applications based on 2D antiferromagnets.

Talk No. 10

Higher-dimensional spin selectivity in chiral crystals

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Abstract

This study aims to investigate the interplay between chiral-induced spin-orbit coupling along the screw axis and antisymmetric spin-orbit coupling (ASOC) in the normal plane within a chiral crystal, using both general model analysis and first-principles simulations of InSeI, a chiral van der Waals crystal. While chiral molecules of light atoms typically exhibit spin selectivity only along the screw axis, chiral crystals with heavier atoms can have strong ASOC effects that influence spin-momentum locking in all directions. The resulting phase diagram of spin texture shows the potential for controlling phase transition and flipping spin by reducing symmetry through surface cleavage, thickness reduction or strain. We also experimentally synthesized high-quality InSeI crystals of the thermodynamically stable achiral analogue which showed exposed (110) facets corresponding to single-handed helices to demonstrate the potential of material realization for higher-dimensional spin selectivity in the development of spintronic devices.

Talk No. 11 (Brainstorming Session)

What's more on yin-yang flat bands

Feng Liu
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Abstract

I will review on yin-yang flat band systems and related interesting physical properties and applications.

Talk No. 12

$p + ip$ Excitonic Insulator in Flattened Dirac Bands of a Superatomic Graphene

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Abstract

In this work, we study the interplay of topological and excitonic effects in flattened Dirac bands of opposite chirality. Using exact diagonalization of many-excitonic Hubbard Hamiltonians for tight binding model based on a superatomic graphene lattice, we illustrate that bands of opposite chirality are conducive to forming a $p + ip$ excitonic condensate under short-range interactions due to inherent topology of excitons formed between such bands. We calculate many-excitonic formation energies and analyze the many-body ground-state wavefunction to show off-diagonal long-range order of excitons and non-trivial phase of excitonic order parameter. Our work provides interesting avenues to study topological excitonic effects in semiconductors/semi-metals leading to the realization of exotic $p + ip$ excitonic condensate.

G.S, and F.L. acknowledge financial support from US Department of Energy-Basic Energy Sciences (Grant No. DE-FG02- 04ER46148)

Talk No. 13

Observation of Flat Band in Mesoscale Ordered 2D Hydrogen-Bond Organic Framework

Minghu Pan[1] and Feng Liu[2]
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Abstract

Flat bands (FBs), presenting a strongly interacting quantum system, have drawn increasing interest recently. However, experimental synthesis of monolayer FB materials has been challenging and have remained elusive, where the FB arises from destructive quantum interference as predicted in 2D lattice models. Here, we report the growth of a self-assembled monolayer of 2D hydrogen-bond (H-bond) organic frameworks (HOFs) of 1,3,5-tris(4-hydroxyphenyl) benzene (THPB) on Au(111) substrate and the observation of FB. High-resolution scanning tunneling microscopy and spectroscopy shows mesoscale, highly ordered, and uniform THPB HOF domains, while angle-resolved photoemission spectroscopy highlights a FB over the whole Brillouin zone. Density functional-theory calculations reveal that the observed topological FB arises from a hidden electronic breathing-Kagome lattice without atomically breathing bonds. Our findings demonstrate that self-assembly of HOFs provides a viable approach for synthesis of 2D organic topological materials, paving the way to explore many-body quantum states of topological FBs.

Reference：

Minghu Pan *et al.,* Growth of Mesoscale Ordered Two-Dimensional Hydrogen-Bond Organic Framework with the Observation of Flat Band, *Phys. Rev. Lett.* **130**, 036203(2023) (Editors' Suggestion)

Talk No. 14

Orbital physics for the design of low-dimensional quantum materials on substrate

Miao Zhou
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Abstract

Recent progress of orbital physics, utilizing the orbital degree of freedom in addition to the charge and spin of electrons, opens up new opportunities to realize richer extraordinary properties. In this presentation, we will present our recent progress on the theoretical design and understanding of low-dimensional topological quantum materials based on lattice structure and orbital composition. In particular, by tight-binding modeling with first-principles calculations, we demonstrate the electronic structures and topological properties of 1D atomic nanolines and 2D triangular lattices with multi-orbitals. The topological phase diagrams are mapped out, and possible topological phase transitions initiated by substrate are predicted. Real material systems are proposed, which fully capture the salient features of tight-binding parameter space, and can be experimentally prepared and characterized by MBE, STM/STS and ARPES.

Talk No. 15

Topological and Ferroelectric properties of 2D puckered elemental layer

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Abstract

Emergent Dirac fermion states underlie many intriguing properties of graphene, and the search for them constitutes one strong motivation to explore two-dimensional (2D) allotropes of other elements. Phosphorene, the ultrathin layers of black phosphorous, has been a subject of intense investigations recently, and it was found that other group-Va elements could also form 2D layers with similar puckered lattice structure. Here, by a close examination of their electronic band structure evolution, we discover two types of Dirac fermion states emerging in the low-energy spectrum. One pair of (type-I) Dirac points is sitting on high-symmetry lines, while two pairs of (type-II) Dirac points are located at generic k-points, with different anisotropic dispersions determined by the reduced symmetries at their locations. Such fully-unpinned (type-II) 2D Dirac points are discovered for the first time. In addition, combining first-principles calculations and scanning tunneling microscopy/spectroscopy (STM/STS) experimental studies, we report nontrivial 2D TI phases in 2-monolayer (2-ML) and 4-ML Bi(110) films with large and tunable bandgaps determined by atomic buckling of Bi(110) films.

On the other hand, we reveal spontaneous electric polarization and ferroelectricity in two-dimensional elemental Group-V (As, Sb, and Bi) monolayer with the puckered lattice structure similar to phosphorene. These are the first example of elemental ferroelectric materials. The polarization is due to the spontaneous lattice distortion with atomic layer buckling and has quite sizable values, comparable or even larger than that recently found in 2D monolayer compound SnTe. Interestingly, for Bi monolayer, apart from the ferroelectric phase, we find that it can also host an antiferroelectric phase. The Curie temperatures of these elemental materials can be higher than room temperature, making them promising for realizing ultrathin ferroelectric devices of broad interest. A general model is constructed to understand and search for 2D ferroelectric and antiferroelectric materials in future studies.

Acknowledgments

YHLU thank Prof. Shengyuan Yang, Prof.Shengbai Zhang, Prof.Yuanping Feng for valuable discussion.

Talk No. 16

Emergent quantum states in two-dimensional charge density wave materials

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Abstract

Charge Density Waves (CDWs) are a many-body quantum state characterized by periodic modulations of conduction electron densities and the associated lattice distortions. As we venture into the realm of two-dimensional (2D) materials, the intrigue surrounding CDWs has been reignited. Preliminary investigations illuminate that under the constraints of 2D, CDWs display behaviors that diverge markedly from their 3D counterparts, and manifest in tandem with novel quantum states such as superconductivity, ferromagnetism, and Mott insulators. Deciphering the implications of reduced dimensionality on CDWs, alongside unveiling the curious quantum states that appear in conjunction with 2D CDWs, stand as focal points in contemporary research. This report will show our latest progress in exploring the landscape of 2D CDW systems. First, we discover that 1T-$HfTe_2$, which lacks CDWs in its bulk form, unexpectedly exhibits a stable 2 × 2 CDW order in the monolayer format, which can be linked to the enhanced electron–phonon coupling (EPC) in the monolayer. Impressively, Ising superconductivity with a significantly enhanced in-plane critical field can arise once the CDW is suppressed by electron doping[1]. Secondly, topological materials possessing CDW states are still uncommon, particularly in the 2D limit. We have found that a single layer of 1T-$NbTe_2$ can support a QSH or QAH phase with a coexisting CDW[2]. Lastly, we will demonstrate that the stacking order can profoundly influence the quantum phase transitions of layered 1T-$TaSe_2$ with a remarkable 2D CDW order. By manipulating the vertical stacking order of CDWs, bulk 1T-$TaSe_2$ can host a variety of electronic phases, including quasi-1D and 3D metals, and band insulators[3].

References:
[1] Nano Res. 2023, https://doi.org/10.1007/s12274-023-5780-1.
[2] Adv. Funct. Mater. 2022, 32, 2111675
[3] Adv. Funct. Mater. 2023, 33, 2214583

Talk No. 17

Topological Superconductivity of Line Defects in Transition Metal Dichalcogenides

Xiaoming Zhang
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Abstract

Convincible signatures of Majorana zero modes (MZMs) are one necessary requirement for achieving fault-tolerant quantum computations based on topological superconductivity (TSC). In addition to improving fabrication techniques, exploring stoichiometric TSC platform is another route to suppress the influences of trivial in-gap modes on the signatures of MZMs. Stoichiometric transition metal dichalcogenide (TMD) with topological surface states (TSSs) is promising but the field range of inducing magnetic vortices to harbor MZMs is limited by the small perpendicular upper critical field. Here, we propose the line defects of chalcogen vacancies (CVs) embedded in TMDs are the stoichiometric TSC candidates to realizing stable MZMs without needing the TSSs under wide range of in-plane magnetic field. Detailed analysis and calculations on the 1H-MoX2, 1H-WX2, and 1T-PtX2 (X=S, Se or Te) monolayer with CVs line defects indicate the antisymmetric spin-orbit coupling effect, known as the origin of odd-parity pairing, is ensured by non-centrosymmetric point group symmetry. TSC phase diagrams are constructed to facilitate experimental detection of convincible signatures for the MZMs located at both ends of line defect. Our findings enrich the stoichiometric TSC candidates and will promote devices fabrication to manipulating and storing quantum information based on the device-friendly TMDs.

Talk No. 18

Higher-order Topological Point State

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Abstract

Higher-order topological insulators (HOTIs) have attracted increasing interest recently as a unique class of topological quantum materials. One distinct property of HOTIs is the crystalline symmetry-imposed topological state at the lower-dimensional outer boundary, such as the zero-dimensional (0D) corner state of a 2D HOTI, which has been exclusively used as a universal signature to identify the higher-order topology but yet with uncertainty. Strikingly, we discover the existence of inner topological point states (TPS) in a 2D HOTI, as the embedded "end" states of 1D first-order TI, as exemplified by those located at the vacancies in a Kekulé lattice. Most significantly, we demonstrate that such inner TPS can be unambiguously distinguished from the trivial point-defect states, by their unique topology-endowed inter-TPS interaction and correlated magnetic response through spectroscopy measurements, overcoming an outstanding experimental challenge. Furthermore, based on first-principles calculations, we propose γ-graphyne as a promising material to experimentally observe the higher-order TPS. Our findings not only shed new light on our fundamental understanding of HOTIs, but also open an avenue to experimentally distinguishing and tuning TPS in the interior of a 2D sample for potential applications.

Talk No. 19

Divergence of the phonon Edelstein effect

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Abstract

The phonon heat current naturally generates phonon angular momentum (PAM), namely the phonon Edelstein effect. This effect is analogous to the spin Rashba-Edelstein effect and yet displays unique phenomena owing to the bosonic nature of phonons. Specifically, phonons exhibit a large deviation in their lifetimes in terms of eigenfrequency and temperature. In this study, we calculated the phonon Edelstein effect in wurtzite ferroelectrics (AlN and GaN) and graphene-like boron nitride (g-BN) using precise calculations of mode-specific phonon lifetimes. We identified intriguing critical behaviors in which the phonon Edelstein effect diverges under certain temperature and strain conditions. Chiral phonons with large coherence time result in asymmetric accumulation of phonon angular momentum. The keys to understanding these divergent phenomena lie in the phonon dispersion and their anharmonicity.

Keywords: chiral phonon, phonon angular momentum, thermal transport, anharmonicity

Talk No. 20

Non-Native Structures: What, Why & How…?

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Abstract

We demonstrate a material design principle via "non-native structures"[1,2,3] for cathodes in lithium-ion batteries,[4] type-2 heterostructures in photoelectrochemistry[5,6] and electrocatalysis.[7,8] "Non-native" structures differ from the "native" structure of bulk crystals in terms of discrete translational symmetry and they typically have higher energy and free volume. [1,2,3] Hence, they are expected to generate higher discharge potential and better lithium mobility as a cathode as demonstrated via Ramsdellite MnO_2 (r/NN1-MnO_2) thermally phase transformed to Pyrolusite MnO_2 (β/N-MnO_2).[4] Such intimately interfaced (r/NN1-MnO_2)/(β/N-MnO_2) intergrowth structures show higher voltages, a wider voltage plateau, longer cycle life and faster kinetics. We elucidate the underlying molecular mechanisms via experiments and density functional theory simulations (DFTS).[4] Type-2 heterostructure comprised of Native/Non-Native structures play a critical role in the electron-hole separation in photoelectrochemistry and calibrate them via the following criteria: band edges, valence and conduction band alignment, lattice strain and coherency in interfaces.[5,6] We also demonstrate the utility of non-native structures to scale up the "volcano" activity relationships relevant to oxygen and hydrogen evolution electrocatalysis.[7,8] Finally, we present some of the heuristics garnered from fundamental studies on the self-assembly of non-native structure and heterostructures.[9, 10] An important insight in the evolving understanding of the crystal growth of non-native structures points to the fact that there is size-*reduction* during the early stages of *growth*![10]

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