The 21st Taiwan-Japan-Korea Symposium on Strongly Correlated Electron Systems

National Synchrotron Radiation Research Center, Hsinchu Taiwan
April 6-7, 2023

Organizers
National Synchrotron Radiation Research Center, Taiwan
National Tsing Hua University, Taiwan

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National Science and Technology Council, Taiwan
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NSTC 國家科學及技術委員會
National Science and Technology Council

NSRRC 國家同步輻射研究中心
National Synchrotron Radiation Research Center

國立清華大學
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Overview

The National Synchrotron Research Center in Taiwan hosts the twenty-first Taiwan-Japan-Korea Symposium on Strongly Correlated Electron Systems (TJK21) on April 6th and 7th, 2023. The symposia series began as a workshop in October 2000, with a focus on the latest research developments in strongly correlated materials in Japan and Korea. In 2005, Taiwan organized the sixth meeting, and the symposium evolved into a rotating event that cycles through the country names of Japan, Korea, and Taiwan each year, making it an annual tradition. Unfortunately, due to the COVID-19 pandemic, the symposium was temporarily suspended for two years. However, it remains an important event that promotes communication and collaboration among Asian countries in the field of strongly correlated materials.

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THE 21st TAIWAN-JAPAN-KOREA SYMPOSIUM ON STRONGLY CORRELATED ELECTRON SYSTEMS (TJK21)

6 April, 2023 (Thursday)

Session I

08:20		Registration
08:45		Opening Remarks
		Session Chair: Di-Jing Huang
09:00	Keynote Speech	**ARPES to RIXS Studies of High-Temperature Superconductors** *Atsushi Fujimori, University of Tokyo, Japan*
09:40	A1	**Anomalous ordered magnetic moments in Co^{2+} and V^{3+} magnetic systems** *Jae-hoon Park, POSTECH, Korea*
10:10	A2	**Quantum fluctuations of charge order induce phonon softening in $La_{2-x}Sr_xCuO_4$** *Hsiao-Yu Huang, NSRRC, Taiwan*
10:25		Coffee break

Session II

		Session Chair: Ying-Hao Chu
10:40	A3	**Antiferromagnetic domain imaging via linear magnetoelectric effect** *Tsuyoshi Kimura, University of Tokyo, Japan*
11:10	A4	**Strongly correlative ionic transport triggered by oxygen-vacancy ordering transition in a doped multiferroic** *Chan-Ho Yang, KAIST, Korea*
11:40	A5	**Twisted complex oxide lateral homostructures** *Jan-Chi Yang, National Cheng Kung Univ., Taiwan*
12:10		Flash poster session *Session Chair: Cheng-Maw Cheng*
		Group Photo/Lunch/ Poster session (start at 13:10)

6 April, 2023 (Thursday)

Session III

		Session Chair: Way-Faung Pong
14:20	B1	**Quantum anomalous Hall effect in 2D magnetic materials** *Jaejun Yu, Seoul National University, Korea*
14:50	B2	**Enhancement of electronic nematic susceptibility near the first superconducting dome in the kagome superconductor $Cs(V_{1-x}Ti_x)_3Sb_5$** *Kee Hoon Kim, Seoul National University, Korea*
15:20	B3	**Quantum critical 2D Bose gas formation in the honeycomb antiferromagnet $YbCl_3$** *Yosuke Matsumoto, Max Planck Institut, Germany*
15:50	B4	**Observation of the charge density wave gap in CuTe with ARPES** *Ping-Hui Lin, NSRRC, Taiwan*
16:05		**Coffee break**
		Session Chair: Chao-Hung Du
16:20	B5	**Metal-insulator transition and negative magnetoresistance in $Ba_{3-x}Eu_xNb_5O_{15}$** *Takuro Katsufuji, Waseda University, Japan*
16:50	B6	**Superconductivity in Ternary Telluride Sc_6MTe_2 with 3*d*, 4*d*, and 5*d* Transition Metals** *Yoshihiko Okamoto, University of Tokyo, Japan*
17:20	B7	**The Dynamical Charge Response of Plasmons to the Charge-Density-Wave Order in CuTe** *Ming-Wen Chu, National Taiwan University, Taiwan*
17:50	B8	**Dirac nodal line in hourglass semimetal Nb_3SiTe** *Ro-Ya Liu, NSRRC, Taiwan*
18:20		Departure for banquet

7 April, 2023 (Friday)

Session IV

		Session Chair: Atsushi Fujimori
08:30	C1	**Ab initio studies of cuprate superconductors and analyses on the electron fractionalization** *Masatoshi Imada, Waseda Univ./Toyota Phys. Chem. Res. Inst. /Sophia Univ., Japan*
09:00	C2	**New twists in strongly correlated electronic systems: from Kondo screening to unconventional superconductivity** *Chung-Yu Mou, National Tsing Hua University, Taiwan*
09:30	C3	**Revealing the mystery of strange metal states in correlated electron systems** *Chung-Hou Chung, National Yang Ming Chiao Tung University, Taiwan*
10:00	C4	**Unconventional exciton evolution from the pseudogap to superconducting phases in cuprates** *Amol Singh, NSRRC, Taiwan*
10:15		Coffee break

Session V

		Session Chair: Jaejun Yu
10:30	C5	**My story of van der Waals magnets and Prof. Shin** *Je-Geun Park, Seoul National University, Korea*
11:00	C6	**Atomically Resolved Electronic Structure of Copper-Oxide Chains and Planes on Incommensurate Charge Order in $YBa_2Cu_3O_{6+x}$** *Ya-Ping Chiu National Taiwan Univ., Taiwan*
11:30	C7	**First-principles studies of delicate octahedra tilting in cuprates** *Chi-Cheng Lee, Tamkang Univ., Taiwan*
12:00	C8	**Solving high-temperature superconductivity with quantum computers** *Kwon Park, KIAS, Korea*
12:30		Closing Remarks *Session Chair: Di-Jing Huang*
12:50		Lunch & Academic Visit for future cooperation

Poster List

Poster number	Presenter	Affiliation	Poster title
P1	Takayuki Nagai	Univ. of Tokyo	Chemical aspect of ferroaxial order: NASICON systems as a case study
P2	Shigetada Yamagishi	Univ. of Tokyo	Database Screening for Ferroaxial Materials and Experimental Verification
P3	Toshiya Ikenobe	Univ. of Tokyo	Possible surface superconductivity in the nodal-line semimetal NaAlSi
P4	Toshihiko Muroi	Univ. of Tokyo	Magnetic field effects on the quadrupole order of the spin–orbit-coupled insulator Ba_2MgReO_6
P5	Takehito Suzuki	Toho Univ.	Chemical doping effect in a triply degenerate point candidate $PtBi_2$
P6	Haruki Takei	Waseda Univ.	Magnetotransport properties of $Ba_{3-x}R_xTa_5O_{15}$ (R=rare earth)
P7	JaeHwan Shim	Seoul National Univ.	Efficient discovery of multiple minimum action pathways using Gaussian process
P8	Il Young Lee	Seoul National Univ.	First-principles study of morphotropic phases in Zr-doped hafnium oxide thin film on TiN substrate
P9	Giung Park	Seoul National Univ.	Universal methodology for twisted van der Waals homostructures
P10	Yi-Cheng Chen	National Tsing Hua Univ.	Quasi-2D Bismuth Oxy-Selenide: An Emerging Material in Advanced Electronic Devices
P11	Yong-Jyun Wang	National Tsing Hua Univ.	Non-volatile Modulation on the Electronic Potential of the 2D Bi_2O_2Se Layer via Ferroelectric Polarization
P12	Hao-Bang Lu	National Yang Ming Chiao Tung Univ.	Exploring the Electrical Properties of Epitaxial Bi_2O_2Se on Silicon Fabricated by a Simple Wet Method
P13	E-Han Li	National Tsing Hua Univ.	Synthesis of magnetic nanoparticles via Mica Interlayer Intercalation

P14	Chuan Chuang	National Tsing Hua Univ.	Fabrication of the Bi_2O_2S Epitaxy Thin Films and the Novel Optical Properties
P15	Wei-En Ke	National Yang Ming Chiao Tung Univ.	Perpendicular magnetic anisotropy in high entropy $(Fe, Co, Ni, Cr, Mn)_3O_4$ oxide driven by single-element orbital anisotropy
P16	Yu-Cheng Cheng	National Yang Ming Chiao Tung Univ.	Creation of Novel Composite Materials: Magnetic and Conductive Muscovite
P17	Jen-Hua Chang	National Tsing Hua Univ.	A new form of thermochromism materials: VO_2 Intercalated Muscovite
P18	Shu-Hua Kuo	National Tsing Hua Univ.	Fabrication of superconductive muscovite via MgB_2 intercalation
P19	Bo-Sheng Chen	National Tsing Hua Univ.	Novel 2D Layered Composite Materials: Modification of Muscovite by Intercalation
P20	Hung-Chi Lai	National Yang Ming Chiao Tung Univ.	Epitaxial High Entropy Oxide Films with High Dielectric Tunability and Superior Thermal Stability
P21	Pin-Ying Chen	National Tsing Hua Univ.	The $Pb(Zr_{0.52}Ti_{0.48})O_3$ Thin Film on Muscovite for the Application of Flexible Electronics
P22	Yu-Hao Tu	National Tsing Hua Univ.	MICAtronics - Muscovite van der Waals Epitaxy
P23	Jia-Wei Chen	National Yang Ming Chiao Tung Univ.	The role of lattisce in the transport and magnetic properties of high entropy alloy films
P24	Jia-Syuan Su	National Yang Ming Chiao Tung Univ.	Momentum-resolved RIXS studies on high-temperature superconductor Bi2212
P25	Chun-I Wu	National Tsing Hua Univ.	RIXS studies on the kagome metal YMn_6Sn_6
P26	Jun Okamoto	NSRRC	Novel X-ray circular dichroism in a collinear antiferromagnet on a chiral lattice
P27	Yao-Wen Chang	National Cheng Kung Univ.	

P28	Sheng-Zhu Ho	National Cheng Kung Univ.	
P29	Rong-Zhu Lin	National Cheng Kung Univ.	
P30	Yun-Chung Chen	National Taiwan Univ.	Chern dartboard insulator: sub-Brillouin zone topology and skyrmion multipoles
P31	Chun-Liang Lin	National Yang Ming Chiao Tung Univ.	Temperature-Dependent Electronic Structures of TMD Weyl Semimetals
P32	Naoya Kawakami	National Yang Ming Chiao Tung Univ.	Unique dewetting growth of Si layers on Ag (111)
P33	Wan-Hsin Chen	National Yang Ming Chiao Tung Univ.	Investigation of the Superconductivity in Buckled Plumbene-Au Kagome Superstructure
P34	Jyun-Yu Wu	National Yang Ming Chiao Tung Univ.	Tomography Scan of Charge Density Wave in $NbSe_2$
P35	Wei-Xuan Lin	Tamkang Univ.	Origin of the ferromagnetic transition in $Co_{1.55}ZrSn$ Heusler alloy Weyl semi-metal
P36	Chin-Wei Li	Tamkang Univ.	
P37	Sambhu Charan Das	Tamkang Univ.	
P38	Chun-Hao Lai	Tamkang Univ.	Neutron Powder Diffraction Study of the Helimagnet $YBaCuFeO_5$ with B-site Disorder
P39	Yu-Hui Liang	Tamkang Univ.	Study of the Phase Transition in the Intermetallic Compound Ir_2In_8Se Using X-ray Scattering
P40	Surajit Ghosh	Tamkang Univ.	Structural Instability and Charge Transfer mediated Transition in $Pr_3Co_4Sn_{13}$: A Synchrotron Radiation Spectroscopy Based Study

Keynote Speech

ARPES TO RIXS STUDIES OF HIGH-TEMPERATURE SUPERCONDUCTORS

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In this talk, we start from early x-ray absorption (XAS) and resonant photoemission (RPES) studies on transition-metal compounds with Prof. Shik Shin [1] at SOR-RING, the first storage ring dedicated to spectroscopy. A brief overview is given how soft x-ray spectroscopies, namely, RPES, XAS, and ARPES, not only synchrotron-radiation-based but also laser-based, have contributed to our understanding of transition-metal compounds, particularly, the cuprate high-temperature superconductors including theoretical modeling [2]. Then we focus on the resonant inelastic x-ray scattering (RIXS) technique [3] and its successful applications to cuprates at TPS 41A of NSRRC: electron fractionalization in the pseudogap phase [4], static and fluctuating charge-density wave near QCP [5], and acoustic plasmon excitation [6].

We thank fruitful collaboration with A. Singh, H. Y. Huang, J. Okamoto, M. Imada, T. Watanabe, S. Komiya, T. K. Lee, C. Y. Mou, A. Chainani, K. Sheshadri, D. Malterre, and C. T. Chen.

[1] S. Shin *et al.*, Phys. Rev. B **41**, 4993 (1990).
[2] K. Sheshadri *et al.*, Phys. Rev. B **107**, 085125 (2023).
[3] For an early review, see A. Kotani and S. Shin, Rev. Mod. Phys. **73**, 203 (2001).
[4] A. Singh *et al.*, Nat. Commun. **13**, 7906 (2022).
[5] H. Y. Huang *et al.*, Phys. Rev. X **11**, 041038 (2021).
[6] A. Singh *et al.*, Phys. Rev. B **105**, 235105 (2022).

A1

Anomalous ordered magnetic moments in Co^{2+} and V^{3+} magnetic systems

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In the 3d transition metal compound magnetic insulator, the ordered moment is, in general, mainly determined by the ground state spin quantum value S, i.e. $\mu \approx 2S\mu_B$ since the orbital moment is mostly quenched. On the other hand, the triplet t_{2g} orbital can be regarded as an effective orbital angular moment $L_{eff} = 1$ state, and thus a considerable orbital moment ΔL can survive and contribute to the ordered moment in the system with a partially filled t_{2g} orbital configuration due to the spin-orbit coupling, virtually following the Hund rule, i.e. $\mu \approx (2S \mp \Delta L)\mu_B$. This phenomenological simple concept has commonly been applied to understand the magnetic ordered moment and indeed reasonably well explains the order moments of most 3d transition metal magnetic insulators. We explicitly examine this simple concept using the cluster model calculations including the configuration interactions, atomic full multiplets, crystal fields, and spin-orbit coupling. We found that the simple concept can be invalid in some systems especially with either Co^{2+} ($3d^7$; t_{2g}^2 + a half full) or V^{3+} (3d2; t_{2g}^2) magnetic ions. In this talk, I will discuss the model calculation results inconsistent with the simple concept together with real examples such as Ba_3CoSbO_9 (Co^{2+}) and VI_3 (V^{3+}).

A2

Quantum Fluctuations of Charge Order Induce Phonon Softening in $La_{2-x}Sr_xCuO_4$

Hsiao-Yu Huang[1], Amol Singh[1], Chung-Yu Mou[2], Steve Johnston[3], Alexander F. Kemper[4], Jeroen van den Brink[5], Peng-Jen Chen[6,7], Ting-Kuo Lee[8,9], Jun Okamoto[1], Yen-Yi Chu[1], Jung-Han Li[10], Seiki Komiya[11], Alexander Komarek[12], Atsushi Fujimori[1,10,13], Chien-Te Chen[1], Di-Jing Huang[1,10]

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Quantum phase transitions play a crucial role in shaping the phase diagram of high-temperature cuprate superconductors, which possess intertwined orders that interact strongly with superconductivity. Among these orders, charge-density waves (CDWs) have recently attracted renewed interest. However, evidence for the quantum critical point associated with the charge order in the superconducting phase remains elusive. In this study, we investigate short-range charge orders and the spectral signature of quantum fluctuations in $La_{2-x}Sr_xCuO_4$ (LSCO) near optimal doping using high-resolution resonant inelastic x-ray scattering. Through a diagrammatic framework, we find that charge correlations significantly soften several branches of phonons. We demonstrate clear quantum critical scalings of charge fluctuations in the temperature domain, consistent with the speculation of a quantum critical point. Our results provide evidence for the role of charge order in the LSCO compound and elucidate quantum critical scaling and discommensurations associated with charge order.

[1] H. Y. Huang *et al*., Phys. Rev. X **11**, 041038 (2021)

A3

Antiferromagnetic domain imaging via linear magnetoelectric effect

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The Faraday effect and the magneto-optical Kerr effect observed in ferromagnetic materials breaking time-reversal symmetry are representative nonreciprocal optical effects, that is, optical responses which are different for counter-propagating light beams. In addition to such conventional effects, unconventional nonreciprocal optical effects occur in materials with broken not only time-reversal symmetry but also space-inversion symmetry, which are ascribed to a linear magnetoelectric (ME) coupling. In this presentation, we focus on four types of unconventional nonreciprocal effects: directional dichroism, electric-field-induced Faraday effect (*E*-induced Faraday), electric-field-induced magnetic circular dichroism (*E*-induced MCD), and nonreciprocal rotation of reflected light (NRR). One of the fundamental features of these effects is that they can be used to distinguish domain states even in fully compensated antiferromagnetic materials. We investigated the abovementioned unconventional nonreciprocal optical effects in several ME antiferromagnets including Cr_2O_3 [1] and Bi_2CuO_4 [2]. By microscope observations of these effects, we succeeded in visualizing antiferromagnetic domains in these antiferromagnets.

[1] T. Hayashida *et al.*, Phys. Rev. Research **4**, 043063 (2022).
[2] K. Kimura *et al.*, Nat. Commun. **13**, 697 (2022).

A4

Strongly correlative ionic transport triggered by oxygen-vacancy ordering transition in a doped multiferroic

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Long-range correlated fluctuations in order parameters occur at phase transition points, revealing emergent functionalities such as the morphotropic-phase-boundary driven high-k dielectrics, large piezoelectricity, and quantum paraelectricity. Likewise, the correlation length of thermal and quantum fluctuations of atomic positions can be large at the critical point, leading to rapid and coherent ionic conduction. However, the lack of a lattice system that exhibits competing defect orderings has hindered the study of the feasibility of this general thermodynamic wisdom. Here, we demonstrate a route toward coherent thermionic conduction in solids, by exploiting the lowered activation energy associated with oxygen transport in Ca-substituted bismuth ferrite ($Bi_{1-x}Ca_xFeO_{3-\delta}$) thin films. Our demonstration relies on the finding that a compositional phase boundary between two isostructural phases with oxygen vacancy channel orderings competitively along the <100> or <110> crystal axes emerges at a chemical doping ratio (x_{Ca} ~ 0.45). Regardless of the atomic-scale irregularity in defect distribution at the compositional boundary, the activation energy is largely suppressed to 0.43 eV, compared with the ~0.9 eV measured in otherwise rigid phases. From first-principle calculations, we clarify that the effective short-range attraction between two positively charged oxygen vacancies sharing lattice deformation is the driving force of the long-range order and collective diffusion in the system. The collective phase evolution is necessary to understand the suppression of ionic activation energy. Our findings open a new avenue into strongly correlative ionics.

A5

Twisted complex oxide lateral homostructures

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Epitaxial growth, thin film deposition by which the crystalline layers with well-defined orientations grown atop single crystal substrates, is indispensable in condensed matter science and semiconductor industry, given that it delivers high quality films comparable to single crystals. Over the past decades, epitaxial growth has enabled efficient interface and strain engineering of functional materials, which has played a key role in renovating modern science and a wide spectrum of technically important applications. In terms of epitaxial growth, the selection of single crystal substrates determines the foundation template for the deposited materials. Namely, the lattice constrains and crystalline orientations of deposited materials are subject to selected template beneath, thus the allowed epitaxial degrees of freedom is determined once a specific substrate is chosen.

In this talk, using multiferroic $BiFeO_3$ as a model system, we propose an efficient approach to fabricate twisted lateral homostructures with various conjunction tunabilities, including crystalline orientation, epitaxial constrain and phase stability. With a patterned prototype device, we will further demonstrate that the proposed approach is not only compatible with conventional lithography and etching processes, but also generic for fabricating various twisted complex materials. Additionally, we show that the lateral homostructures can also be assembled by combining structurally-different polymorphs, forming interfaces with unconventional physical properties. Our results evidence the excellent controllability and unbounded conjunction tunability of the lateral homostructures using the proposed method, allowing epitaxial films to be assembled at particular position in the plane, as if they were artificially “weaved”. Such an approach not only provides a new way to design twisted lateral homostructures, but also depicts an different scene of epitaxial growth.

B1

Quantum anomalous Hall effect in 2D magnetic materials

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Recently, two-dimensional (2D) magnetic materials composed of transition metal (TM) atoms have garnered significant attention due to their intriguing physical properties. While some transition metal chalcogenides and halides exhibit exciting features in their electronic band structure, resulting in novel magnetic interactions and topological characteristics, there is still a lack of systematic understanding of the electronic configurations of 3*d* TM atoms and their correlation with the magnetic ordering in 2D compounds. In contrast to transition metal oxides, the strong hybridization between metal and ligands can lead to unexpected behavior in the spin state of the transition metal atoms. In this study, we utilize first-principles electronic structure calculations to demonstrate a systematic correlation between the 3*d* TM *d* configuration and the effective magnetic exchange interactions, proposing a common effective magnetic exchange mechanism in 2D magnetic materials. In addition to the intriguing magnetism, we observe Chern insulating phases emerging from 2D magnetic materials. For instance, we find the quantum Hall effect under charge doping in a single layer of layered chalcogenide $CrSiTe_3$, a transition metal trichalcogenides (TMTC) material. Due to the strong hybridization with Te *p* orbitals, the spin-orbit coupling effect opens a finite band gap. This results in a nontrivial topology of the Cr e_g conduction band manifold with higher Chern numbers. Our calculations demonstrate that quantum anomalous Hall effects can be achieved by adding one electron in a formula unit cell of $Cr_2Si_2Te_6$. An external magnetic field can regulate the doping-induced anomalous Hall conductivity by tuning the spin-orbit coupling in a spin-orientation-dependent manner. Hence, $CrSiTe_3$ can be an intriguing platform for realizing Chern insulating systems with higher Chern numbers.

*in collaboration with Sungmo Kang, Seungjin Kang, and Heungsik Kim

[1] Sungmo Kang, Seungjin Kang, Heung-Sik Kim and Jaejun Yu, npj 2D Mater. Appl. **7**, 13 (2023)
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[3] S. Kang, S. Kang, and Jaejun Yu, J. Electron. Mater. 48, 1441 (2019)
[4] S. Baidya, Jaejun Yu, and C. H. Kim, Phys. Rev. B 98, 155148 (2018).

B2

Enhancement of electronic nematic susceptibility near the first superconducting dome in the kagome superconductor $Cs(V_{1-x}Ti_x)_3Sb_5$

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Abstract

Elastoresistance has been systematically investigated in high-quality single crystals of $Cs(V_{1-x}Ti_x)_3Sb_5$ to uncover the intricate evolution of electronic nematic susceptibility near their charge-density-wave (CDW) ordering temperature T_{CDW}. The temperature dependence of the nematic susceptibility below T_{CDW} exhibits the Curie–Weiss behavior in low Ti doped $Cs(V_{1-x}Ti_x)_3Sb_5$ crystals ($0 \leq x \leq 0.03$). With increase of Ti doping x, the extracted Curie–Weiss temperature, found at 30 K for $x = 0$, is monotonically suppressed and changes its sign to become negative around $x = 0.009$. Furthermore, the Curie constant is found to become maximum at $x = 0.01$, showing enhanced nematic susceptibility near the putative nematic quantum critical point (NQCP) at $x = 0.009$. Strikingly, the superconducting transition temperature and Meissner volume fraction exhibit an unusual double-dome feature as a function x, in which the center of the first dome is located in the vicinity of NQCP. This points to a crucial role of nematic fluctuation in enhancing the superconductivity in a low doping regime of $Cs(V_{1-x}Ti_x)_3Sb_5$.

B3

Quantum critical 2D Bose gas formation in the honeycomb antiferromagnet $YbCl_3$

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Bose-Einstein condensation (BEC) in quantum magnets is that of the hard-core bosons introduced by Matsubara-Matsuda transformation of spins [1, 2]. While a three-dimensional (3D) XY ordering nearby the saturation field is regarded as a BEC, the fully polarized (FP) state can be viewed as vacuum. By tuning magnetic field, one can study the quantum phase transition (QPT) between the two states in detail. The effect of the reduced dimensionality is one of the attractive extension of such studies. Especially, in 2D, one can expect Berezinskii-Kosterlitz-Thouless (BKT)-type characteristics and its interplay with the QPT. However, there has been no clear example to date due to the lack of model materials with an easily accessible saturation field.

$YbCl_3$ is a pseudo-spin 1/2 honeycomb Heisenberg antiferromagnet with intra-layer coupling of $J \sim 5$K and exhibits a transition to a FP state at an in-plane saturation field $H_s = 5.93$ T [3-5]. We will discuss that the long range ordering right below H_s is a BEC in the 2D-limit stabilized by an extremely small interlayer coupling of the order of $10^{-5}J$ [6]. The quantum critical fluctuations at H_s are well described as a highly mobile bose gas in the 2D limit. The reduced boson-boson interaction estimated at H_s indicates the logarithmic correction inherent to 2D systems. Thus, $YbCl_3$ is established as an ideal arena for a quantum critical BEC in the 2D limit. We will further discuss the possible BKT characteristics in the thermal fluctuations.

[1] V. Zapf, M. Jaime, and C. D. Batista, Rev. Mod. Phys. **86**, 563 (2014).
[2] T. Matsubara and H. Matsuda, Prog. Theor. Phys. **16**, 569(1956).
[3] G. Sala *et al*., Phys. Rev. B **100**, 180406(R) (2019).
[4] J. Xing *et al*., Phys. Rev. B **102**, 014427 (2020).
[5] G. Sala *et al*., Nat Commun **12**, 171 (2021).
[6] Y. Matsumoto *et al*., arXiv:2207.02329.

B5

Metal-insulator transition and negative magnetoresistance in $Ba_{3-x}Eu_xNb_5O_{15}$

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$Ba_3Nb_5O_{15}$ with a tetragonal tungsten bronze structure has 0.2 electron per Nb in the 4*d* orbitals, and exhibits one-dimensional conduction. Intriguing properties of this compound with various types of substitutions are discussed, in particular, the metal-insulator transition with the substitution of divalent ions for Ba [1] and a large negative magnetoresistance reaching $\rho(0)/\rho(H)\sim5000$ in $Ba_{3-x}Eu_xNb_5O_{15}$ [2].

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B6

Superconductivity in Ternary Telluride Sc_6MTe_2 with 3*d*, 4*d*, and 5*d* Transition Metals

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d-electron superconductors, such as cuprates and iron arsenides, exhibited various unique superconductivities that have attracted attention in condensed matter physics. They are realized by the cooperation between various features of *d* electrons of transition metals, such as strong electron correlation, spin-orbit coupling, and spin and orbital fluctuations. However, such *d*-electron superconductivities appeared only in materials with the specific combination of transition metal elements and crystal structure, which prevents complete understanding of them based on the systematic experimental studies.

Here we report the discovery of bulk superconductivity in Sc_6MTe_2, where *M* is seven transition-metal elements. They crystallize in the hexagonal Zr_6CoAl_2 type with the *P*–62*m* space group without inversion symmetry. The critical temperatures for *M* = 3*d* elements were higher than those for *M* = 4*d* and 5*d* ones, as shown in the Table, reaching the highest T_c = 4.7 K for *M* = Fe. The superconductivity in Sc_6FeTe_2 is suggested to be strong coupling, and the first principles calculation results indicated the Fe 3*d* electrons have considerable contribution to the electronic state at the Fermi energy. The upper critical field H_{c2} also has a pronounced element dependence, where Sc_6MTe_2 with *M* = Os and Ir showed the high $H_{c2}(0)$ violating the Pauli limit. These results clearly show that Sc_6MTe_2 is a unique *d*-electron superconductor family that showed superconductivity in all 3*d*, 4*d*, and 5*d* cases, where the electron correlation and spin-orbit coupling of *d* electrons might play roles.

Table. T_c and $H_{c2}(0)$ of Sc_6MTe_2.

3*d* element	Mn	Fe	Co	Ni
T_c (K)	< 0.1	4.7	3.5	2.6
$\mu_0 H_{c2}(0)$ (T)		8.7	6.2	2.7
4*d* element		Ru	Rh	
T_c (K)		1.9	1.9	
$\mu_0 H_{c2}(0)$ (T)		3.6	3.5	
5*d* element		Os	Ir	
T_c (K)		2.4	2.0	
$\mu_0 H_{c2}(0)$ (T)		5.2	5.0	

The work was done in collaboration with Y. Shinoda, Y. Yamakawa, D. Hirai, K. Takenaka (Nagoya Univ.) and H. Matsumoto (Univ. Tokyo).

B7

The Dynamical Charge Response of Plasmons to the Charge-Density-Wave Order in CuTe

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CuTe harbors a quasi-one-dimensional crystal structure, with the onset of charge density wave (CDW) below 335 K [1,2]. This CDW order satisfies all the essential ingredients of the uniaxial lattice modulation, Fermi-surface nesting, and Kohn anomaly in the classical context of the Peierls instability [1].
Conversely, plasmons, being the quanta of dynamical charge oscillations in matters, have been shown to be sensitive to the CDW order by the presence of a negative momentum(q)-dependent dispersion, which reflects the softening of the dynamical response by the CDW [3]. A very recent q-dependent electron-energy loss spectroscopy (q-EELS) study, however, refutes this scenario of the CDW-induced plasmon condensation and points out a rather quadratic q-dispersion in close interaction with the CDW gap [4]. CuTe, with the plasmon excitation at ~2.5 eV [2] and the gap size at the way lower energy scale of ~150 meV [1], stands out as an ideal system for mitigating the direct impact of the single-particle gap excitation on the collective plasmon [4] and could readily unveil the most fundamental aspect on the dynamical charge response in the electronic order of CDWs [2-4]. Using the joint force of q-EELS and atom-resolved EELS (Å-EELS), we have resolved the plasmon dispersions in CuTe as a function of temperatures below 335 K, along with the atomistic insight into the wave modulation in real space. An exotic plasmon-dispersion characteristic in response to the concomitant CDW order-parameter strength was unambiguously observed and will be thoroughly presented in the meeting in light of disentangling the complex physics of the dynamical plasmon response in the presence of the static CDW order.

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C1

Ab initio studies of cuprate superconductors and analyses on the electron fractionalization

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We discuss recent numerical studies on several cuprate high-T_c superconductors by applying highly accurate quantum many-body solvers to first principles Hamiltonians [1,2]. We find a principal component that controls the superconducting order parameter and T_c. By extending the Hamiltonians beyond the *ab initio* parameters, we discuss how the superconductivity can be further enhanced.

The solutions of the *ab initio* Hamiltonians support the fractionalization of electrons [3], which is also supported by theoretical model studies [4] as well as by machine learning studies of photoemission experiments [5]. The fractionalization has a further consequence in exciton dynamics which can be tested in independent measurements by resonant inelastic X-ray scattering [6,7].

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C2

New twists in strongly correlated electronic systems: from Kondo screening to unconventional superconductivity

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In this talk, I will discuss some new issues arising in strongly correlated electronic systems including the puzzlement of observing quantum oscillation in Kondo insulators and how to realize unconventional superconductivity. I will present our theory to resolve the puzzlement of quantum oscillations in Kondo insulators and show how to realize *p*-wave superconductivity by using topology of geometry.

C3

Revealing the mystery of strange metal states in correlated electron systems

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A major mystery in strongly interacting quantum systems is the microscopic origin of the "strange metal" phenomenology, with unconventional metallic behavior that defies Landau's Fermi liquid framework for ordinary metals. This state is found across a wide range of correlated quantum materials, including rare-earth intermetallic compounds and unconventional superconductors at finite temperatures (T) near a magnetic quantum phase transition. It shows a quasilinear-in-temperature resistivity and a logarithmic-in-temperature specific heat coefficient. In this talk, I will present two theoretical studies to reveal the mystery of strange metal state in $CePd_{1-x}Ni_xAl$, a geometrically frustrated Kondo lattice compound, as well as in $Ce_{1-x}Nd_xCoIn_5$, a heavy-electron quantum critical superconductor. (i) $CePd_{1-x}Ni_xAl$. Recently, an enigmatic behavior pointing toward a stable strange metal ground state (phase) was observed in $CePd_{1-x}Ni_xAl$. Here, we propose a mechanism for such phenomena driven by the interplay of the gapless fermionic short-ranged antiferromagnetic spin correlations (spinons) and critical bosonic charge (holons) fluctuations near a Kondo breakdown quantum phase transition [1]. Within a dynamical large-N approach to the Kondo–Heisenberg lattice model, the strange metal phase is realized in transport and thermodynamic quantities. It is manifested as a fluctuating Kondo-scattering–stabilized critical (gapless) fermionic spin-liquid metal. It shows ω/T scaling in dynamical electron scattering rate, a signature of quantum criticality. Our results offer a qualitative understanding of the $CePd_{1-x}Ni_xAl$ compound [2] and suggest a possibility of realizing the quantum critical strange metal phase in correlated electron systems in general. (ii) $Ce_{1-x}Nd_xCoIn_5$. An even more mysterious Planckian metal state[3], a particular type of strange metal state, showing perfect T-linear resistivity associated with universal scattering rate, $1/\tau = \alpha\, k_B T/\hbar$ with $\alpha \sim 1$, has been observed in the normal state of various strongly correlated superconductors close to a quantum critical point. However, its microscopic origin and link to quantum criticality remains an outstanding open problem. Here, we observe quantum-critical T/B-scaling of the Planckian metal state in resistivity and heat capacity of heavy-electron superconductor $Ce_{1-x}Nd_xCoIn_5$ in magnetic fields near the edge of anti-ferromagnetism at the critical doping xc ~ 0.03. We present clear experimental evidences of Kondo hybridization being quantum critical at xc. We provide a generic microscopic mechanism to qualitatively account for this quantum critical Planckian state within the quasi-two dimensional Kondo-Heisenberg lattice model near Kondo breakdown transition. We find α is a non-universal constant and depends inversely on the square of Kondo hybridization strength [4]. Our observation and proposed mechanism offer the first microscopic understanding of the Planckian dissipation limit in a quantum critical system. The applications of our studies in these two systems for the understanding of the Planckian strange metal state observed in high-Tc cuprate superconductors are discussed.

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C4

Unconventional exciton evolution from the pseudogap to superconducting phases in cuprates

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Electron quasiparticles play a crucial role in simplifying the description of many-body physics in solids with surprising success. Conventional Landau's Fermi-liquid and quasiparticle theories for high-temperature superconducting cuprates have, however, received skepticism from various angles. A path-breaking framework of electron fractionalization has been established to replace the Fermi-liquid theory for systems that show the fractional quantum Hall effect and the Mott insulating phenomena; whether it captures the essential physics of the pseudogap and superconducting phases of cuprates is still an open issue. Here, we show that excitonic excitation of optimally doped $Bi_2Sr_2CaCu_2O_{8+\delta}$ with energy far above the superconducting-gap energy scale, about 1 eV or even higher, is unusually enhanced by the onset of superconductivity. Our finding proves the involvement of such high-energy excitons in superconductivity. Therefore, the observed enhancement in the spectral weight of excitons imposes a crucial constraint on theories for the pseudogap and superconducting mechanisms. A simple two-component fermion model which embodies electron fractionalization in the pseudogap state provides a possible mechanism of this enhancement, pointing toward a novel route for understanding the electronic structure of superconducting cuprates.

C5

My story of van der Waals magnets and Prof. Shin

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Two-dimensional (2d) magnetism has been central to decades-long research as it offers the cleanest test bed for new ideas and physics. The discovery of van der Waals(vdW) magnets reported in 2016 by my group and others in the following years has completely transformed the field of 2d magnetism by providing natural 2d magnets that can be experimentally studied using many tools. Despite their short lifetime, van der magnets have been used for excitingly interesting reports and ideas.

When I started this crazy idea in early 2010, I did not know where it was heading. But slowly, I moved in my ideas and gave the first public presentation of my idea in a JKT meeting at Tokyo Univ. in 2013. I remember some of the warm and kind encouragement I had from friends attending the meeting. I admit now that I desperately needed such moral support then, as I was uncertain about the project. Then I gave my second presentation about these vdW magnets at the TJK meeting in 2015, where Prof. Shin proposed an exciting idea of measuring my vdW magnets using his then new machine of laser PEEM machine to study the magnetic domain in these 2d magnets.

It began years of collaborations between Prof. Shin and me, with several research visits to the Kashiwa campus by my students and me. I will share my warm memory of this collaboration with you in this talk.

C6

Atomically Resolved Electronic Structure of Copper-Oxide Chains and Planes on Incommensurate Charge Order in $YBa_2Cu_3O_{6+x}$

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Abstract

Charge ordering (CO) was identified as a key factor in competition with superconductivity of high-temperature cuprate superconductors. However, a fundamental application of a spatially resolved technique capable of giving direct insight into the nature of CO in the benchmark high-temperature cuprate $YBa_2Cu_3O_{6+x}$ is still lacking. In the work,[1] we correlate the atomically-resolved electronic structure of CuO chains and planes and the incommensurate CO by using cross-sectional scanning tunneling microscopy. The direct access to electronic CO states in $YBCO_{6.81}$ along the ***c*** direction indicates the stabilization of the CO involves both chain and planes layers with comparable wave amplitude, wavelength, and local density of states in YBCO. Meanwhile, our observation highlights the hopping process of electrons into the neighboring layers is not only through CuO_2 bilayers, but also CuO chain layers. This approach may open new directions for exploring the CO correlation in the fundamental mechanism of superconductivity, and more discussions will be reported at the meeting.

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Keywords: Charge ordering, Superconductivity, Atomically-resolved electronic structure, Cupper-oxide chains and planes, Cross-sectional scanning tunneling microscopy

C7

First-principles studies of delicate octahedra tilting in cuprates

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Cuprates are well-known high-temperature superconductors. Although the structures of cuprates have been extensively studied, new findings concerning the structures involving the delicate tilts of CuO_6 octahedra could still be revealed. In our recent study on the original cuprate, $La_{2-x}Sr_xCuO_4$, the low-temperature less-orthorhombic (LTLO) structure with the *Pccn* symmetry has been identified as the ground-state structure for the optimally doped $La_{1.875}Sr_{0.125}CuO_4$ within the generalized gradient approximation of density functional theory [1], which was against the well-established low-temperature orthorhombic (LTO) structure for $La_{2-x}Sr_xCuO_4$. While the La_2CuO_4 was generally thought to have the orthorhombic structure with the *Bmab* symmetry, newer neutron scattering experiments [2] showed that LTLO plus a subtle monoclinic distortion [3] could explain the measured data. In this talk, I will discuss the tiny energy differences among the structures with different octahedra tilting in $La_{1.875}Sr_{0.125}CuO_4$ based on our first-principles calculations and how phonon instability can be used to distinguish the stable structures. Then I will discuss the energy competition among those structures for the undoped La_2CuO_4 together with addressing the effect of strengths of on-site Coulomb repulsion that can enhance the magnetism in the system.

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C8

Solving high-temperature superconductivity with quantum computers

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High-temperature superconductivity is the holy grail of quantum many-body problems with a seemingly unsurmountable obstacle of the exponentially increasing Hilbert space as a function of the system size. Realizing Feynman's vision of the quantum simulation that nature should be simulated quantum mechanically, high-temperature superconductivity is a perfect example that can benefit from quantum computers harnessing the power of quantum mechanics to make the exponentially increasing Hilbert space tractable. For the success of the quantum simulation, however, it is critical to prepare a good trial state that can have a sizable overlap with the exact ground state. In this talk, I show that, serving as a good trial state for high-temperature superconductivity, the resonating valence bond state can be efficiently prepared by using the quantum algorithm for the Gutzwiller projection implemented via the fixed-point amplitude amplification method. Moreover, this method can be applied to various different types of the spin liquid state formulated in the form of the Gutzwiller-projected Fermi Sea.

P1

Chemical aspect of ferroaxial order: NASICON systems as a case study

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Ferroaxial (or ferro-rotational) order has been recently classified as a new ferroic order, which is characterized by a ferroaxial moment **A** defined as a vortex of electric dipoles [1, 2]. The **A** is an axial vector invariant under both time-reversal and spatial inversion operations while mirror symmetry parallel to **A** is broken. Despite its less electromagnetic activity, the ferroaxial materials have been attracting attention because it can be a platform for exploring unique physical phenomena (e.g., transverse response to input field or longitudinal spin current generation) [3, 4]. Thus, it is desirable to develop new ferroaxial materials, but so far, there has been no chemical information on what kind of crystalline materials exhibit ferroaxial order.

In this study, we propose a guideline for realizing ferroaxial order in crystalline materials, comprising two concepts: staggered structure and Second-order Jahn-Teller (SOJT) theory extended to electronic band structure. The effectiveness of our proposals is demonstrated in Na-superionic conductor (NASICON) systems $NaM_2(PO_4)_3$ as a case study. We point out that the staggered structure composed of MO_6 octahedra and PO_4 tetrahedra in NASICON systems plays a crucial role in realizing the ferroaxial order. Furthermore, our calculations and theoretical analyses using the group theory reveal that the ferroaxial phase transition occurs only in the NASICON with a SOJT-active electronic structure. The present study provides new insight into the exploration of ferroaxial materials.

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P2

Database Screening for Ferroaxial Materials and Experimental Verification

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In recent years, 'ferroaxial' order is discussed as a new class of ferroic states [1,2]. This order is a structural order characterized by a partial rotational distortion introduced by R.D. Johnson *et al*. in 2011 [1]. It has been attracting increased interests because of its potential for unconventional physical phenomena and new functionalities such as transverse responses in which input external fields induce output conjugate physical quantities along the perpendicular direction [3]. However, only a few ferroaxial materials have been reported to date, such as $NiTiO_3$ [4,5] and $RbFe(MoO_4)_2$ [5].

In this work, we sought new ferroaxial materials by formula-based screening using regular expression search and symmetry detection algorithm. As a result, we found that a glaserite-type compound, $K_2Zr(PO_4)_2$, is one of the promising candidates for ferroaxial materials. In addition, our *ab initio* phonon calculations suggest that this compound undergoes a ferroaxial transition. Experimentally, by the structural analysis using neutron powder diffraction measurements, we demonstrate that $K_2Zr(PO_4)_2$ shows a ferroaxial transition at about 700 K. The ferroaxial nature of $K_2Zr(PO_4)_2$ is further confirmed by the observation of its domain structures using a linear electrogyration effect, that is, optical rotation in proportion to an applied electric field [6]. In this poster presentation, the details of the database screening and experiments will be presented.

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P3

Possible surface superconductivity in the nodal-line semimetal NaAlSi

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In recent years, superconductivity has been studied from the viewpoint of topology, revealing novel properties of superconductors. We focus on the possibility of superconductivity in topological surface states. Nodal-line semimetals may have drumhead surface states that appear on the crystal surface. It has been pointed out that a flat band with a large density of states is formed there, which causes surface superconductivity with a high T_c [1].

NaAlSi is an s-wave superconductor with $T_c \sim 7$ K crystallizing the anti-PbFCl-type layered structure [2,3]. First-principles calculations show the existence of nodal-lines near the Fermi energy E_F and a drumhead-type surface state on the (001) surface of the crystal [4]. Recently, a partial superconductivity, in addition to the bulk superconductivity, was observed in electrical resistivity measurements under magnetic fields [5], but its origin remained unclear (Fig.1). We will show the possibility of surface superconductivity based on the magnetic field angle dependence of B_{c2}, which exhibits a characteristic electrical current dependence.

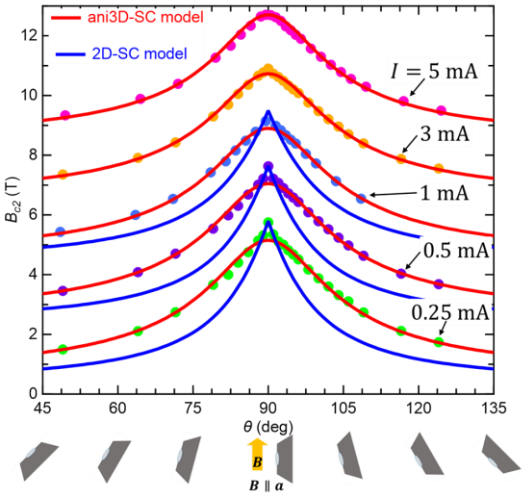

Fig.1 B_{c2} angle dependence at various current values, offset by 2 T with respect to the $I = 0.25$ mA data. Red lines are anisotropic 3-D superconductor model and blue lines are 2-D superconductor model.

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P4

Magnetic field effects on the quadrupole order of the spin–orbit-coupled insulator Ba_2MgReO_6

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Strong spin–orbit coupling (SOC) and electron correlations in 5d transition metal oxides are attracting attention [1]. The double perovskite compound Ba_2MgReO_6 (BMRO) with the electron configuration of $5d^1$ is a good candidate for multipole ordering [2]. BMRO undergoes phase transitions to a quadrupole-ordered phase at T_q = 33 K and to a canted antiferromagnetic phase at T_m = 18 K [3, 4]. As a result of the two transitions, both structural and magnetic domains are formed below T_m.

In this study, X-ray diffraction experiments under magnetic fields up to 7.5 T were performed. It is revealed that structural domains that normally cannot be controlled by magnetic fields are aligned by applying magnetic field below T_m (Fig. 1). We have also discovered that magnetic field affects the quadrupole-ordered phase above T_m. These characteristics are likely to originate from the spin–orbit-entangled electronic state of BMRO. We will discuss the unique magnetic field effects on BMRO in terms of multipolar physics.

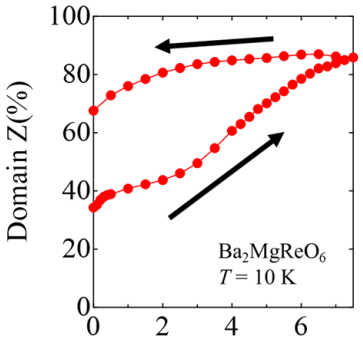

Fig. 1 Alignment of structural domains below T_m. The vertical axis shows the volume fraction of one of the three structural domains.

[1] W.Witczak-Krempa *et al*. Annu. Rev. Condens. Matter Phys. 5, **57** (2014).
[2] G. Chen *et al*. Phys. Rev. B **82**, 174440 (2010).
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[4] D. Hirai *et al*. Phys. Rev. Res. **2**, 022063 (2020).

P5

Chemical doping effect in a triply degenerate point candidate $PtBi_2$

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A crossing of linearly dispersing bands gives rise to exotic material properties [1]. These include the presence of a topologically protected surface state (called Fermi arc), unusual negative longitudinal magnetoresistance and anomalous Hall effect, which originate from the fact that the electronic state near the crossing point can be described effectively by relativistic quantum mechanical equations of motion. The well-known types of the crossings are the four-fold degenerate Dirac nodes and the doubly degenerate Weyl nodes that can be considered as a material realization of the Dirac and Weyl particles of high energy physics, respectively. In addition to such fundamental crossings, it has been recently revealed that a material system can possess advanced ones that do not have a counterpart in high energy physics [2]. One of the examples is triply degenerate point which is obtained by crossing the symmetrically protected doubly degenerate band and nondegenerate band [3]. Though this crossing is characterized as an intermediate of the Dirac and Weyl nodes, the physics including topology and material properties inherent to the crossing has been yet to be understood.

Here we report a single crystal growth of the pristine and chemically-doped trigonal $PtBi_2$, where the pristine one is theoretically proposed to have a triply degenerate point ~0.3 eV above the Fermi level [4], and discuss the chemical doping effect on the transport properties.

[1] N. P. Armitage et al., Rev. Mod. Phys. **90**, 015001 (2018).
[2] B. Bradlyn et al., Science **353**, aaf5037 (2016).
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[4] W. Gao et al., Nat. Commun. **9**, 3249 (2018).

P6

Magnetotransport properties of $Ba_{3-x}R_xTa_5O_{15}$ (R=rare earth)

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$Ba_3Nb_5O_{15}$ with a tetragonal tungsten bronze (TTB) structure exhibits one-dimensional anisotropy with a higher conductivity along the c axis [1]. If Ba^{2+} is replaced with rare earth ions, a large magnetoresistance was observed for R=Eu [2], which is caused by the interaction between Nb 4d electrons and R 4f moments. We expect more interesting phenomena in $Ba_3Ta_5O_{15}$ with R substitution caused by a larger coupling between Ta 5d and R 4f, and thus, we grew single crystals of $Ba_{3-x}R_xTa_5O_{15}$ and investigated their physical properties. We found that $Ba_3Ta_5O_{15}$ exhibits an anisotropy with a higher conductivity along the c axis, similarly to $Ba_3Nb_5O_{15}$. We also found a decrease in the number of carriers with R substitution caused by offstoichiometry. Negative magnetoresistance was observed for $Ba_{3-x}Eu_xTa_5O_{15}$, suggesting the existence of a large interaction between Ta 5d and Eu^{2+} 4f.

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[2] K. Iwamoto, W. Sekino, S. Ito, Y. Katayama, K. Ueno, and T. Katsufuji, J. Phys. Soc. Jpn. **91**, 033702 (2022).

P7

Efficient discovery of multiple minimum action pathways using Gaussian process

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We present a new efficient transition pathway search method based on the least action principle and the Gaussian process regression method. Most pathway search methods developed so far rely on string representations, which approximate a transition pathway by a series of slowly varying system replicas. Such string methods are computationally expensive in general because they require many replicas to obtain smooth pathways. Here, we present an approach employing the Gaussian process regression method, which infers the shape of a potential energy surface with a few observed data and Gaussian-shaped kernel functions. We demonstrate a drastic elevation of computing efficiency of the method about five orders of magnitude than existing methods. Further, to demonstrate its real-world capabilities, we apply our method to find multiple conformational transition pathways of alanine dipeptide using a quantum mechanical potential. ab initio calculations on that of Owing to the improved efficiency of our method, Gaussian process action optimization (GPAO), we obtain the multiple transition pathways of alanine dipeptide and calculate their transition probabilities successfully with ab initio accuracy. In addition, GPAO successfully finds the isomerization pathways of small molecules and the rearrangement of atoms on a metallic surface.

[1] J. Shim, J. Lee, J. Yu, *J. Phys. Commun.* **7**, 025004 (2023).

P8

First-principles study of morphotropic phases in Zr-doped hafnium oxide thin film on TiN substrate

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To gain insights into the morphotropic phase boundary (MPB) observed in Zr-doped hafnia systems, we conducted density-functional-theory calculations for various structural phases of $(Hf,Zr)O_2$, subject to lattice strain imposed by substrates that simulate the geometry of thin films on electrodes. By assessing the thermodynamic stability of the system, considering the bulk, surface, and interface energies, as well as temperature, we modeled the free energy of $(Hf,Zr)O_2$ over TiN electrodes, taking into account Zr composition, film thickness, and temperature. Our first-principles analysis reveals that thin films tend to grow along the tetragonal long axis, and the lattice strain by the electrode plays a crucial role in the non-polar-to-polar phase transition that contributes to the morphotropic phase boundary of $Hf_{0.5}Zr_{0.5}O_2$. Furthermore, our model predicts the appearance of the MPB even at a temperature as low as 400 K for ZrO_2, which is lower than the process temperature. Understanding the origin of the morphotropic phase boundary can have significant implications for device applications of dielectric materials.

P9

Universal methodology for twisted van der Waals homostructures

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Abstract

The field of discovering new physics as we control the angle has been active not only theoretically but also experimentally, with the discovery of the superconducting phase in Twisted Graphene in 2018, and recently, there are many attempts to expand not only graphene but also various material groups. Accurate angle control is required to realize twisted physics, but it is almost impossible to align samples separated from each other substrates with accuracy within 0.1 degree by stacking them on different substrates. In order to solve these problems, it is essential to control one sample in pieces. However, existing tear and stack methods have various limitations in making a moire structure except for a specific material group. We report a method that can be applied to a variety of material families while adhering to the tear and stack using PCL. Through the above method, it was confirmed that accurate angle control and clean interfaces could be maintained for various material groups, and it was confirmed that various measurement options could be expanded by selecting the presence or absence of a capping layer. Through the above method, it is expected that it will help to experimentally realize moire physics for 2d materials with different crystal structures and different phases, such as magnetic van der Waals materials, as well as easy access to SPM measurement that were previously difficult to approach.

P10

Quasi-2D Bismuth Oxy-Selenide: An Emerging Material in Advanced Electronic Devices

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Bismuth oxy-selenide (Bi_2O_2Se) is an emerging layered quasi-2D material in low-dimension devices due to its fascinating physical properties and excellent performance in various applications. These novel properties can be attributed to several factors, including lattice symmetry, high mobility, tunable transport properties, optoelectronic properties, band structure engineering potential, and spin-orbital coupling. Moreover, the native oxide layer of bismuth oxy-selenide (Bi_2O_5Se) exhibits a high dielectric constant, is air-stable, and can be directly formed on the bismuth oxy-compound surface by proper thermal treatment. The similar structure of the conventional SiO_2/Si but a much higher dielectric constant makes the bismuth oxy-compound system an attractive material in the field effect transistor development. We fabricated these bismuth oxy-compounds into epitaxy thin films to fully utilize these intriguing physical properties. Additionally, we have successfully integrated the bismuth oxy-selenide along with its inherent high dielectric oxide layer into advanced electronic devices, demonstrating its potential for further technological applications.

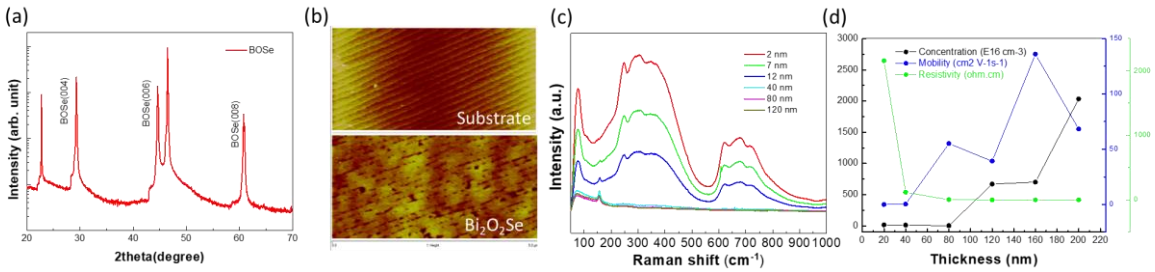

Fig. 1 (a) Structural, (b) morphology, (c) optical, and (d) transport properties.

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[2] Xiang, D. et al., Matter 5.12 4274-4314. (2022)

P11

Non-volatile Modulation on the Electronic Potential of the 2D Bi_2O_2Se Layer via Ferroelectric Polarization

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The novel 2D semiconducting material systems with high electron mobility, and suitable bandgap has become the main trend in modern electronics, leading to the scalable fabrication of high-performance devices. Bi_2O_2Se (BOSe), a 2D material with various astonishing physical properties, is a good candidate for further investigation. Currently, the control of carrier mobility and electronic structure has been achieved via the electric field effect. However, it is essential to extend the new control concepts to gain non-volatile and reversible capabilities. This work adds a ferroelectric PbZr0.2Ti0.8O3 (PZT) layer near the BOSe layer to alter band structure. Inside the BOSe/ PZT heterostructure, the position of the Fermi level in the BOSe layer could be modulated by the ferroelectric polarization of the PZT layer. Two opposite ferroelectric polarization states (P_{up} and P_{down} states) are expected to change the band structure, further affecting the binding energy and electric mobility. In conclusion, the idea for tuning the electronic properties of BOSe via non-volatile and reversible concept is provided, delivering an avenue for modifying the novel material system.

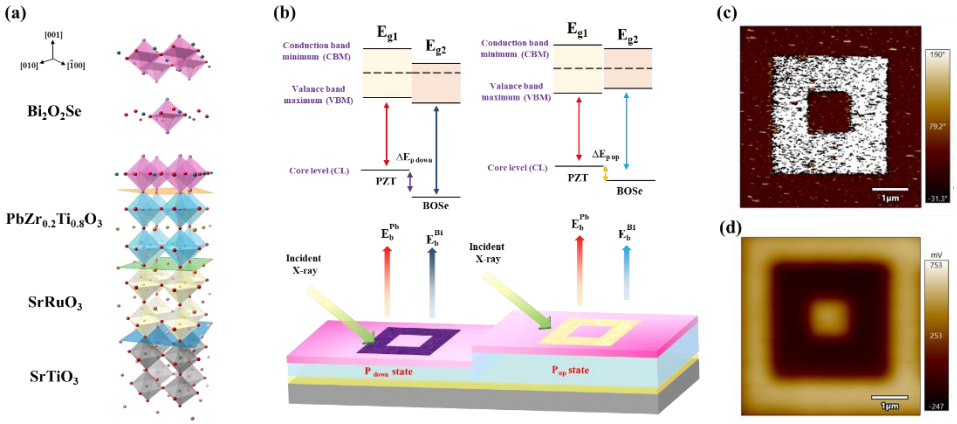

Figure 1. (a) The heterostructure of BOSe/PZT/SRO/STO. (b) The band alignment of BOSe/PZT during P and P state. (c) PFM out-of-plane phase image and (d) KPFM image for surface potential after poling process.

[1] Wu, J., et al, *Nature Nanotechnology*, "High electron mobility and quantum oscillations in non-encapsulated ultrathin semiconducting Bi2O2Se" *12*(6), 530-534 (2017).

P12

Exploring the Electrical Properties of Epitaxial Bi_2O_2Se on Silicon Fabricated by a Simple Wet Method

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In recent years, Bi_2O_2Se has emerged as a promising two-dimensional material with high mobility.[1,2] It possesses spontaneous oxide high-k material Bi_2SeO_5, which is similar to the relationship between Si and SiO_2 in semiconductors.[3] However, silicon or other 3D semiconductors' scaling leads to reduced mobility and increased short-channel effects.[4] Two-dimensional materials present fewer scaling problems compared to their three-dimensional counterparts. This makes them highly attractive for practical applications in various industries. Silicon is a commonly used substrate for two-dimensional materials in the industry due to its favorable properties and compatibility with standard microfabrication processes. We successfully transferred Bi_2O_2Se onto a silicon substrate by using free-standing techniques in this experiment.[5] Structural analysis using X-ray diffraction (XRD) indicated the transfer technique's potential on Si-based devices. The completion of this experiment provides a method for further research on Bi_2O_2Se on Si, with potential applications in various fields.

[1] Wu J, et al. Nat. Nanotechnol.12, 530-4. (2017)
[2] Ding X, et al. Matter. 5, 4274-314. (2022)
[3] Illarionov YY, et al. Nat. Electron. 3, 442-3. (2020)
[4] Li T, et al. Acc. Mater. Res. 2, 842-53. (2021)
[5] Chiabrera FM, et al. Ann.Phys. 534, 2200084. (2022)

P13

Synthesis of magnetic nanoparticles via Mica Interlayer Intercalation

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Intercalation in 2-dimensional (2D) materials is a rapidly growing area of research to develop next-generation energy-storage and optoelectronic devices, including batteries, sensors, transistors, and electrically tunable displays. The existence of van der Waals (vdW) gaps in 2D materials offers an opportunity for external species to intercalate, which can significantly modulate the intrinsic properties of 2D materials and enrich their applications. Researchers attempt to test various materials to see if they can get a tunable device. Muscovite mica is a 2D layered oxide with extraordinary optical transparency and mechanical flexibility. In order to alter the properties of muscovite, the following materials are used. They are synthetic mica, Tricobalt tetroxide, and Cobalt Selenide. Tricobalt tetroxide is a black powder with magnetic properties and can be used to make catalysts and supercapacitors. Cobalt Selenide is both a magnetic and conductive material. If we can synthesize an intercalated mica with magnetic or conductive particles as the intercalants, the properties of mica can be significantly elevated. A fascinating flexible electronic and magnetic carrier can even be desired.

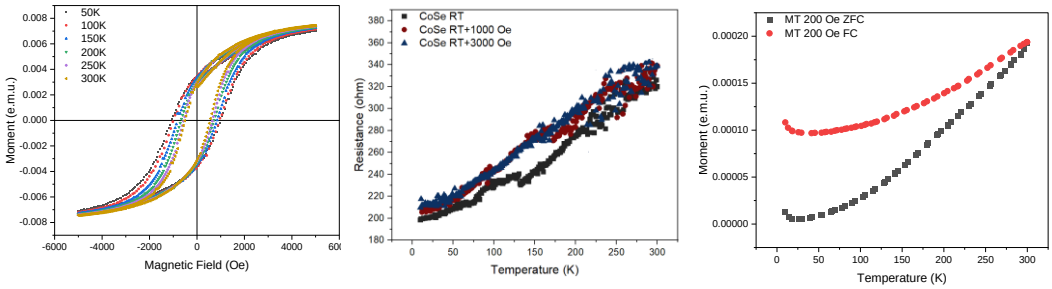

Fig. The plots of (a) CoSe MH loops, (b) CoSe RT loops, and (c) CoSe MT loops.

[1] Huang et al. Effect of structure: A new insight into nanoparticle assemblies from inanimate to animate. Sci. Adv. 6, eaba1321 (2020)

P14

Fabrication of the Bi_2O_2S Epitaxy Thin Films and the Novel Optical Properties

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Bismuth oxychalcogenides Bi_2O_2X (X = S, Se, Te) compounds are now attracting much research due to their remarkable electronic, optoelectronic, and thermoelectric properties. [1] The semiconductors with an Eg value around 1–1.8 eV are suitable for absorbing most solar light (UV, visible, and some NIR light). The studies show that the band gap of Bi_2O_2S (Eg = 1.12 eV) falls in this region. [2] In addition, Bi_2O_2S is an intrinsic semiconductor, meaning it has p-type and n-type characteristics depending on the doping and preparation methods. In its pristine form, Bi_2O_2S is often reported as an n-type semiconductor. However, p-type doping of Bi_2O_2S has been investigated in recent research to enhance its electronic and photocatalytic properties. Therefore, the conductivity type of Bi_2O_2S depends on the doping elements and the conditions of preparation and treatment. Moreover, a recent study demonstrated a high-performance solar cell based on a Bi_2O_2S absorber layer. The solar cell showed a power conversion efficiency of 5.08%, which is relatively high for a thin-film solar cell based on a Bi-based absorber layer. This indicates that Bi_2O_2S has the potential for use in high-performance solar cells. As for thermoelectric materials, Bi_2O_2S, one of the bismuth chalcogenides with a layered structure, is believed to have excellent photoelectric properties. [3] However, there are still very few studies on Bi_2O_2S properties. In this study, the epitaxy Bi_2O_2S thin film has been fabricated. The crystal structure was confirmed by x-ray diffraction through a phi scan, rocking curve. We also did the optical measurement. These properties make Bi_2O_2S a promising material for various applications, including solar cells, photocatalysts, and electronic and optoelectronic devices. This result paves a new avenue for advanced optoelectronics.

[1] M. J. Pitcher et al., J. Mater. Chem. A, 3, 17376-17382 (2015).
[2] Y. Liu et al., ACS Appl. Mater. Interfaces, 7, 7924-7930 (2015).
[3] J. Li et al., J. Mater. Chem. C, 7, 1209-1215 (2019).

P15

Perpendicular magnetic anisotropy in high entropy (Fe, Co, Ni, Cr, Mn)$_3$O$_4$ oxide driven by single-element orbital anisotropy

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Multicomponent material design has captured considerable attention due to the ability to tailor functional properties in the past few years. In this study, we study the magnetic behavior of high entropy oxide (HEO) composed of iron, cobalt, nickel, chromium, and manganese. The magnetic interactions are expected to be complex and isotropic due to different types and magnitude variation of exchange interactions.[1] [2] But, substrate induced strain is introduced as a knob to alter the orbital occupation of Mn^{3+}, providing a source of magnetic anisotropy and dominating the overall magnetic performance. With the element-specific x-ray absorption spectroscopy analysis, the cause of the magnetic anisotropy difference can be determined. This study demonstrates single-element driven properties on HEO to overcome the random distribution of atoms and magnetic interaction, providing a design rule for high entropy materials.

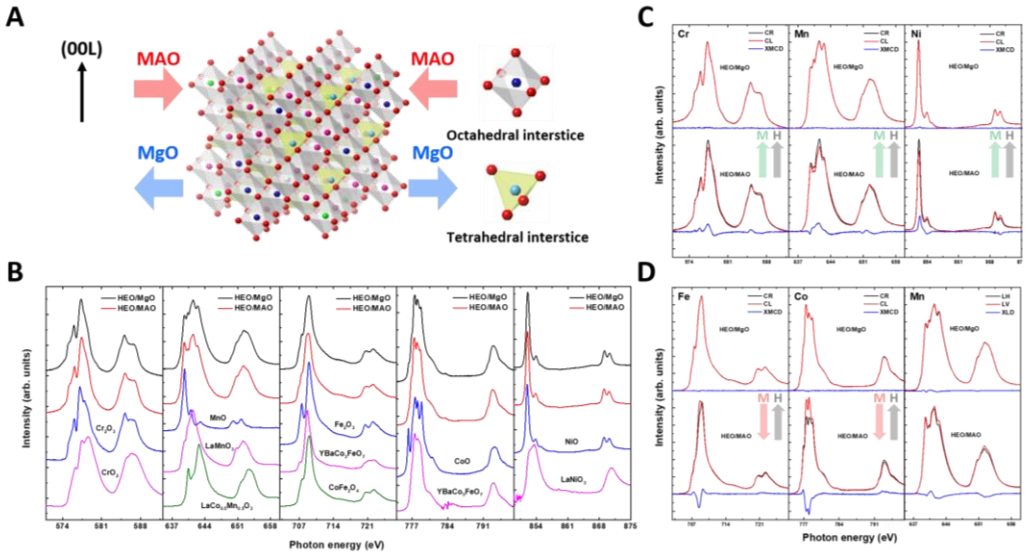

Figure. (A) The schematic of HEO structure under MAO compressive strain and MgO tensile strain. (B) XAS spectra of HEO/MAO and HEO/MgO structures. (C) Cr, Mn, Ni XAS-XMCD spectra. (D) Fe, Co XAS-XMCD and Mn XAS-XLD spectra.

[1] C. M. Rost, E. Sachet, T. Borman, A. Moballegh, E. C. Dickey, D. Hou, J. L. Jones, S. Curtarolo, and J. P. Maria, Nat. Commun. **6**, 8 (2015).

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P16

Creation of Novel Composite Materials: Magnetic and Conductive Muscovite

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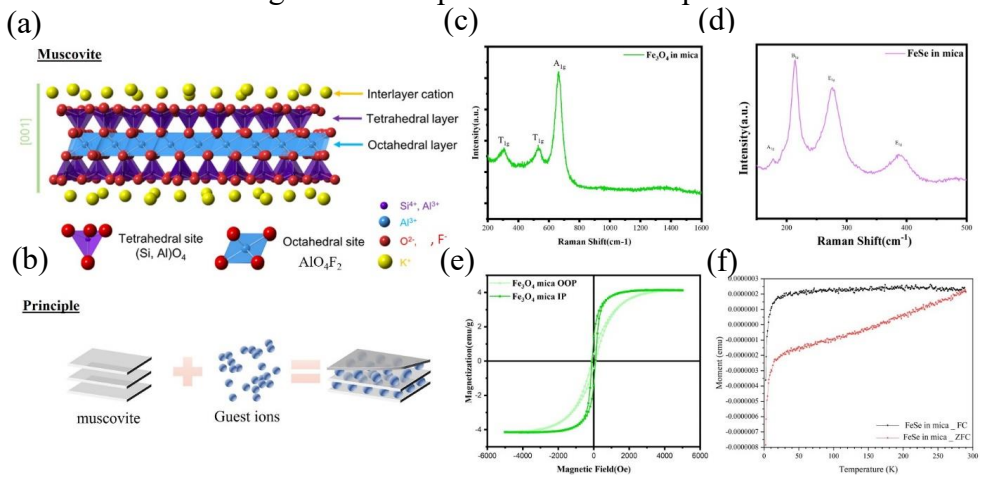
Two-dimensional layered materials are composed of van der Waals forces between the layers and exhibit unique physical and chemical properties. Due to the weak interaction between adjacent layers, space exists between them, called the “van der Waals gap”. With these gaps, foreign ions or nanoparticles can be inserted into the gap to modify the electronic, optical, magnetic, and mechanical performance of the 2D materials. This modification technique by inserting foreign atoms is called intercalation. Muscovite is a layered silicate, and a single layer of muscovite consists of two tetrahedral sheets and one octahedral sheet. In addition, muscovite exhibits plenty of characteristics, including flexibility, transparency, and good chemical stability, making it a promising platform for developing flexible devices. Therefore, to extend the application of muscovite, we intercalate the transition element, “Fe”, to modify the insulated and diamagnetic muscovite into the ferromagnetic and superconductive composite.



Figure(a) Structure of muscovite; (b)illustration of intercalation method; (c, d) Raman spectroscopy of Fe_3O_4 and FeSe inserted into muscovite; (e) hysteresis loop of Fe_3O_4 in muscovite;(f) temperature-dependent magnetization of FeSe in mica

[1] Zhou, J, et al., *Adv. Mater.* 2021, 33, 2004557.

P17

A new form of thermochromism materials: VO_2 Intercalated Muscovite

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Vanadium(IV) oxide is a fascinating material for its low metal−insulator transition (MIT) point around room temperature. The MIT of VO_2 couples with the optical transmittance strongly. It exhibits excellent reversible thermochromic during the phase transformation, making VO_2 suitable for intelligent windows. Muscovite, 2D layered oxide, exhibits remarkable properties such as optical transparency, mechanical flexibility, and chemical stability, suggesting a superior carrier for window applications. Taking advantage of the layered structure, the force between the muscovite layers is van der Waals's force, providing an environment to intercalate guest materials. In this study, we apply a gas phase intercalation to insert VO_2 into interlayers. Through X-ray diffraction and Raman spectroscopy, we found that VO_2 crystallizes between the mica layer and exhibits thermochromism and optical transmittance, indicating the potential for a new perspective of intelligent windows.

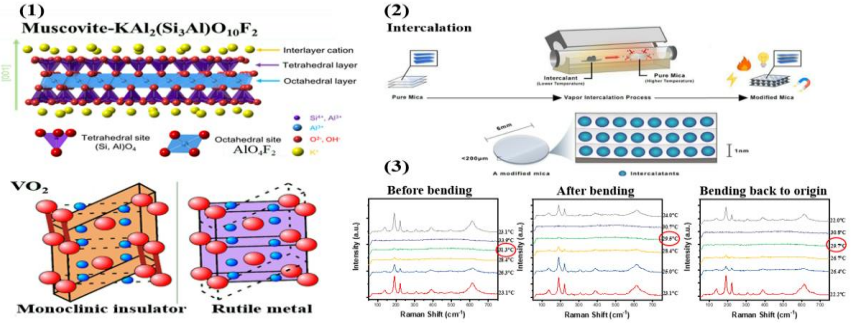

Fig.(1) The structure of Muscovite and VO_2. **Fig.(2)** Experiment process: First, V_2O_5 was inserted into muscovite by vapor phase intercalation process. Then, the samples were annealed in hydrogen. Finally, modified muscovite with VO_2 was obtained. **Fig.(3)** Raman spectrum: the intercalant in muscovite can be confirmed by the Raman spectrum.VO_2 muscovite was observed. And with different temperatures, we found the metal-insulator transition temperature.

[1] C. I Li et al., van der Waal Epitaxy of Flexible and Transparent VO_2 Film on Muscovite, Chem. Mater. 28, 11 (2016).
[2] J. Y. Zhou et al., Layered intercalation materials, Adv. Mater. 33, 25, (2021).

P18

Fabrication of superconductive muscovite via MgB_2 intercalation

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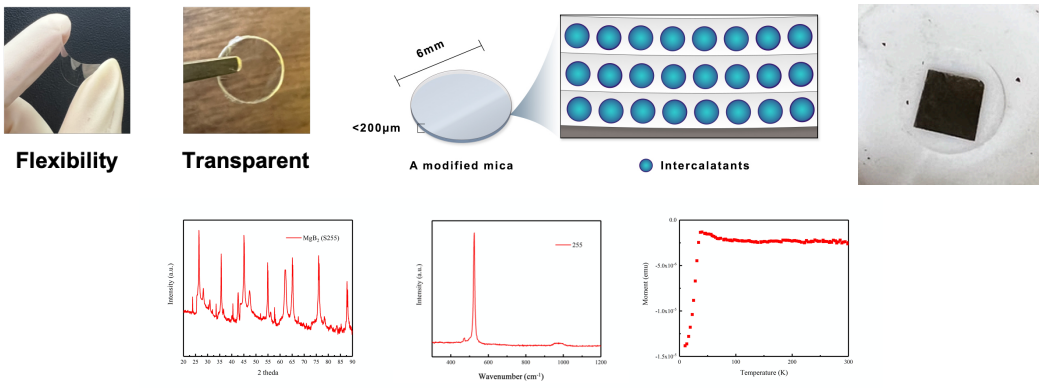
Muscovite, a flexible and natural layered clay mineral with large lateral dimensions and interlayer spaces in a small volume, provides an ideal platform for intercalation. Muscovite interlayers covalently bond atomic lattices by weak van der Waals interactions, in which various foreign species may be inserted without breaking the in-plane covalent bonds through intercalation processes. Those intercalant species introduce unusual physical and chemical properties to muscovite, making it perform unique functions. Magnesium diboride (MgB_2) exhibits superconductivity at a critical temperature of approximately 39K. The simple crystal structure, considerable coherence lengths, high critical current densities and fields, and transparency of grain boundaries to current make it an auspicious material for a wide range of applications, including large-scale applications and electronic devices. Herein, we designed the experiments of intercalating MgB_2 into muscovite and obtained a superconductive muscovite with high crystallization quality in a continuous large area (up to 1x1cm). We aim to control its critical temperature to realize flexible and large-scale functional muscovite for next-generation devices.



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[2] C. Buzea, et al., Sci. Technol. **14**, R115 (2001).

P19

Novel 2D Layered Composite Materials: Modification of Muscovite by Intercalation

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2D layered compounds have attracted great interest for researchers due to the distinctive features originating from strong in-plane covalent bonds and weak out-of-plane van der Waals force between neighboring layers. Moreover, tuning properties and creating novel 2D layered compounds with unique electronic and heat transport let 2D materials have opportunities to overcome the limitation of thickness for next-generation electronic devices. Intercalation is a widely used strategy to modify 2D layered materials. The weak van der Waals bonding between atomic layers provides gaps that can be considered 2D space to insert guest species with host materials. Numerous intriguing physical properties are expected to be induced by the insertion of foreign species. In the development of new 2D layered material, muscovite is a potential candidate with a 2D layered structure bonded by van der Waals interaction and features optical transparency and mechanical flexibility. However, muscovite was used as a substrate and strain source in past studies. Thus, this program implements intercalation chemistry to create a novel 2D layered composite for innovation based on muscovite. Some nickel-related materials, including NiO, $NiFe_2O_4$, $NiSe_x$, and Ni, were successfully intercalated into the layers of muscovite after a series of treatments. Various outstanding physical properties emerged in the new composites, such as metal conductivity and ferromagnetism differed from pure muscovite. Furthermore, the epitaxy features were revealed in the Ni, NiO, and $NiFe_2O_4$ muscovite system. In conclusion, this work provides a new design of 2D layered composite, showing great potential for application in the field of energy, wearable electronics, and semiconductors.

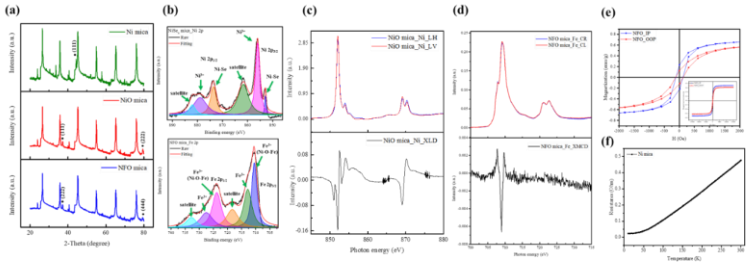

Fig.1 (a) XRD of Ni, NiO, and NFO intercalated muscovite (b) XPS of $NiSe_x$ and NFO intercalated muscovite (c) XAS and XMCD of NFO intercalated muscovite (d) XAS and XLD of NiO intercalated muscovite (e) MH loop of NFO intercalated muscovite (f) R-T curve of Ni intercalated muscovite.

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P20

Epitaxial High Entropy Oxide Films with High Dielectric Tunability and Superior Thermal Stability

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The compositional diversity is the advantage of a high entropy system, stabilizing the single-phase structure because of the configurational disorder. The system has excellent thermal tolerance and the potential to develop electrical components. In this work, relaxor-based materials are utilized to fabricate the epitaxial high entropy oxide (HEO) thin films with the benefits of dielectric and high entropy simultaneously. Relaxor ferroelectrics are widely used in many applications due to their outstanding features, such as energy storage capacity, energy conversion efficiency, and dielectric constant. Substitutional doping is an effective strategy to manipulate the characterizations of this class material. The manufacture of epitaxial HEO films is carried out by pulsed laser deposition (PLD) technique. The films deposited on the $SrTiO_3$ (STO) substrates are mixed with the relaxor-based materials and the dopants. According to the analysis results, the epitaxial HEO films exhibit higher dielectric tunability and better thermal stability than the classical tunable material (Ba, Sr)TiO_3 (BSTO).

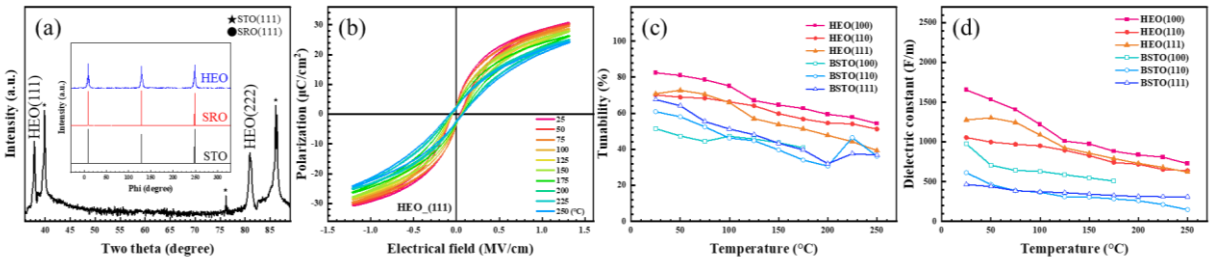

Fig. 1 (a)XRD patterns (in set: phi-scan results). Temperature-dependent, (b)hysteresis loops, (c) dielectric tunability, and (d) dielectric constant.

P21

The $Pb(Zr_{0.52}Ti_{0.48})O_3$ Thin Film on Muscovite for the Application of Flexible Electronics

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The strongly correlated electron system (SCE) contributes to various physical properties of multiferroic materials. For perovskite structure, behaviors of electrons cannot be deemed independent due to the Columbic interactions between electrons in the d-orbitals. With the complex interactions of electrons, perovskite materials often demonstrate exciting properties, such as ferroelectricity and magnetism, and are applied widely. Consequently, this research's primary goal is to dig into the possibility of ferroelectric perovskites. In this research, the perovskite material $Pb(Zr_{0.52}Ti_{0.48})O_3$ is chosen not only from its ferroelectric property but its piezoelectricity that shows outstanding electromechanical effect. The specific ratio of Zr and Ti was determined by the morphotropic phase boundary in the phase diagram, where the rhombohedral and tetragonal phases coexist, causing the best performance in the piezoelectric effect. In this study, the PZT 52/48 thin film was fabricated by magnetron sputtering on muscovite, a 2-D material. Free dangling bonds on the muscovite surface allow this functional film to obtain better electronic properties.

In the aspects of properties analyses, the polarization loops measuring was also conducted, besides using XRD to assure the epitaxy of PZT 52/48 thin film. Our sample could distinguish different sources and respond respectively was also discussed. Moreover, flexibility can be obtained if the number of layers of muscovite is reduced. Hence, determining the electronic stability after bending is the critical point in this experiment, bringing about the possibility of ferroelectric materials in the field of flexible electronic apparatus.

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P22

MICAtronics - Muscovite van der Waals Epitaxy

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In the fabrication of epitaxial heterostructures, strain has always been an important factor to be considered. The lattice mismatch between the substrate and thin film must be controlled within a certain range; otherwise, the epitaxial structure cannot be formed. To solve this problem, the concept of van der Waals epitaxy[1] was proposed. With no dangling bonds on the substrate surface, the only bonding force between the substrate and film is van der Waals force, which is much weaker than other chemical bonds. Hence, we can obtain a virtually strain-free thin film.

Among the various kinds of substrates used in van der Waals epitaxy, muscovite[2] is one of the potential options. As an abundant natural mineral, muscovite is cheap and easy to obtain. Under an adequate thickness, muscovite can show great transparency and flexibility. Besides, it also has high thermal and chemical stability, which can survive in extreme environments. Due to its advantages, it has been combined with all kinds of materials and performed numerous characteristics, such as metal-insulator transition[3], transparent conductive oxide[4], and deep ultraviolet photodetection[5]. In this work, we are going to introduce various kinds of research results of muscovite van der Waals epitaxy and its possible applications, bringing a better understanding of the potential of muscovite.

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P23

The role of lattice in the transport and magnetic properties of high entropy alloy films

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High entropy alloys (HEAs), complex systems with many elements, are a thriving research topic in materials science. [1] However, this highly disordered system is hard to analyze by the physical models. When considering the role of entropy in HEA, extrinsic factors such as the existence of grains and different phases should be separated from intrinsic configurations of the atomic lattice. Here, we fabricate $CoCrFeNi_2Al_{0.5}$ HEA/muscovite heterostructures, with some prepared as epitaxial bilayers and others as an amorphous system. These two systems are classified into atomic-site disordered (ASD) and structurally disordered (SD) states without extrinsic effects to isolate the role of the crystal lattice in high-entropy states. In this study, we uncover the lattice role in correlation to the structural, electronic, and magnetic properties of the HEA using a combination of X-ray diffraction, transmission electron microscopy, magneto-transport, ultrafast dynamics spectroscopy, and X-ray absorption spectroscopy with magnetic circular dichroism. The ASD state shows a fully metallic behavior with intense magnetic saturation, whereas the SD state displays metallic with Kondo-like behavior under 50K. X-ray absorption and magnetic circular dichroism are used to understand the interaction of magnetic elements in the ASD and SD states. The difference between the saturation magnetic moment and the electron relaxation behavior in the ASD and SD states results from the existence of the lattice affecting the atomic distance and periodicity to modify the exchange interaction [2] and tune the electron-phonon interaction for scattering.

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P24

Momentum-resolved RIXS studies on high-temperature superconductor Bi2212

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We used momentum resolved measurements of Cu L_3-edge resonant inelastic x-ray scattering (RIXS) to investigate the quasiparticle excitations of optimally-doped $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi2212). Our findings indicate that momentum-resolved RIXS can measure the dynamical structure factor. The energy dispersions of our RIXS data are in good agreement with the charge susceptibility previously reported, which are explicitly calculated using a tight-binding band structure and the SC order parameter. Additionally, our study revealed that the CDW excitations of Bi2212 remain robust with Q near (0.25, 0) at an energy up to ~0.25 eV.

P25

RIXS studies on the kagome metal YMn_6Sn_6

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S-W Cheong,[4] S. Poteryaev, [5] A. Ushakov, [5] S. V. Streltsov, [5]
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We performed RIXS measurements on YMn_6Sn_6 using various incident photon energies across the Mn L_3 edge, and the obtained data revealed two distinct RIXS spectral signatures: fluorescence-like and Raman-like RIXS features. The fluorescence-like signature reflects the transitions of the 3d bands crossing the Fermi level, while the Raman-like signature originates from Mn dd excitations. Additionally, the self-energy calculations show that three of the Mn 3d bands are metallic, while the other two are insulating-like. These results provide spectral evidence for the existence of orbital-selective Hund's metal in the kagome metal YMn_6Sn_6.

P26

Novel X-ray circular dichroism in a collinear antiferromagnet on a chiral lattice

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X-ray circular dichroism (CD), which reflects the dependence of absorption on photon helicity, measures the magnetization of ferromagnetic materials [1] and the handedness of chiral crystals [2]. A collinear antiferromagnet should exhibit no x-ray magnetic circular dichroism (XMCD) because of time-reversal symmetry. Here, we report on observing a new type of x-ray CD at the Ni L edge in the structurally chiral, collinear antiferromagnet Ni_3TeO_6 [3] without an external magnetic field, where only a tiny natural CD is expected. The observed x-ray CD changes sign between domains of opposite crystal chirality, indicating that the crystal chirality acts as an effective “magnetic field” on the Ni spins. To explain this new type of x-ray CD, which is distinct from XMCD in noncoplanar antiferromagnets [4], we propose a mechanism based on the local crystal chirality due to oxygen ions at the non-centrosymmetric sites bridging spin-up and spin-down Ni ions, in analogy to spontaneous Hall effect in another collinear antiferromagnet [5]. The coupling of such chirality to spin causes spin-dependent hybridization between the two Ni ions, breaking of time-reversal symmetry, and hence the magnetically-enhanced x-ray CD in Ni_3TeO_6.

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P30

Chern dartboard insulator: sub-Brillouin zone topology and skyrmion multipoles

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Topology plays a crucial role in many physical systems, leading to interesting states at the surface. The paradigmatic example is the Chern number defined in the Brillouin zone that leads to the robust gapless edge states. Here we introduce the reduced Chern number, defined in subregions of the Brillouin zone (BZ), and construct a family of Chern dartboard insulators (CDIs) with quantized reduced Chern numbers in the sub-BZ (sBZ) but with trivial bulk topology. CDIs are protected by mirror symmetries and exhibit distinct pseudospin textures, including (anti)skyrmions, inside the sBZ. These CDIs host exotic gapless edge states, such as Möbius fermions and midgap corner states, and can be realized in photonic crystals. Our work opens up new possibilities for exploring sBZ topology and nontrivial surface responses in topological systems.

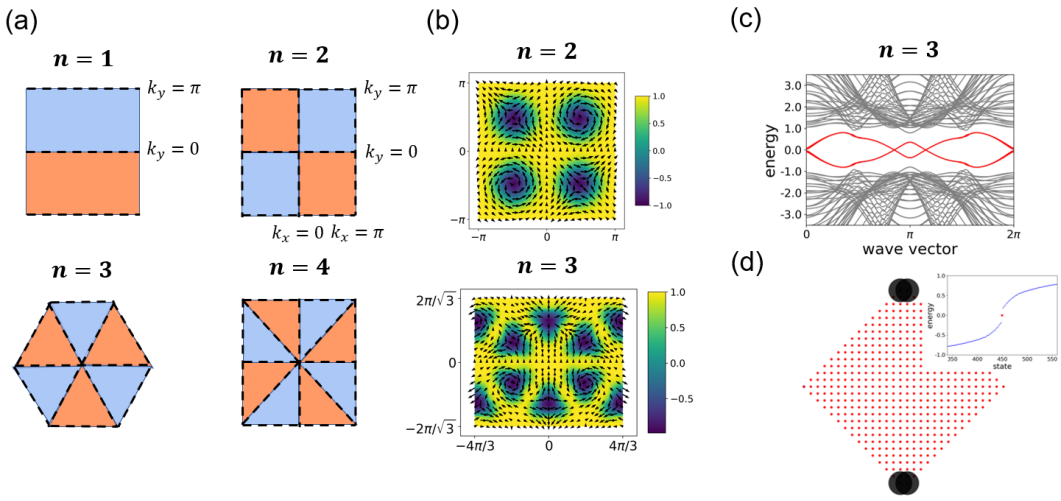

Fig. 1. (a) SBZ topology of CDIs. The red and blue color denote the sBZs with opposite signs of reduced Chern number. (b) Pseudospin textures of CDIs. Arrows denote the magnitude of n_x and n_y, while color denotes the magnitude of n_z. (c) Mobius fermions in the gapless edge modes of the Type I $n = 3$ CDI. (d) Probability distribution of the midgap corner states in the Type I $n = 1$ CDI.

P31

Temperature-Dependent Electronic Structures of TMD Weyl Semimetals

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Transition metal dichalcogenides (TMDs) are layered materials with chemical compositions described as MX2. Most TMDs are semiconducting with valley degrees of freedom to generate an application in information processing. On the other hand, $MoTe_2$ and WTe_2 are TMDs and have been proposed as candidates for Weyl semimetals [1, 2]. Both of them have gathered a great deal of attention because of the quasiparticles on their crystal surface behave as massless chiral fermions −Weyl fermions. One of the unique characteristics of Weyl semimetals is the emergence of a topologically protected surface state called Fermi arc, which can be observed by Angle-resolved photoemission spectroscopy (ARPES) and scanning tunneling microscopy (STM) based quasiparticles interference (QPI). Besides, it also obtains novel characteristics related to noncentrosymmetry [3].

Recently temperature-dependent transport properties of both WTe2 and MoTe2 are reported [4, 5]. Therefore, it is urgent to reveal the temperature-dependent electronic structures of these TMD Weyl Semimetals. By using STM and STM-QPI, both structure and electronic structures of $MoTe_2$ and WTe_2 are clearly revealed. Surprisingly, huge variations are found in between the results measured at 5K and 77K. For WTe_2, slight shifts of both two Fermi arc surface states (SS1 and SS2) and Weyl points (WPs) are obseverd. Much large variations are found in the results of $MoTe_2$. The current work provides valuable insights into the temperature-dependent properties of TMD semimetals.

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P32

Unique dewetting growth of Si layers on Ag(111)

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Two-dimensional (2D) materials show various exotic characteristics. For extending the field of 2D materials, the synthesis of large crystals is essential. However, 2D materials often grow unconventionally because of the anisotropic bonding. A representative example is the silicene growth on Ag(111). SIlicene is a 2D honeycomb sheet of Si atoms, first synthesized on Ag(111) in 2011. Experimental studies revealed that although silicene covers the whole surface at the beginning of the growth, further deposition leads to the aggregation of Si atoms by exposing Ag(111) substrate. We call this phenomenon dewetting. The dewetting is exceptional in the conventional epitaxial growth modes. Understanding the dewetting should promote controlling the growth of 2D materials.

In this study, we revealed the underlying mechanism of the dewetting of silicene on Ag(111) by combining experimental studies using scanning tunneling microscopy (STM) and a simulation based on the kinetic Monte Carlo (KMC) method [2]. The STM observation clarified that the dewetting happens after the completion of silicene. After three monolayer depositions, about half of the bare Ag(111) surface was exposed. The coverage change during the deposition is well reproduced by the KMC simulation, in which the difference in the diffusion barrier on each layer is considered.

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P33

Investigation of the Superconductivity in Buckled Plumbene-Au Kagome Superstructure

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Since the discovery of graphene, two-dimensional (2D) materials with honeycomb structures have been widely discussed. As a member of the carbon family, lead (Pb) has a similar structure to graphene, called plumbene [1]. Due to its heavy atomic mass, plumbene is expected to exhibit a strong spin-orbit coupling (SOC) effect. Indeed, the strong SOC has been confirmed in 2D superconductivity exhibited by ultrathin Pb films on Si [2]. Theoretical predictions suggest that tuning the buckling and spin-orbit couplings in 2D materials may enhance the superconducting critical temperature [3, 4]. Therefore, investigating the possibility of superconductivity in other plumbene-based superstructures is highly intriguing. In this work, the superconductivity in buckled plumbene-Au kagome superstructure is investigated. Additionally, the enhanced T_c in this system is further explained by the theoretical calculation.

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P34

Tomography Scan of Charge Density Wave in $NbSe_2$

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Charge density wave (CDW) resulted from a small distortion in the lattice is able to create new orders beyond the original lattice. In *2H*-$NbSe_2$, one of layered transition metal dichalcogenides (TMD), the 3×3 charge order appears in two-dimensional (2D) layers. Although CDW is usually described by a sine wave, the spatial distribution within a 2D layer has never been systematically visualized in the lattice. Here by using scanning tunneling microscopy (STM) and density functional theory (DFT), we have monitored the evolution of 3×3 CDW along c-axis and realized a nearly tomography scan of CDW. The results show that the strength of 3×3 charge order varies while increasing the tunneling current. The 3×3 charge order is relatively strong at the outermost Se level and decreases while probing in between Se and Nb levels. Interestingly, the 3×3 charge order gets strong again as reaching Nb level but with a phase shift. We further calculated the orbital charge distributions and found that both CDW intensity modulation and phase shift are strongly correlated to the distribution of Se *p* orbitals and Nb *d* orbitals.

P35

Origin of the ferromagnetic transition in $Co_{1.55}ZrSn$ Heusler alloy Weyl semi-metal

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This investigation aims to understand the evolution of ferromagnetic transition, and Weyl semi-metallic behavior, in $Co_{1.55}ZrSn$ Heusler alloy single crystal sample by X-ray absorption spectroscopic techniques. Magnetization and resistivity measurements respectively reveal paramagnetic-to-ferromagnetic (T_c) and insulator-to-metal (T_{IM}) transitions near ~170 K. Resonant inelastic x-ray scattering spectra at Co $L_{2,3}$ edge at 80 and 300 K show localized *d-d* excitation and fluorescence feature similar to Co $L_{2,3}$ edge in standard Co metal. Analysis of the extended X-ray absorption fine structure spectra at Sn *K*-edge also show an increase in static disorder due to out-of-plane local lattice distortion (LLD), below ~ 170 K, for the incident x-ray polarization parallel to the out-of-plane direction of the sample (**E** // [222]). However, similar measurements along the in-plane (**E** $\perp$ [222]) direction show the in-plane LLD at/below 190 K. This coincides with the temperature (T_h ~ 190 K) at which the preferential hole occupancy in the Co 3*d* in-plane orbital states begins to increase. Therefore, it is evident that the in-plane lattice-orbital correlation at/below 190 K triggers out-of-plane LLD, and subsequently paramagnetic-to-ferromagnetic transition due to possible spin-lattice-orbital coupling below 170 K. A finite temperature difference between T_{IM} and T_h indicates that the breakdown of time reversal symmetry near 170 K is responsible for the semi-metallic behavior.

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Neutron Powder Diffraction Study of the Helimagnet $YBaCuFeO_5$ with B-site Disorder

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Magnetic properties of various Cu/Fe ratios x of the double perovskite $YBa(Cu_{1-x}Fe_x)_2O_5$ were investigated by using neutron powder diffraction (*NPD*) and susceptibility measurements. The crystal structures of all the samples are formed in a space group of *P*4/*mmm* within the x range between 0.45 and 0.55. Susceptibility measurements of $YBaCuFeO_5$ single crystal exhibited two antiferromagnetic (AFM) transitions at T_{N1} ~ 450 K and T_{N2} ~ 175 K, accompanied by two unusual spin ordering, but these only happen when an external field applied vertically to the *c*-axis implies that the moments are constrained in the *ab*-plane [1]. The Rietveld refinement results revealed a collinear magnetic ordering {+, −, −, +} between T_{N1} and T_{N2}, which as a commensurate (CM) phase with propagation vector k_{c1} = (½ ½ ½), and below T_{N2}, two satellites of incommensurate (ICM) phase with k_i = (½ ½ ½ ± δ) were observed from the separation of commensurate peaks, indicating the emergence of a helical magnetic structure. Furthermore, these experiments suggested that T_{N2} is very sensitive to the concentration of Iron, and explained the paradox of transition temperatures in past reports. For $x \geq 0.510$, additional magnetic reflections with a propagation vector k_{c2} = (½ ½ 0) have been proved as a collinear magnetic ordering {+, −, +, −}, which replaces the ICM phase below T_{N2}. Recently, a group proposed their simulation results with a superlattice consisting of at least 2 % of Fe-O-Fe impurities randomly distributed. Below T_{N2}, these impurity bonds produce a strong AFM superexchange along the *c*-axis and create spin frustration, which further leads to a helical spin ordering [2].

[1] Y.-C. Lai, C.-H. Du, C.-H. Lai, Y.-H. Liang, C.-W.Wang, K. C. Rule, H.-C.Wu, H.-D. Yang,W.-T. Chen, G. J. Shu, and F.-C. Chou, J. Phys. Condens. Matter 29, 145801 (2017).
[2] A. Scaramucci, H. Shinaoka, M. V. Mostovoy, M. Müller, C. Mudry, M. Troyer, and N. A. Spaldin, Phys. Rev. X 8, 011005 (2018).

P39

Study of the Phase Transition in the Intermetallic Compound Ir_2In_8Se Using X-ray Scattering

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Intermetallic compound Ir_2In_8Se (IIS) undergoes an anomaly transition at T^* ~ 203 K that was reported to be due to the formation of a charge-density wave (CDW). In order to confirm the existence of the CDW modulation, a high-resolution x-ray scattering experiment was conducted. Using high-resolution x-ray scattering on the beamline TPS09A, a modulated structure was observed to have a size of six times of the host lattice in $a \times b$ plane. From our single crystal diffraction pattern, there is a modulated structure at 100 K been observed. Further using x-ray scattering experiments, there are two kinds of low-temperature modulation structures with q_{CDW} ~ (0.23 0.23 0) and q_{Phonon} = (0.5 0.5 0). In addition, judging from the half-width of the two modulation structures, one is related to CDW and the other is related to phonons. The inverse order-disorder transition was observed in the *H*, *K*, and *L* directions of the phonon-related peaks. However, there is no such phenomenon in the CDW peak. In contrast to the ref. [1], the CDW signal was measured from the lowest temperature to room temperature. The system has a great interaction between electrons and phonons, and is currently trying to integrate with calculations in the hope of establishing a more complete mechanism.

[1] J. F. Khoury, A. J. E. Rettie, I. Robredo, M. J. Krogstad, C. D. Malliakas, A. Bergara, M. G. Vergniory, R. Osborn, S. Rosenkranz, D. Y. Chung and M. G. Kanatzidis, Journal of the American Chemical Society **142** (13), 6312-6323 (2020).

P40

Structural Instability and Charge Transfer mediated Transition in $Pr_3Co_4Sn_{13}$: A Synchrotron Radiation Spectroscopy Based Study

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Single crystal ternary stannide materials with an $R_3T_4Sn_{13}$ stoichiometry, where R = La, Sr or Ca and T = Ir, Rh or Co are recently being studied for many interesting properties like, Heavy fermions, Kondo effect, superconductivity, and three-dimensional charge-density-wave (CDW) instability etc. Earlier report on $Pr_3Co_4Sn_{13}$ predicted a CDW like transition at ~ 138 K via specific heat and nuclear magnetic resonance studies [1]. This study aims to clarify the physics behind the 2nd order transition observed in the material at low temperature by means of synchrotron radiation based spectroscopic techniques like, X-ray scattering (XRS), X-ray diffraction (XRD), X-ray absorption near-edge structure (XANES), Extend X-ray absorption fine structure (EXAFS) and valence band photoemission (VB-PES), and resonant inelastic X-ray scattering (RIXS) etc. Appearance of satellite peaks in XRS study indicated a modulation in the structure along a new *q* vector (0.5, 0.5, 0) below 120 K. XANES spectra of Sn *K* edge revealed a charge transfer process at low temperature. Study of 2nd coordination number i.e., the next nearest neighbor from Sn *K*-edge EXAFS also suggested a distortion in the Sn sites at low temperatures. The VB-PES study along with the theoretical calculation following DFT+U method could not detect any significant change in the band gap of the material around the transition. All the results therefore suggested that the transition originated due to charge transfer process in the Sn sites followed by a diffusion less modulation/distortion in the structure.

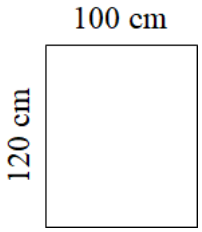
[1] Liu H F (2016) Single crystal synthesis and nuclear magnetic resonance study of $R_3Co_4Sn_{13}$ (R= La, Ce, Pr, Yb) intermetallics [Doctoral dissertation, National Cheng Kung University, Taiwan] [NCKU depository https://hdl.handle.net/11296/vkn2z7]

Poster presentation

(1) The poster session will be held in room **D260** on the 2nd floor of the Activity Center from **13:10** to **14:20** on **April 6th** (Thu).

(2) Please display your poster on the board assigned to your poster number.
The poster number assignment will be available on the poster number list.

(3) The poster size should be smaller than **120 cm × 100 cm**.
Double-sided tapes are prepared in the poster session area.



(4) There will be a poster flash session from **12:10** to **12:40**: a one-minute oral presentation for each poster.

(5) Please prepare the power-point file or the PDF file that can run on Windows for the poster flash session.

(6) Before the session, upload your presentation file with a filename starting with your poster number, e. g. P23***.ppt.

(7) Remove your poster from the board before the closing remarks of the meeting.

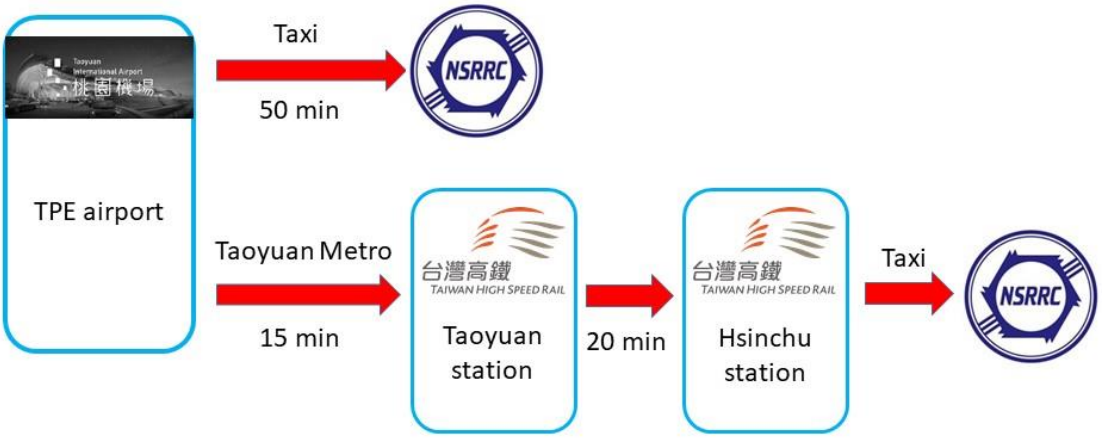
Travel to NSRRC

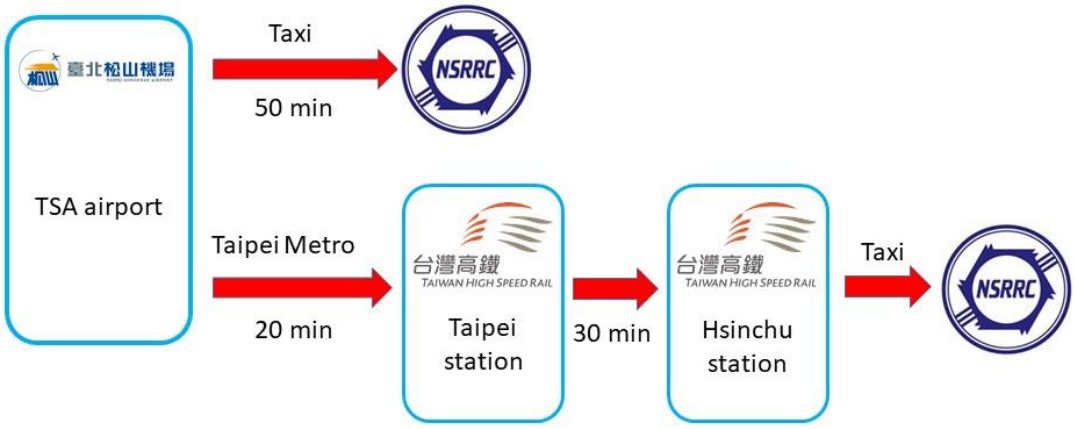
Hsinchu, commonly known as the “Windy City,” is located in northwestern Taiwan, approximately 80 km south of the capital city, Taipei. Hsinchu is about 50 km from the TPE Airport , where most international flights land.

There are two other international airports in Taiwan, TSA Airport in Taipei, and KHH Airport in Kaohsiung. There are several ways to get to Hsinchu from the Airports. If you will take public transportation, you can link or download the schedules below. In case you need a taxi, it is advised to approach the taxi services at airports and train stations.

Public Transportation Schedules:

1. **Taiwan High Speed Rail:** https://en.thsrc.com.tw/
2. **Taipei Metro :** https://english.metro.taipei/
3. **Kaohsiung Metro :** https://www.krtc.com.tw/eng/
4. **Taoyuan Metro :** https://www.tymetro.com.tw/tymetro-new/en/index.php





The way to take Taipei metro to Taipei high speed rail station or Nangang high speed rail station