PROGRAM BOOK

제 22 회 고등과학원 전자구조계산학회

2026 년 7 월 9 일(목) - 7 월 10 일(금)

고등과학원 1 호관 대강당

초청연사

김인구 (삼성전자)
강승훈 (한국과학기술정보연구원)
고아라 (전남대)
김민재 (전북대)
김선우 (한양대)
김영재 (강원대)
김용훈 (한국과학기술원)
김충현 (아주대)
안성수 (한국과학기술원)
이광렬 (한국과학기술연구원)
이승준 (경희대)
서호성 (성균관대)
신용진 (단국대)
신승재 (울산과학기술원)

자문위원회

고아라 (전남대), 권영균(경희대), 김수란 (경북대), 김용현 (KAIST), 김용훈 (KAIST), 류훈 (금오공대), 심지훈 (포항공대), 유재준 (서울대), 이승미 (표준과학연구원), 이재광 (부산대), 정유성 (서울대), 최형준 (연세대), 한상수 (KIST), 한승우 (서울대)

조직위원회

김세중 (홍익대), 손영우 (KIAS), 최상국 (KIAS), 한명준 (KAIST)

연락처

류애리 (고등과학원) 이메일: arryu20@kias.re.kr

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7월 9일 (목) – 7월 10일 (금) · 고등과학원 전자구조계산학회

7월 9일 (목) — Day 1

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10:10 ~10:50	**고아라** · 전남대 *Active learning and data-driven approaches in Hamiltonian-diagonalization DMFT*
10:50 ~11:30	**안성수** · KAIST *Machine learning Hamiltonians with equivariant flow matching*
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Session 2	**Correlated Oxide Materials**
좌장: 김흥식 (KENTECH)	
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13:40 ~14:20	**김민재** · 전북대 *Orbital-selective electronic correlations and emergent phenomena in quantum materials*
14:20 ~15:00	☕ Coffee Break
Session 3	**Device Physics and Chemistry**
좌장: 최영우 (서강대)	
15:00 ~15:40	**이승준** · 경희대 *Electronic structure engineering in 2D materials through layer stacking: physics of band nesting and band alignment models*
15:40 ~16:20	**김영재** · 강원대 *Manipulation of quantum dynamics at extremely ultrafast time scales*
16:20 ~17:00	**신승재** · UNIST *Constant potential electrochemistry modelling in atomic scale*
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7월 10일 (금) — Day 2

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좌장: 박진수 (POSTECH)	
11:20 ~12:00	**신용진** · 단국대 *Discovery of ferroic properties in oxygen-deficient perovskites with long-range vacancy orderings*
12:00 ~12:40	**김선우** · 한양대 Toward a Predictive Theory of Charge Density Waves in Kagome Metals
12:40 ~14:00	🍱 점심식사
Session 6	**Spin Physics and Quantum Information**
좌장: 진호섭 (UNIST)	
14:00 ~14:40	**서호성** · 성균관대 *First-principles investigations of spin qubit decoherence in two-dimensional crystalline materials*
14:40 ~15:20	**강승훈** · KISTI *Magnetic and crystal symmetry control on spin Hall conductivity in altermagnets*

POSTER LIST

1. 포스터 발표자 이름, 포스터 제목
2. 포스터 발표자 이름, 포스터 제목
3. 포스터 발표자 이름, 포스터 제목
4. 포스터 발표자 이름, 포스터 제목

POSTER LIST

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2. 포스터 발표자 이름, 포스터 제목
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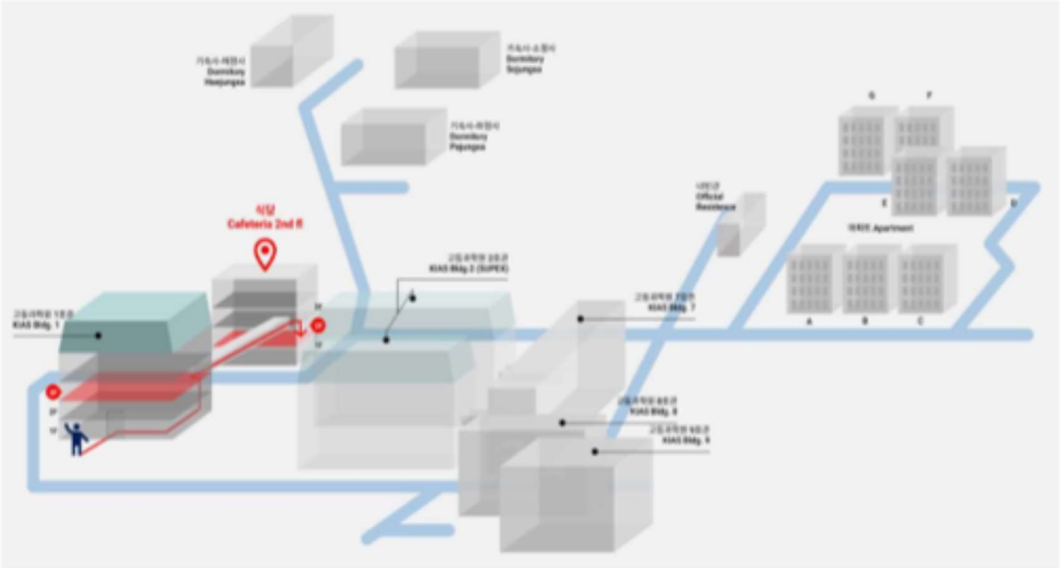
4. 포스터 발표자 이름, 포스터 제목

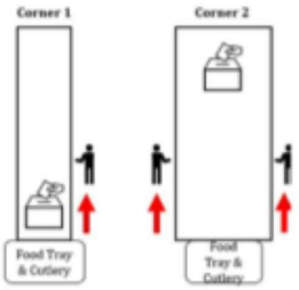
Bldg.1 to Cafeteria

1. Go downstairs to the 3rd floor of the main building(Bldg.1).
2. Use the passageway that connects the buildings. Just go straight forward and if you see Woori-Bank, it means that you arrived at the student union building 3rd floor correctly.
3. Go downstairs one more time. The cafeteria is one the 2nd floor of the student union building.

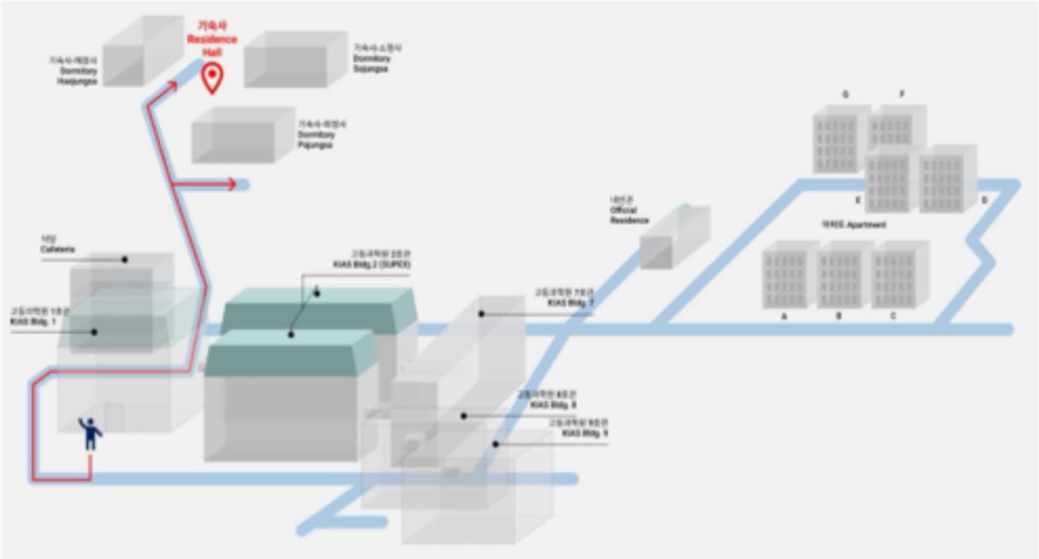


Lunch Coupon Usage

- You can pick up lunch coupons at the reception desk in front of the 1503 seminar room.
- These coupons can be used at the KIAS cafeteria only during lunch time (12:00~13:00).
- Today's menu is displayed outside the cafeteria and each corner has different menu. Please choose one.
- Please put the lunch coupon inside the transparent ticket box. Box location is different by Corners. (Please refer to the image)



Bldg.1 to Residence Hall



Transportation

Bus – 201, 273

- Get off at 'KAIST /Hong-neung Elementary School'.

Metro – line no.1

- Get off at 'Cheongnyangni' or 'Hoegi' Station.

From Hoegi Station

1. From exit No. 1, turn left and follow the sidewalk on the right until you reach the intersection and crosswalk.
2. Cross the street and turn right.
3. Go straight until you see the bus stop.
4. Take No.273 and get off at 'KAIST /Hong-neung Elementary School'.

From Cheongnyangni Station

1. When you get out through exit No. 2, ignore the bus stop you see right away and follow the way without making turns until you see another bus stop.
2. Take No. 201 and get off at 'Hong-neung Elementary School' bus stop.
3. You will see KIAS(KAIST campus) across the street.

ABSTRACTS OF INVITED TALKS

Talk No.1

Scientific Communication in the Future AI-Dominated Era

Kwang-Ryeol Lee[1]

[1]*Comptutational Science Research Center, Korea Institute of Science and Technology, Seoul, Korea*

As we are witnessing today, the term "AI transformation" is emerging beyond "digital transformation" across many fields of science and technology. Significant changes have occurred as AI and machine learning technologies are actively utilized in various scientific domains. In relation to the theme of this symposium, considering the transferability and accuracy of machine learning potentials, there are even debatable predictions that first-principles calculations will eventually be replaced by this technology. Whether we want it or not, scientific and technological research is likely to evolve in a very different way in the future.

In this new era of scientific research, the exchange of data itself will play a crucial role. From this perspective, the current system for exchanging scientific and technological achievements—where research data is compiled and disseminated in the form of academic papers—is highly inefficient. This inefficiency stems from the current limitation of having to communicate through human language systems. Consequently, we go through a redundant process where researchers' data is converted into human-readable information, only to be converted back into machine-readable data. In an AI-transformed future, it will be much more efficient for machines to directly recognize and interpret the raw data to generate knowledge, which can then be exchanged in the form of another data.

This presentation will discuss data schemas and vocabulary standardization as the future language for scientific exchange. In particular, it will explain the concept of the data language system being developed in the field of materials science, highlighting past achievements in standardization and outlining future challenges.

Talk No.2

Active Learning and Data-Driven Approaches in Hamiltonian-Diagonalization DMFT

Ara Go[1]

[1]*Department of Physics, Chonnam National University*

Dynamical mean-field theory (DMFT) combined with density functional theory has become a standard framework for studying correlated materials, but Hamiltonian-diagonalization–based impurity solvers still face practical limitations. Two issues are particularly relevant in realistic calculations: the rapid growth of the many-body Hilbert space and the numerical difficulty of fitting a continuous hybridization function with a finite bath. In this talk, I will discuss recent work addressing these problems by incorporating simple machine-learning–based strategies into existing many-body workflows. The first part introduces an active-learning–based truncation configuration interaction (ATCI) scheme for quantum impurity models. By iteratively identifying important determinants during the diagonalization procedure, the method constructs a compact Hilbert space while maintaining the accuracy expected from Hamiltonian-diagonalization approaches.

The second part concerns the bath discretization step in DMFT. Instead of solving the bath fitting problem from scratch at every iteration, we formulate it as a data-driven regression task and use a model trained on physically motivated tight-binding systems to provide good initial bath parameters. This significantly stabilizes and accelerates the fitting procedure without changing the underlying DMFT algorithm. The overall aim is not to replace standard many-body techniques, but to show that relatively modest machine-learning components can be used to reduce computational overhead in practical DMFT calculations. The talk will focus on the algorithmic ideas and their possible role in future electronic-structure workflows.

Talk No.3

Machine Learning Hamiltonians with Equivariant Flow Matching

Sungsoo Ahn[1]

[1]*KAIST, Graduate School of AI*

Machine learning interatomic potentials (MLIPs) have become a standard tool for fast energy and force prediction, but they do not provide access to electronic-structure quantities such as electron densities and orbital energies. Machine learning Hamiltonian (MLH) models offer an alternative: by predicting the Kohn-Sham Hamiltonian directly from molecular geometry, one can obtain energies, forces, and electronic-structure information simultaneously. A natural question is whether MLH models can match the energy-force accuracy that MLIPs already achieve. In this talk, I present a benchmark that computes energies and forces directly from predicted Hamiltonians and show that the answer is yes. Our model QHFlow2 is the first Hamiltonian predictor to reach MLIP-level force accuracy on MD17/rMD17 while achieving up to 20× lower energy error than NequIP, and reduces energy error by up to 20× compared to MACE on QH9. I also demonstrate consistent scaling behavior with model size and training data, and show that predicted Hamiltonians can accelerate SCF convergence by roughly 50%. These results suggest that MLH models are a promising direction for atomistic simulations where both physical accuracy and electronic-structure access are needed.

Talk No.4

From Jahn-Teller Distortions to Spin-Orbital Entanglement: Pathways to Mott Metal-Insulator

Choong Hyun Kim[1]

[1]*Department of Physics, Ajou University, Suwon, Republic of Korea*

Mott metal-insulator transition (Mott MIT) is one of the most prominent emergent phenomena in strongly correlated systems. Unlike conventional band insulators, Mott MIT arises from the interplay of Coulomb interaction, spin-orbit coupling, and lattice distortion, leading to novel phase transitions and electronic states. In multi-orbital systems, the lifting of orbital degeneracy plays a crucial role in determining the MIT. This can be driven by Jahn-Teller distortion, spin-orbit coupling, or a complex interplay of Hund's coupling and Coulomb U, which can either compete or cooperate in shaping the phase transition. In this presentation, we will discuss how key factors such as Coulomb U, lattice distortion, Hund's coupling, and spin-orbit coupling interact to produce intriguing phase diagrams in strongly correlated materials. Specifically, we will focus on two systems: the $CuAl_2O_4$ spinel, where strong spin-orbit coupling leads to a novel spin-orbital-entangled state, and monolayer $SrRuO_3$ thin films, where a new type of Jahn-Teller distortion drives the metal-insulator transition. These cases highlight the rich physics underlying Mott MIT and provide insights into the broader implications for correlated electron systems.

Talk No.5

Orbital-Selective Electronic Correlations and Emergent Phenomena in Quantum Materials

Minjae Kim[1]

[1] *Jeonbuk National University, Department of Semiconductor Science and Technology*

Quantum materials with strong electronic correlation have diverse emergent phenomena, including metal-insulator transition, magnetism, superconductivity, and topological phases. In many cases, emergent phenomena involve multi-orbitals of the correlated subshell, and, depending on crystalline symmetry and dimensionality, those orbitals experience orbitally-selective electronic correlation from Hubbard interactions and Hund's coupling [1].

In this talk, I discuss our recent progress in understanding the role of the orbital-selective electronic correlations for the emergent phenomena in quantum materials where the multi-orbital nature is essential. For quasi-two-dimensional ruthenate materials, the orbital-selective electronic correlations inherit the emergence of magnetism and the metal-insulator transition [2,3,4]. For the iron-based superconductor of $FeSe_{1-x}Te_x$, the strong orbital-selective electronic correlations govern the topological transition connected to the emergence of the topological superconductivity [5,6]. For atomically thin $LaNiO_3$ films under compressive strain, the emergence of an orbital-selective Mott transition is demonstrated, where strong spin fluctuations in the localized orbital suggest an intriguing opportunity to engineer new emergent phases [7]. These progresses imply that orbital-selective electronic correlations have a pivotal role in controlling the emergent phenomena in various quantum materials.

[1] A. Georges, L. Medici, J. Mravlje, Annu. Rev. Condens. Matter Phys. 4, 137-178 (2021)
[2] M. Kim, C.-J. Kang et al., Phys. Rev. B 106, L201103 (2022)
[3] S. G. Jeong, M. Kim, J. Y. Oh et al., Appl. Phys. Rev. 12, 041406 (2025)
[4] J. Kim et al., Nano Lett. 26, 395-400 (2026)
[5] M. Kim et al., Phys. Rev. Lett. 132, 136504 (2024)
[6] Y. Kim et al., arXiv:2507.17656
[7] B. Sohn, M. Kim, S. Lee et al., Phys. Rev. Res. 7, 043132 (2025)

Talk No.6

Electronic Structure Engineering in 2D Materials through Layer Stacking: Physics of Band Nesting and Band Alignment Models

Seungjun Lee[1]

[1]*Department of Applied Physics, Kyung Hee University.*

The interlayer interaction and layer stacking in van der Waals (vdW) materials provides a wide degree of freedom for tailoring their electronic structures. In this talk, I discuss how layer stacking controls the electronic structures of both vdW homo- and hetero-bilayers, offering a pathway to optimize future optoelectronic and nanoelectronic applications.

We first discuss the achievement of near-perfect light absorption at room temperature using only two or three atomic layers of transition metal dichalcogenide (TMD) homobilayers by optimizing layer stacking and band nesting. Our theoretical calculations confirm that when TMDs are stacked in a configuration where interlayer coupling is minimized, the system offers optimal band nesting. We demonstrate two feasible routes to controlling this interlayer coupling: twisted TMD bilayers and TMD/buffer-layer/TMD trilayer heterostructures. These theoretical predictions are clearly verified by follow-up experimental demonstrations. [1]

Second, we transition to the broader challenge of interfacial design by vdW heterostructures (vdWHs) and discuss a universal band alignment model. Based on first-principles calculations for approximately ~10^3 vdWHs, we introduce a generalized linear response (gLR) model that that incorporates interfacial charge spillage dipoles through a quantum capacitance term. With only two intuitive input parameters, the charge neutrality level offset and the sum of the isolated-layer bandgaps, the gLR reproduces density functional theory (DFT) band alignments with high accuracy ($r^2 \sim 0.9$) across type-I, -II, and -III stackings. Our model is further validated through machine learning analysis, confirming that these physical input features play a pivotal role in the band alignment of vdWHs. [2]

[1] S. Lee et al., *Nature communications* **14** (1), 3889 (2023)
[2] S. Lee et al., *ACS nano* **19** (43), 37749-37757 (2025)

Talk No.7

Manipulation of quantum dynamics at extremely ultrafast time scales

Youngjae Kim[1,2]

[1] *Department of Semiconductor Physics, Kangwon National University, Chuncheon 24341, Republic of Korea*

2 School of Physics, Korea Institute for Advanced Study (KIAS), Seoul 02455, Korea

Manipulation of quantum dynamics at extremely ultrafast time scales is a key challenge for next-generation electronic and valleytronic technologies, where device performance is fundamentally limited by intrinsic material properties. In this talk, I show that quantum geometric semimetals, such as quadratic band touching systems and singular flat bands, enable an unprecedented regime of ultrafast charge dynamics. In these systems, an electric current is generated instantaneously when a bias field is applied, reaching a steady value within only a few femtoseconds and outperforming conventional metals, semiconductors, and graphene. This behavior originates from interband quantum dynamics governed by the quantum distance, together with a finite density of states at the band-touching point. I then demonstrate how light can be used to manipulate quantum dynamics in momentum space on comparable ultrafast time scales. By engineering light-matter interactions, valley degrees of freedom can be selectively controlled beyond conventional approaches limited to specific valleys. This all-optical control enables high-fidelity manipulation of valley populations across an exceptionally broad frequency range, from terahertz to petahertz. Together, these results establish quantum geometry and tailored light fields as powerful tools for controlling charge and valley dynamics at the ultimate speed limits of condensed-matter systems.

Talk No.8

Constant Potential Electrochemistry Modelling in Atomic Scale

Seung-Jae Shin[1]

[1] *School of Energy and Chemical Engineering, UNIST*

Theoretical frameworks have given a general guideline to electrochemists for understanding the multiscale nature of electrochemical reactions. The Nernst equation, Butler-Volmer equation, and Nernst-Planck equation are the major frameworks to understand thermodynamics, kinetics, and transport phenomena. However, these key theories are not efficient enough to figure out every detail with the development of rapid nanotechnologies, the enormously expanded material space, different cell configurations, and versatile reactions.

Computational electrochemistry investigates electrochemical phenomena, including the interface, charge transfer, and mass transport. It can effectively address many intriguing questions with the help of different levels of theories and computational approaches.

Atomic-scale computational chemistry has gained attention since Professor Nørskov successfully explained the 'origin of overpotential' at different oxide materials for oxygen evolution reactions. After this theory, a.k.a., d-band theory, the computational electrochemistry in atomic resolution has been widely developed by many theoretical electrochemistry groups worldwide.

In this talk, I will talk about the development of modelling electrochemical system at constant potential including utilisation of machine learning potential. Implementation of computational potentiostat into the QM/ML framework will be mainly discussed.

Talk No.9

Machine Learning and Human Learning of Local Chemical Bonding Characters

Ryong-Gyu Lee and Yong-Hoon Kim

School of Electrical Engineering, Korea Advanced Institute of Science and Technology (KAIST), Daejeon, Korea

The self-consistent field (SCF) density functional theory (DFT) calculation relies on the idea that the ground-state electron density encodes the essential physics of chemical bonding, yet extracting and utilizing that bonding information efficiently remains a central challenge in electronic structure theory [1].

In this presentation, I will first discuss the DeepSCF machine learning framework, which learns the mapping from the sum of neutral atomic densities to the converged self-consistent density using a three-dimensional U-Net convolutional neural network [2]. By targeting the residual density $\delta\rho$ rather than the total density itself, DeepSCF is trained to recognize the spatial signatures of local chemical bonding, revealing how the nearsightedness of electronic structure can be naturally represented through the locality of machine learning models.

Looking beyond density prediction, I will further discuss our ongoing effort toward the development of a density functional exchange-correlation formalism that identifies local bonding characters directly in real space and applies a local self-interaction correction according to a quasiparticle-total energy consistency (QTC) principle [3,4]. Taken together, we emphasize that local chemical bonding character is the essential ingredient that both machine learning and human reasoning converge upon when seeking to improve the accuracy and efficiency of DFT.

References

[1] J. C. Slater, *The Self-Consistent Field for Molecules and Solids: Quantum Theory of Molecules and Solids, Vol. 4* (McGraw-Hill, New York 1974)).
[2] R.G. Lee and Y.-H. Kim, npj Comput. Mater. **10**, 248 (2024).
[3] R.G. Lee and Y.-H. Kim (in preparation).
[4] Y.-H. Kim, M. Städele, R. M. Martin, Phys. Rev. A **60**, 3633 (1999).

Talk No.10

Very-Large-Scale Density Functional Theory on Massively Parallel GPUs

Inkoo Kim

CSE Team, Semiconductor R&D Center, Samsung Electronics

Modern graphics processing units (GPUs) provide an unprecedented level of computing power, enabling significant advancements in quantum chemistry. In this talk, I will present a high-performance multi-GPU implementation of the Kohn–Sham density functional theory (DFT) and time-dependent DFT (TDDFT), along with their analytical nuclear gradients. The discussion will focus on algorithms optimized for efficient Fock matrix construction on massively parallel systems, leveraging multiple parallel models (MPI, OpenMP and CUDA) in tandem to achieve optimal scalability with increasing material size, considerably reducing computational time. To illustrate the effectiveness of this approach, I will present a benchmark TDDFT study on a biological protein consisting of 4,353 atoms with 40,518 Gaussian-type atomic orbitals, performed at the range-separated hybrid GGA level of theory. This study demonstrates favorable parallel efficiencies, with >70% efficiency on up to 64 GPUs and approximately 30% with 256 GPUs, using a high-speed distributed system equipped with the state-of-the-art GPUs. These results highlight the potential of modern high-performance computing systems to tackle very-large-scale quantum chemical simulations efficiently.

Talk No.11

Discovery of ferroic properties in oxygen-deficient perovskites with long-range vacancy orderings

Yongjin Shin[1]

[1]*Department of Semiconductor Convergence Engineering, Dankook University, Yongin-si, Gyeonggi-do, South Korea*

Transition metal oxides offer a rich platform for discovering emergent properties through sensitive coupling between charge, spin, orbital, and lattice degrees of freedom. Using first-principles calculations, we demonstrate various emergent properties stabilized in oxygen-deficient perovskites. First, we establish a simple structural descriptor to predict distortive behavior in brownmillerites with $ABO_{2.5}$ chemistry. The brownmillerite structure is a perovskite derivative where ordered oxygen vacancies convert half of the octahedral units into tetrahedral units, which exhibit exotic distortions not captured by the standard Goldschmidt tolerance factor. By surveying a range of $ABO_{2.5}$ brownmillerites, we show that a modified tolerance factor based solely on the *B*-ion radius in tetrahedral coordination effectively predicts these distortions. This refinement is justified by the fact that octahedral sites relax readily under Imma symmetry, leaving tetrahedral *B* cations as the key determinant of *A*-ion bond valence optimization. This descriptor serves as an a priori tool for guiding the discovery of ferroelectric materials in oxygen-deficient perovskites. Second, we predict that tunable ferroelectricity can be realized in oxide perovskites with ordered oxygen vacancies. Specifically, $R_{1/3}A_{2/3}FeO_{2.67}$ solids (where *R* is a rare-earth ion and *A* an alkaline-earth cation) exhibit stable polar phases with spontaneous polarization tunable by an appropriate choice of *R* and *A*. Together, these findings provide broad insights into the discovery of emergent properties within oxygen-deficient perovskites.

Talk No.12

Toward a Predictive Theory of Charge Density Waves in Kagome Metals

Sun-Woo Kim

Department of Physics, Hanyang University

Charge density waves (CDWs), periodic modulations of charge density arising from electron-electron interactions and/or electron-phonon coupling, have long been a central theme of modern condensed matter physics. They have been extensively studied in a wide range of materials, including transition metal dichalcogenides, cuprates, and nickelates. More recently, kagome metals have emerged as a particularly rich platform, hosting competing CDWs with unconventional properties such as time-reversal symmetry breaking and a strong interplay with superconductivity and nematicity.

In this talk, I will present our recent theoretical studies of diverse CDW phenomena in kagome metals. From bilayer kagome metals to recently discovered flat-band kagome superconductors, I will discuss how first-principles calculations provide microscopic insights into the emergence, competition, and tunability of CDW states in these materials, achieving quantitative agreement with experiments. Furthermore, I will show how these calculations uncover the microscopic electronic conditions required for time-reversal-symmetry-breaking loop-current order, providing new insights into its underlying mechanism.

References

[1] K. Wang, S. Chen, S.-W. Kim*, and B. Monserrat*, *Nat. Commun.* **15**, 10428 (2024).

[2] P. Král, J. N. Graham, V. Sazgari, …, S.-W. Kim* & Z. Guguchia*, *Nat. Commun.* **17**, 1121 (2026)

[3] H. Lim, K. Wang, B. Monserrat, and S.-W. Kim*, under revision in *JACS.*

[4] O. Gerguri, P. Král, M. Spitaler, …, S.-W. Kim* & Z. Guguchia*, arXiv:2603.27408

Talk No.13

First-principles investigations of spin qubit decoherence in two-dimensional crystalline materials

Hosung Seo[1,2]

[1]*Department of Quantum Information Engineering, Sungkyunkwan University, Suwon, Gyeonggi 16419, Republic of Korea*

[2]*SKKU Advanced Institute of Nanotechnology, Sungkyunkwan University, Suwon, Gyeonggi 16419, Republic of Korea*

Understanding and mitigating spin decoherence is a central challenge in solid-state quantum technologies. Two-dimensional crystalline materials such as hexagonal boron nitride (h-BN) and transition metal dichalcogenides (TMDCs) provide a promising platform for spin qubits, where atomic-scale thickness and host-dependent nuclear spin environments give rise to distinctive coherence phenomena. Their compatibility with electrostatic gating and van der Waals heterostructures further enables attractive routes toward quantum device integration. Yet, the microscopic origins of spin coherence in these atomically thin systems remain insufficiently understood. In this talk, we present a first-principles computational framework that integrates hybrid density functional theory (DFT) with quantum many-body spin dynamics simulations based on the cluster correlation expansion (CCE) method to quantitatively predict spin decoherence times in realistic material environments. For h-BN, we discuss the decoherence of boron vacancy centers [1] and carbon-related defects [2] embedded in dense nuclear spin baths with varying isotopic compositions. We identify magnetic-field-dependent transitions in the dominant decoherence mechanisms, distinguishing regimes governed by independent nuclear spin dynamics from those dominated by pairwise flip-flop processes. For TMDCs, I show how the interplay among dilute yet high-spin nuclear species, defect-specific hyperfine interactions, and quadrupolar effects leads to unconventional decoherence behavior, including early coherence collapse (ECC) driven by single-nuclear-spin dynamics [3]. Together, these studies establish a unified, materials-specific understanding of spin decoherence in 2D crystalline hosts. The presented first-principles framework provides predictive guidelines for defect identification, isotopic engineering, and magnetic-field optimization, accelerating the development of scalable 2D quantum sensing and quantum information platforms.

Reference:

[1] J. Lee, H. Kim, H. Park, and H. Seo, Advanced Functional Materials, e11274 (2025).
[2] H. Kim, J. Lee, H. Park, and H. Seo, in preparation (2026).
[3] T. Park, J. Lee, H. Park, and H. Seo, to be submitted (2026).

Talk No.14

Magnetic and Crystal Symmetry Control on Spin Hall Conductivity in Altermagnets

Seoung-Hun Kang

Korea Institute of Science and Technology Information

Altermagnets can efficiently convert charge current into spin current while maintaining almost zero net magnetization. However, the full spin Hall conductivity (SHC) tensor is hard to predict because crystal and magnetic symmetries can allow or forbid different tensor components and can produce "unusual" signals. In this talk, we present a symmetry-based method that splits SHC in the Kubo formula into a time-reversal-even part (Fermi-sea) and a time-reversal-odd part (Fermi-surface), and we derive clear rules that include antiunitary symmetries like T_g as well as (non)symmorphic operations. With this, we can directly tell which SHC components are allowed, which are blocked, and which appear only when magnetic order lowers the symmetry.

We apply these rules to rutile RuO_2, CrSb, and MnTe using first-principles calculations with spin–orbit coupling and Wannier-based interpolation. We show that some "unconventional" SHC can come from a simple choice of coordinate frame, while other parts are truly intrinsic and are turned on by the easy-axis direction that changes the magnetic symmetry. We also map how the SHC changes with direction, which is important for spin–orbit-torque setups. Because the SHC picture for bulk RuO_2 depends on its debated magnetic ground state, we add a high-accuracy many-body energy test that helps reduce the gap between experiment and standard theory, thereby making the RuO_2 analysis more consistent.

ABSTRACTS OF POSTERS

Poster No.1

Statistical Accessibility of Fluorite-Based HfO_2 and ZrO_2 Polymorphs from Exhaustive Configuration Sampling

Dohyun Kim[1,2], Taeyoung Jeong[1,2], Seungjae Yoon[1,2], Yunjae Kim[1,2] and Jung-Hae Choi[1]

[1]*Electronic and Hybrid Materials Research Center, Korea Institute of Science and Technology, Seoul 02792, Korea*

[2]*Department of Materials Science and Engineering, and Inter-University Semiconductor Research Center, Seoul National University, Seoul 08826, Korea*

A fluorite structure serves as the structural framework for most polymorphs of hafnium oxide (HfO_2) and zirconium oxide (ZrO_2). In the fluorite structure, cations occupy the fcc lattice and anions fill the tetrahedral sites. The anions can either remain at the centers of tetrahedral sites to be 4-fold coordinated to neighboring cations, or be displaced toward a tetrahedral vertex to become 3-fold coordinated. The configuration of these displacements distinguishes each polymorph. This study exhaustively examines all possible configurations of the eight anions in the fcc unit cell. Structural relaxations are performed on all 61,781 physically allowed configurations, with different choices of cations (Hf and Zr) and exchange-correlation functionals (PBE, PBEsol, and LDA). The resulting potential energy surface (PES) is partitioned into basins of attraction, and exhaustive configuration sampling enables the estimation of PES geometry and basin sizes. Counting the number of configurations that relaxed into each polymorph provides a statistical measure of polymorph accessibility beyond energetic stability alone. While the ground monoclinic mI phase dominates, the experimentally observed stabilization of the polar orthorhombic oIII phase and the stronger preference of ZrO_2 toward the tetragonal tI phase can be explained. The LDA calculations are more appropriate for the HfO_2 and ZrO_2 systems. On the other hand, PBE calculations for HfO_2 over-stabilize larger-volume structures, leading to TiO_2-like polymorphs such as rutile and anatase. These phases can also be interpreted within the fluorite-based structural framework, providing a unified description of Group 4 dioxide polymorphs.

Poster No.2

Dielectric Responses and Phase Stability at Finite Temperatures Investigated using a Universal Machine Learning Interatomic Potential

Akihiro Nagoya

Matlantis Corporation, Japan

Predicting the dielectric response and structural stability of functional materials at finite temperatures is critical for the development of advanced electronic devices. In particular, for ferroelectric materials, capturing both the temperature-dependent dielectric response and their phase stability is indispensable for understanding their functional behavior. While first-principles molecular dynamics (MD) provides fundamental microscopic insights, the high computational cost restricts its applicability to small system sizes and short timescales, rendering it insufficient for studying complex phenomena such as strongly anharmonic behavior and phase transitions.

In this study, we combine density functional theory (DFT)-based electronic structure analyses with PreFerred Potential (PFP), a universal machine learning interatomic potential (uMLIP), to accelerate the investigation of dielectric and ferroelectric materials. Our approach leverages the high-fidelity predictive power of MLIPs to perform large-scale MD simulations, while DFT is utilized to provide accurate electronic properties.

To address the requirements of dielectric and structural evaluation, we first use Green-Kubo (GK) analysis to compute the frequency-dependent dielectric function. We utilize DFT to compute Born effective charge (BEC) tensors; by treating these BECs as constant effective charges during MD trajectories, the dielectric functions are evaluated. While this workflow successfully predicts the dielectric functions of simple paraelectric materials in agreement with reported experimental data, some deviations are observed for ferroelectric materials, where complex phase stability is involved. To address this sensitivity in ferroelectric systems, we integrate crystal structure prediction (CSP) to evaluate the thermodynamic stability and convex hulls of these complex phases at finite temperatures. Our results demonstrate that this combination of uMLIP-MD, crystal structure prediction, and complementary DFT calculations provides a robust framework for analyzing complex dielectric materials, bridging the gap between atomistic simulations and experimental observations.

Poster No.3

Phase transition of CoPS3 under pressure

CHOI Seong Jae, KIM Heung-Sik

Interdisciplinary Program in Earth Environmental System Science & Engineering,, Kangwon National University

Department of Energy Engineering, Korea Institute of Energy Technology, Naju-si, 58330

Tricobalt trisulfide (CoPS3) undergoes pronounced pressure-driven structural and electronic evolution. Using first-principles electronic-structure and phonon calculations, we track the orbital character of Co states and identify two distinct metastable states accessible at the same pressure, reflecting pressure-path dependence. Experimentally, $CoPS_3$ exhibits an insulator–metal transition near 8 GPa, while our calculations predict band-gap closure around 6 GPa. With further compression, interlayer P–P orbital overlap emerges near 12 GPa, and the magnetic moment per Co collapses to zero by ~16 GPa. We also find a marked hysteresis: under increasing pressure the P-31m phase is stable around 8 GPa, whereas on decompression the system favors a transition to C2/m with lower enthalpy and finite magnetization. Phonon dispersions reveal clear pressure-induced mode splitting consistent with the observed structural transitions, providing microscopic support for the phase sequence. Extending the analysis to multiple candidate space groups further indicates additional pressure-induced transitions, consistent with experimental reports. In parallel, we reinterpret the reported P-3$\bar{1}$m structure within a distorted framework, where tilted P–P dimers induce local symmetry lowering and enable competing metastable configurations. A distorted C2/m phase emerges as the most stable state at low pressure, consistent with the observed irreversibility. The system follows distinct pathways under compression and decompression, giving rise to hysteresis. With increasing pressure, the distorted C2/m phase becomes unstable and evolves toward a P-3$\bar{1}$m-related structure, while symmetry lowering persists in the high-pressure regime.

Poster No.4

Diverse spin textures in coplanar compensated magnets

Sangyun Lee[†], Junhee Shin[†], Hogyun Jeong[*] & Hosub Jin[*]

Department of Physics, Ulsan National Institute of Science and Technology, Ulsan 44919, Korea

Distinct from conventional antiferromagnetism, altermagnetism hosts a unique spin texture in momentum space, opening new possibilities for spintronic applications. Here, we propose a way to combine several spin textures in noncollinear compensated magnetic systems. Using one-dimensional helimagnetic chains as a building block, we show that a (p+f)-wave spin texture in a three-dimensional hexagonal lattice, which blends in-plane f-wave and out-of-plane p-wave spin-momentum locking. First-principles calculations confirm the existence of the (p+f)-wave spin texture in a real material system. Furthermore, additional spin canting induces even-parity mixing. Our results establish noncollinear compensated magnets as an interesting platform for complex spin-momentum locking beyond single-parity spin textures.

Poster No.5

Singular Flat Bands and Coexisting Boundary States in a Two-Dimensional SSH Lattice

Myung-Chul Jung[1,2], Hee Chul Park[3], Jung-Wan Ryu[4], Jun-Won Rhim[5], and Nojoon Myoung[1,2]

[1] *Department of Physics Education, Chosun University, Gwangju, 61452, Republic of Korea*

[2] *Institute of Well-Aging Medicare & Chosun University G-LAMP Project Group, Chosun University, Gwangju, 61452, Republic of Korea*

[3] *Department of Physics, Pukyong National University, Busan 48513, Republic of Korea*

[4] *Center for Theoretical Physics of Complex Systems, Institute for Basic Science, Daejeon 34126, Republic of Korea*

[5] *Department of Physics, Ajou University, Suwon 16499, Republic of Korea*

Flat bands are characterized by dispersionless energy in momentum space, resulting in quenched kinetic energy and enhanced interaction effects that can give rise to exotic quantum phases such as superconductivity and ferromagnetism. The localized nature of flat-band states is described by compact localized states (CLSs), which arise from destructive interference of hopping processes[1,2]. When a flat band touches a dispersive band at certain momenta, however, the Bloch wave function becomes singular, preventing CLSs alone from forming a complete basis of the flat-band Hilbert space. In this case, additional extended eigenstates, known as non-contractible loop states (NLSs), are required. In finite systems, these NLSs manifest as robust boundary modes (RBMs), providing a direct signature of the singular flat band[1-3].

Here, we propose a two-dimensional Su-Schrieffer-Heeger (SSH) lattice with intra-cell next-nearest-neighbor hopping that realizes a singular flat band. For appropriate hopping parameters, finite lattices exhibit RBMs, confirming the singular character of the flat band. Remarkably, these RBMs coexist with conventional topological edge states, demonstrating the simultaneous presence of geometric topology associated with flat-band singularity and band topology protected by lattice symmetry. The topological properties are characterized by a quantized Zak phase arising from parity symmetry. Furthermore, by tuning onsite energies and hopping amplitudes, the system undergoes topological phase transitions while enabling control over the singularity of the flat band.

Our results establish a versatile platform for investigating the interplay between flat-band geometry and band topology, providing new opportunities for flat-band engineering and future quantum-device applications.

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Poster No.6

Electronic structures of Cd doped ZnS; A First-Principles Study

Rsool Shujaat and Junhyeok Bang

Department of Physics, Chungbuk National University, Cheongju 28644, Republic of Korea

ZnS is a wide bandgap semiconductor with an experimental band gap of about (3.91) eV, making it relevant for optoelectronic, photocatalytic, and photovoltaic applications, although its large band gap restricts visible light absorption. In this study, $Cd_xZn_{1-x}S$ alloys are investigated over the full Cd concentration range, $0 \leq x \leq 1$, using first-principles DFT calculations. The calculations are performed within the LDA framework using Quantum ESPRESSO. ZnS Wurtzite ZnS is found to be more stable than the zinc blende phase, with cohesive energies of (-3.24) and (-2.41) eV/atom, respectively. Cd atoms were substituted at Zn sites in random and layer-by-layer configurations. At (x=0.062), both configurations show nearly identical formation energies, while for higher concentrations the random configuration is energetically more stable. The maximum difference occurs near (x=0.50), with an energy difference of about (0.628) eV/Cd. The calculated band gap decreases from (2.34) eV for ZnS to about (1.63) eV at Cd0.5Zn0.5S, indicating improved visible-light absorption and photocatalytic potential.

Poster No.7

Hybrid functional calculation of erbium and its complexes in silicon

Hyungwoo Lee[1], and Minseok Choi[1,2*]

[1]*Department of Physics, Inha university, Incheon 22212, Korea,*

[2]*Institute of Quantum science, Inha University, Incheon 22212, Korea*

Abstract:

Erbium has attracted attention for long-distance quantum communication because its optical transition $^4I_{13/2} \rightarrow {}^4I_{15/2}$ occurs at 1530 nm, within the telecom C band, enabling low-loss transmission through optical fibers. Several optically detected magnetic resonance (ODMR) experiments have reported optical inhomogeneous linewidths below 0.1 GHz, homogeneous linewidths of several tens of kHz, and Hahn-echo coherence times of 0.8 ms and 1.2 ms at ~ 11 mT. Despite these advantages, the stable configurations of the doped Er in Si and their microscopic properties remain unclear. In addition, undesirable effects such as Er segregation are reported to cause a low photon emission efficiency of ~1%. In this work, we performed hybrid functional calculation to investigate the doped Er in Si by evaluating the formation energy, migration barrier, and interaction with native defects. Our results can offer valuable insight into the microscopic picture of Er in silicon.

Acknowledgement:

This work was supported by the government of the Republic of Korea (MSIT) and the National Research Foundation of Korea (RS-2024-00442710, RS-2025-25443942, RS-2025-16068832). We also acknowledge the National Supercomputing Center with supercomputing resources including technical support (KSC-2025-CRE-0596).

Poster No.8

Type-Ⅱ multiferroicity in a van der Waals NiI_2 monolayer

Junhee Shin†, Sangyun Lee† & Hosub Jin*

Department of Physics, Ulsan National Institute of Science and Technology, Ulsan 44919, Korea

The NiI2 monolayer is a type-II multiferroic van der Waals material in which helical magnetic ordering breaks inversion symmetry, inducing ferroelectric polarization. In this study, we reveal that four-state degenerate ferroelectricity emerges from the tilted angle between the spin-rotating plane and the propagation vector in NiI2. Based on first-principles (DFT) calculations, the existence of four symmetry-related magnetic configurations is identified. Polarizations have both parallel and perpendicular components with respect to the propagation vector. These four degenerate magnetic configurations induce corresponding polarization states. Furthermore, the evolution of the polarizations with respect to the rotation of the spin-rotating plane follows a sinusoidal function x, y, and z components of the polarization. This behavior suggests the possibility of independent control over the two polarization components and extends beyond conventional two-stable ferroelectricity, enabling four-stable ferroelectricity and suggesting potential applications in multi-state functional devices.

Poster no.9

Machine Learning Interatomic Potential Approaches for High-Entropy NVP Cathode Materials

Wonjun Choi[1], Chan Woo Lee[2], Jong Min Yuk[1]

[1]Department of materials science and engineering, KAIST

[2]Department of energy and materials engineering, Dongguk university

Machine learning interatomic potentials (MLIPs) have enabled atomistic simulations with near-DFT accuracy and significantly reduced computational cost compared to conventional DFT. Universal MLIP models trained on large-scale, multi-fidelity datasets have shown strong transferability across diverse chemical systems, often without additional fine-tuning. However, their high predictive accuracy is generally achieved using large model architectures with numerous trainable parameters, resulting in increased inference time and limited efficiency for large-scale configurational screening.

To overcome this limitation, fine-tuning lightweight MLIP models for target material systems offers a practical strategy for balancing accuracy and computational efficiency. Instead of directly relying on computationally expensive universal models for repeated structural relaxation and sampling, a compact model can be adapted to the chemical and configurational space of high-entropy sodium vanadium phosphate (HE-NVP) cathodes using a limited but representative dataset. This approach reduces inference cost while retaining the essential accuracy required to describe the local atomic environments, transition-metal disorder, and Na-ion/vacancy configurations in HE-NVP systems.

In this work, relaxation-based and molecular-dynamics-based datasets are compared for fine-tuning lightweight MLIP models for HE-NVP cathodes. The relaxation-based dataset captures structural pathways during geometry optimization, while the MD-based dataset includes thermally perturbed configurations reflecting local atomic fluctuations. This comparison clarifies how dataset construction influences model accuracy, data efficiency, and computational cost in MLIP-assisted simulations of complex high-entropy cathode materials.

Poster No.10

Understanding Adsorption Properties of Alcohol Molecules in Zn–Siloxane Cluster-Based Metal–Organic Framework Using Machine-Learning Interatomic Potentials

Minhyeok Park[1] and Jung-Hoon Lee[1,2]

[1]KU-KIST Graduate School of Converging Science and Technology, Korea University, Seoul, Korea

[2]Computational Science Research Center, Korea Institute of Science and Technology (KIST), Seoul, Republic of Korea

Despite recent advances in the synthesis of Zn–siloxane-based metal–organic frameworks (MOFs), a comprehensive understanding of their gas adsorption properties remains lacking. The large primitive cell of this MOF, comprising 4,530 atoms, renders first-principles density functional theory (DFT) calculations computationally intractable, precluding direct atomistic insight into adsorption mechanisms at the molecular level. To overcome this limitation, we employ machine learning interatomic potentials (MLIPs) to systematically evaluate the adsorption energies of different alcohol molecules across distinct binding sites within the primitive cell of Zn–siloxane-based. Our MLIP calculations show that the oxygen site in the Zn-siloxane cluster serves as the dominant adsorption site for alcohol molecules. These findings offer atomistic-level insight into the selective adsorption behavior of alcohol molecules, providing a mechanistic foundation for the rational design of MOF-based separation processes. Furthermore, this work establishes MLIP as a powerful and efficient computational framework for probing the adsorption properties of structurally complex, large-scale MOF systems, paving the way for future investigations into dynamic adsorption processes and multi-component selectivity.

Poster No. 11

Feasibility of Realizing a Polar Metal by High-Concentration La Substitution into Ferroelectric $BaTiO_3$ Evaluated with the Universal Neural Network Potential PFP

Yuta Aoki

Matlantis Corporation

Elemental substitution is a powerful strategy for tailoring the electronic properties of a material and endowing it with new functionalities. In atomistic simulation, however, the number of symmetrically distinct dopant arrangements grows combinatorially with supercell size and dopant concentration, making an exhaustive first-principles evaluation of every configuration prohibitively expensive. The universal neural network potential PFP[1] removes this bottleneck, reproducing density-functional-theory-level accuracy while cutting the cost of each relaxation and energy evaluation by orders of magnitude, thereby enabling an exhaustive search over all symmetrically unique substituted structures.[2,3] As a test case to demonstrate an efficient screening of substituted structures at 0 K, we focus on polar metals — materials that sustain both metallic conduction and a polar (non-centrosymmetric) symmetry.[4,5] Because free carriers normally screen the dipoles that break inversion symmetry, this coexistence is rare and was long thought contradictory, yet it is of great interest: the broken inversion symmetry can enable nonlinear optical responses, unconventional superconductivity and spin transport useful for next-generation electronic and spintronic devices, provided the host can be made metallic while retaining its polar symmetry. One route to realize such materials is to dope a high concentration of carriers into a ferroelectric, which already possesses the required polar symmetry.[6] Such heavy doping may, however, collapse that symmetry, so the key question is how much dopant can be dissolved before the polar space group is lost.

We study $BaTiO_3$, a prototypical ferroelectric perovskite with a tetragonal polar structure. La was chosen as the dopant: its ionic radius is close to that of Ba, favouring Ba-site substitution, while La^{3+} (vs. Ba^{2+}) supplies carriers. Using MTCSP program,[7] we generated and relaxed all symmetrically unique $Ba_{1-x}La_xTiO_3$ configurations and tracked the space-group symmetry as a function of La content. We find that La can substitute the Ba site up to $x = 0.2$ while preserving the polar space-group symmetry; higher concentrations drive the structure toward the centrosymmetric $LaTiO_3$ structure and destroy the polarity. This result sets a concrete upper bound on the carrier concentration available in a polar-metallic $BaTiO_3$-based solid solution. Furthermore, this study demonstrates that an exhaustive, PFP-accelerated substituted-structure search can quantitatively assess polar-metal feasibility with a reasonable computational cost. The workflow, combining systematic configuration generation via MTCSP and high-throughput evaluation via PFP, transfers readily to other host–dopant systems, offering an efficient route to design a wide range of functionally substituted materials.

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Poster No.12

Wannier Hopping Changes and SOC-Driven Band Folding in CsV_3Sb_5: 1×1×1 vs 2×2×1 CDW

GO Myungjun[1], KIM heungsik[*1]
[1]Physics, Kangwon National University
[2]Department of Energy Engineering, KENTECH

Abstract:

By using the Maximally Localized Wannier Function (MLWF) method, we construct Wannier tight-binding (TB) models for the kagome metal CsV_3Sb_5 before and after the in-plane charge density wave (CDW) formation. Our TB parameters faithfully reproduce the DFT bands both in non-CDW and CDW phases. By systematically comparing the in-plane hopping amplitudes before and after the transition, we reveal how symmetry lowering lifts the degeneracy of equivalent hopping paths and quantify the magnitude of each change Δt. In parallel, we present consistent band-structure calculations with and without spin–orbit coupling (SOC) to disentangle SOC-induced splittings from CDW-induced band folding and gap opening. This analysis demonstrates that the CDW transition in CsV_3Sb_5 is accompanied by a profound reorganization of the in-plane bonding network, while SOC plays a decisive role in shaping the final reconstructed electronic structure.

Keywords:

CsV_3Sb_5, kagome, CDW, band reconstruction

Poster No.13

Adaptive Oxygen Sublattice in H-Ta_2O_5 Revealed by Machine-Learning Interatomic Potential Simulations

Seung-Bin Kwon, Kyu-Hyuk Park, Sung-Hoon Lee

Department of Applied Physics, Kyung Hee University, Yongin, Korea

Despite its widespread technological use, the crystal structure of Ta_2O_5 remains unresolved, particularly the oxygen sublattice of its high-temperature phase (H-Ta_2O_5). Resolving this ambiguity requires sampling a large oxygen configurational space in a long-period cell, which is impractical using first-principles calculations alone. Here, we combine a MACE machine-learning interatomic potential with first-principles validation to determine the stable structure and oxygen dynamics of H-Ta_2O_5. We find quasi-one-dimensional oxygen channels hosting multiple channel-confined configurations. Enumeration of these configurations reveals a family of nearly degenerate structures: 18 DFT-converged candidates span only 17.9 meV per formula unit. The lowest-energy member, the κ structure with space group No. 92, is dynamically stable. This shallow configurational landscape also gives rise to adaptive defect behavior: an oxygen vacancy introduced into a channel is collectively accommodated by the soft oxygen sublattice, delocalizing over ~60 Å and migrating with a barrier of only ~0.033 eV. These results establish a ground-state structural model for H-Ta_2O_5 and reveal an adaptive oxygen sublattice capable of channel-confined rearrangement and facile vacancy motion.

Poster No.14

Electronic Structure of Diamond Under Pressure

Hyeongi Kwon[1] and Minseok Choi [1,2]*

[1] *Department of Physics, Inha University, Incheon 22212, Korea*

[2] *Institute of Quantum Science, Inha university, Incheon 22212, Korea*

Quantum sensors based on NV centers in diamond are widely used to probe pressure-induced magnetic properties, such as the superconductivity of hydrides [1,2]. To correctly interpret these magnetic properties, it is essential to understand the stress response of the host diamond itself. Previous studies have shown that diamond exhibits behavior distinct from that of conventional semiconductors under applied stress [3,4]. In particular, experiments have demonstrated that the band gap of diamond increases with stress. In this study, we investigated pressure-induced changes in the band edges of diamond by analyzing deformation potentials using density functional theory calculations. Our results reproduce the experimentally observed increase in the band gap. We further find that the band-gap response depends on periodic trends across the elements and on the availability of unoccupied *d* states.

This work was supported by the government of the Republic of Korea (MSIT) and the National Research Foundation of Korea (RS-2024-00442710, RS-2025-25443942, RS-2025-16068832). We also acknowledge the National Supercomputing Center with supercomputing resources including technical support (KSC-2025-CRE-0596).

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Poster No.15

Filling-enforced topological semimetal phase in square-net material LaZnBi2: first-principles study

Mingeoung Kim[1] and Se Young Park[1, 2]

1. Department of physics, Soongsil University

2. Department of Physics and Origin of Matter and Evolution of Galaxies, Soongsil University, Seoul, 06978, Korea

We investigate the structural and electronic properties of $LaZnBi_2$. The system consists of the Bi-square net sandwiched by La layers with ZnBi spacer layers, having *p*-derived bands from the Bi-square net dominating the states around the Fermi energy. Depending on the configuration of the La atoms around the Bi square net, symmorphic *I4/mmm* and non-symmorphic *P4/nmm* phases can be stabilized. Using the first-principles density functional theory, we find that the total energy of the *P4/nm*m phase is lower than that of *I4/mmm*. Our band structure calculations show the nodal lines protected by the non-symmorphic symmetry of the *P4/nmm* space group that are maintained in the presence of the spin-orbit coupling. Combined with band-filling, the topologically protected band structures enforce the metallic phases. Our findings demonstrate the role of symmetry in determining the phase of matter, which can be applied to other square-net materials with non-symmorphic symmetry.

Poster No.16

Effective Interaction Model for Anisotropic Adatom Distributions on Black Phosphorus

Sangwan Kim, Seung-Hun Kang and Young-Kyun Kwon

Departments of Physics, Kyung Hee University, Seoul, Korea

Disordered dopants on crystalline substrates can give rise to electronic structures that are absent in conventional crystals, including a pseudogap accompanied by backward-bending band dispersion. Alkali metal adatoms deposited on black phosphorus provide a promising platform for investigating the microscopic origin of this phenomenon. Previous work has interpreted these observations using a single-site multiple-scattering model, in which resonance scattering from alkali metal ions produces quasi-bound states and renormalizes the electronic band dispersion.

However, this electronic picture still relies on the spatial distribution of adatoms as a key structural input, and the microscopic origin of that distribution remains insufficiently understood. The spatial arrangement of adatoms is governed not only by well-known interactions such as dipole-dipole repulsion and Friedel oscillations, but also by an experimentally observed deep attractive region along the armchair direction. This deep attractive region, which is not captured by existing structural models, promotes quasi-one-dimensional chain-like adatom arrangements and plays a critical role in shaping the overall adatom distribution.

To capture these distribution dependent features, we develop a simulation framework that incorporates the relevant interaction mechanisms. We employ simulated annealing on an effective potential energy landscape, including theoretical Friedel oscillation terms, to model adatom configurations on the BP surface. In addition, we perform density functional theory calculations to evaluate total energies as functions of interatomic distance and dopant concentration, allowing us to identify the microscopic interaction responsible for the deep attractive region. This study offers fundamental insight into the role of electronic interactions in dopant organization on anisotropic two-dimensional materials and presents a pathway for realistic modeling of disorder in quasi-two-dimensional systems.

Poster No.17

Ab Initio Study on Inhomogeneous Switching Pathway and Coercive Field of Wurtzite AlN

Yunjae Kim[1,2], Kun Hee Ye[1,2], Taeyoung Jeong[1,2], Seung Jae Yoon[1,2], Dohyun Kim[1,2], and Jung-Hae Choi[1,*]

[1]*Electronic and Hybrid Materials Research Center, Korea Institute of Science and Technology, Seoul 02792, Korea*

[2]*Department of Materials Science and Engineering and Inter-University Semiconductor Research Center, Seoul National University, Seoul 08826, Korea*

Ferroelectric materials have attracted significant attention as promising candidates for next-generation semiconductor devices owing to their remanent polarization (P_r), which can be retained even in the absence of an external electric field. In addition to P_r, the coercive field (E_c), defined as the electric field required to reverse the polarization state, is a key physical property governing the operation and reliability of ferroelectric devices. For wurtzite AlN-based ferroelectric materials, previous theoretical studies have mainly focused on homogeneous polarization switching based on Nudged Elastic Band (NEB) calculations [1, 2]. However, NEB typically constructs intermediate structures through linear interpolation between the initial and final polarization states, therefore cannot fully consider domain-mediated inhomogeneous switching (IS) processes. To overcome this discrepancy with experiments, this study systematically investigates an IS pathway in wurtzite AlN by employing domain-mediated structural models. During the IS process in wurtzite AlN, 60°, 120°, and 180° domain walls (DWs) are formed, and the angular dependence of the DW energy is systematically evaluated. The calculated DW energies increase with decreasing DW angle, indicating that minimizing the formation of 60° DWs is energetically favorable. Also, path-dependent DW surface area affects the energy of the DW structure. By incorporating the energetic stability of the DWs with the calculated kinetic barriers, the most favorable IS pathway is identified. Furthermore, by combining the predicted switching pathway with experimentally reported breakdown fields, the theoretical E_c of wurtzite AlN is also estimated with classical nucleation theory and the Vopsaroiu equation [3].

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Poster No.18

QTSpin: A Quantum Toolkit for Simulating Finite-Temperature Properties of Quantum Spin Systems

Taehyeon Kim and Ara Go*

Chonnam National University

We present QTSpin (Quantum Toolkit for Spin systems), a computational package for simulating quantum spin systems. QTSpin provides a flexible framework for constructing spin Hamiltonians from exchange interactions, long-range interactions, and external fields on lattices of arbitrary geometry. Within a single unified interface, the package combines three numerical methods, exact diagonalization (ED) for small systems together with the thermal pure quantum (TPQ) and finite-temperature Lanczos (FTL) methods for larger Hilbert spaces, and exploits symmetry sectors to reduce the computational cost. QTSpin computes thermodynamic properties such as the specific heat and susceptibility, the dynamical spin structure factor, and static properties including eigenstates and spin–spin correlations. As a benchmark, we apply QTSpin to the antiferromagnetic Heisenberg model on the triangular lattice, a geometrically frustrated quantum magnet, where comparing ED, TPQ, and FTL across temperatures and system sizes confirms that the three methods are mutually complementary.

*Corresponding author: arago@jnu.ac.kr

Poster No.19

Cavity-induced Ferroelectricity in SrTiO3 via Flexoelectric

Kim Hanbyul, Shin Dongbin

Department of Physics and Photon Sciences, GIST

We present a multiscale theoretical framework to elucidate the mechanism of cavity-induced ferroelectricity in quantum paraelectric $SrTiO_3$. Based on anharmonic potential energy surfaces extracted from density functional theory (DFT), we construct a microscopic QED Hamiltonian that couples the ferroelectric soft (FES) mode and lattice strain to a single cavity photon mode, incorporating flexoelectric interactions that break inversion symmetry under inhomogeneous strain. Quantum fluctuations of the FES mode and the cavity photon are treated within thermostatted ring-polymer molecular dynamics (TRPMD), capturing essential nuclear quantum effects including zero-point energy and tunneling. We show that the cavity photon field renormalizes the effective mass of the collective phonon mode, thereby suppressing quantum fluctuations and localizing the FES mode wavefunction. In inhomogeneous systems, this dynamical localization enhances ferroelectricity in regions with finite strain gradients via flexoelectric symmetry breaking. However, in a globally homogeneous system without any strain gradient, the cavity alone does not induce a ferroelectric transition. Furthermore, we demonstrate that the strength of the cavity-induced ferroelectric domains grows with increasing light–matter coupling, and that under strong coupling the system can access distinct metastable ferroelectric states selected stochastically by the collective mode dynamics. Our results establish that cavity quantum electrodynamics, combined with flexoelectric symmetry breaking, provides a viable mechanism for controlling ferroelectric phase transitions in quantum paraelectrics.

Poster No.20

A Generalized Framework for Evaluating Dzyaloshinskii–Moriya Interaction Beyond a Single Magnetic Configuration

Hyeong-Ryul Kim, Dameul Jeong and Young-Kyun Kwon*

Department of Physics Kyung Hee University

Noncollinear spin systems, including skyrmions, have emerged as promising candidates for next-generation spintronic applications. The Dzyaloshinskii–Moriya interaction (DMI) is one of the key interactions responsible for stabilizing these spin textures through spin–orbit coupling (SOC). Various density functional theory (DFT)-based approaches have been proposed to evaluate DMI in magnetic materials. However, the resulting DMI parameters generally depend on the magnetic configuration adopted in each calculation. This limitation becomes particularly significant in non-stoichiometric systems, where a unique ground-state magnetic configuration is often difficult to identify. To overcome this challenge, we propose a generalized framework for evaluating DMI beyond a single magnetic configuration. Using first-principles DFT calculations, we investigate the relationship between spin configurations and total energies for self-intercalated $Cr_{1+\delta}Te_2$ with different compositions. From these data, we determine a consistent set of DMI parameters that captures the overall magnetic behavior of the Cr–Te system. This framework provides a more reliable evaluation of DMI across the CrTe family and offers a generalized route for studying noncollinear magnetic systems.

Poster No. 21

Ferroelectric control of tunneling conductance in altermagnetic oxides

Keon Ho Park[1], Hyoung Joon Choi[2*], Se Young Park[1†]

[1]*Department of Physics and Origin of Matter and Evolution of Galaxies (OMEG) Institute, Soongsil University, Seoul 06978, Republic of Korea*

[2]*Department of Physics, Yonsei University, Seoul 03722, Republic of Korea*

Altermagnets are is a type of magnetic phase with zero net magnetization by symmetry but exhibiting spin-split bands without spin-orbit coupling. The band splitting leads to various applications, such as spin-filter devices, where the change in conductance is induced by flipping the relative altermagnetic spin splittings across the junction. Thus, identifying order parameters intimately coupled to the spin splitting is important. In this talk, we demonstrate that the altermagnetic spin splitting can be flipped by polarization switching of $AA'_2B_2O_7$-type Ruddlesden-Popper oxides. It is shown that the coupling between spin splitting and BO_6 octahedral tilts enables ferroelectric control of the spin splitting, as the polarization is driven by hybrid improper ferroelectricity. We examine two potential material systems and discuss properties leading to a large contrast in tunneling conductance, including the energy barriers, interface geometry, and tunneling conductance ratios.

[*]h.j.choi@yonsei.ac.kr [†]sp2829@ssu.ac.kr

Poster No.22

Ferroelectric control of tunneling conductance in altermagnetic oxides

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[*]h.j.choi@yonsei.ac.kr [†]sp2829@ssu.ac.kr

Poster No.23

Vacancy-Driven Local Motif Transformations and Hole-Capture Mechanism in Amorphous In-Ga-Zn-O

Sunho Park[1] and Young-Kyun Kwon[1,2,*]

[1]*Department of Physics and Research Institute for Basic Sciences, Kyung Hee University, Seoul*

[2]*Department of Information Display, Kyung Hee University, Seoul*

Amorphous In-Ga-Zn-O (a-IGZO) is a widely used oxide semiconductor for thin-film transistor applications, where oxygen vacancies and carrier trapping are considered key factors governing electrical instability under bias and illumination stress. In particular, the microscopic origin of hole trapping in the disordered amorphous network remains an important issue because local structural relaxation and charge traps are strongly coupled. In this work, we investigate the atomistic relaxation behavior of oxygen vacancies in a-IGZO using first-principles molecular dynamics simulations and local coordination analysis.

By analyzing neutral and charged vacancy configurations, we examine how vacancy-induced structural motifs evolve in time and how the local metal-oxygen network responds to charged states. The simulations show that oxygen-vacancy relaxation proceeds through cooperative bond rearrangements involving oxygen redistribution around Ga, In, and Zn centers, rather than through a simple local relaxation toward the vacancy site. In charged configurations, under-coordinated oxygen atoms near over-coordinated metal sites become structurally labile and can approach neighboring oxygen atoms, leading to the formation of peroxide-like O–O dimers. This structural transformation is accompanied by the depopulation of O–O antibonding states, which stabilizes the peroxide bond and provides a microscopic hole-capture mechanism. Our results suggest that hole trapping in a-IGZO can be mediated by charge-induced local network reconstruction near oxygen vacancies, where peroxide formation serves as a metastable structural response to excess holes. These findings provide atomistic insight into the interplay between oxygen-vacancy disorder, local coordination changes, and charge-trapping processes in amorphous oxide semiconductors.

Poster No.24

First-principles study on electronic and transport properties of 1D single-chain heterojunctions

Seongbin Park, Young Woo Choi

Department of Physics, Sogang University, Seoul, Republic of Korea

Encapsulation inside carbon nanotubes has emerged as a robust route to realize true one-dimensional crystals, providing a platform in which low-dimensional bonding, band structure, and quantum transport can be studied at the atomic level. In this work, we study a 1D heterojunction formed by inserting a discrete Hf_2Se_9 molecule between two metallic VSe_3 single chains, where the resulting VSe_3–Hf_2Se_9–VSe_3 structure realizes a prototypical metal chain–molecule–metal chain junction. Using density-functional theory together with non-equilibrium Green's function calculations, we determine the relaxed interface structure, band alignment and interfacial charge transfer, projected density of states, transmission spectrum, and zero-bias conductance, and clarify the role of terminal-Se dangling bonds and their hydrogen passivation in stabilizing the physical contact geometry. The results establish a microscopic basis for designing atomically defined 1D molecular junctions and 1D metal–molecule superlattices.

Poster No.25

Modeling of Polarons in $BiVO_4$: Benchmarking DFT+*U* against HSE06

Seyeon Park and Bongjae Kim

Department of Physics, Kyungpook National University, Daegu 41566, Korea

A polaron is formed when an excess electron or hole is localized, coupled with lattice distortion. Accurately describing these localized states requires computational methods that properly account for electron-phonon interactions. $BiVO_4$ is a representative water-splitting photocatalyst whose performance is strongly dictated by such polaron states. In our previous work, we employed the HSE06 hybrid functional to identify multi-centered electron and hole polarons in $BiVO_4$.

While HSE06 provides an accurate description of polaron localization, its high computational cost motivates the employment of the more efficient DFT+*U* approach. In this work, we investigate electron- and hole-doped $BiVO_4$ using DFT+*U* and systematically examine the effect of the Hubbard *U* parameter on charge localization and resulting optical response. The results are directly compared with our previous HSE06 calculations and with available optical and spectroscopic experiments to evaluate the capability of DFT+U to accurately reproduce the polaron states in $BiVO_4$.[1,2]

[1] Seyeon Park, *et al.*, arXiv:2511.19853 (2025)
[2] Chaudhuri, A., et al., *Phys. Rev.* B **97**, 195150 (2018)

Poster No.26

Evolution of boson peak during crystallization of amorphous Ge-Sb-Te

Pyung Jin Park and Seung-Hoon Jhi

Department of physics, Pohang University of Science and Technology, Pohang 37673, Republic of Korea

The boson peak is an excess of low frequency vibrational states over the Debye prediction, commonly observed in disordered materials. However, its microscopic origin remains unresolved. We investigate the evolution of the boson peak during crystallization of amorphous Ge-Sb-Te using large scale molecular dynamics simulations with machine learning interatomic potentials. As crystallization proceeds, the boson peak shifts to higher frequencies and its intensity decreases. The dynamical structure factors show that the boson peak frequency coincides with the transverse Ioffe-Regel crossover frequency, consistent with the quasi-localized nature of the boson peak modes. Atom-resolved analysis demonstrates that boson peak modes are populated preferentially in the mechanically soft, under-coordinated regions, revealing an anticorrelation between local shear modulus and boson peak intensity. These results provide an atomistic picture of the vibrational anomalies associated with structural ordering in GST.

Poster No. 27

Novel topological route beyond Floquet–Volkov paths

Hyosub Park[1] and J. D. Lee[1*]

[1]*Department of Physics and Chemistry, DGIST, Daegu 42988, Republic of Korea*

Quantum path interference between Floquet and Volkov states has recently emerged as a hallmark of time-resolved and angle-resolved photoemission spectroscopy (tr-ARPES), enabling precise access to laser-driven dynamics of the electronic structure. We theoretically identify an additional quantum path arising from the virtual interband excitation in tr-ARPES combined with the reconstruction of attosecond beating by interference of two-photon transitions (RABBIT). In particular, virtual interband excitation path is found to reveal topological information encoded in photoemission delays of the RABBIT sidebands. Our findings pave the way for attosecond spectroscopy of topological quantum phases beyond Floquet–Volkov dynamics in semiconductors.

Poster No.28

Electron-phonon coupling effects in high-harmonic generation

Gimin Bae and J. D. Lee*

Department of Physics and Chemistry, DGIST, Daegu 42988, Republic of Korea

**Email: jdlee@dgist.ac.kr*

High-harmonic generation (HHG) has been extensively studied, and many-body effects such as electron-electron and electron-hole interactions have been shown to significantly influence the harmonic spectra. While recent studies have begun to explore the role of electron-phonon coupling in HHG, a systematic understanding of its impact remains limited. In this work, we solve the time-dependent Schrödinger equation for a one-dimensional Holstein model and investigate the influence of electron-phonon interactions on HHG. We find that the harmonic intensity is enhanced as the electron-phonon coupling strength increases, demonstrating that phonons can strongly modify the nonlinear optical response of the system. Our results provide insight into the role of electron-phonon interactions in HHG and establish the calculation as a useful platform for studying phonon-induced effects in strong-field light-matter interactions.

Poster No.29

Novel topological route beyond Floquet–Volkov paths

Hyosub Park[1] and J. D. Lee[1*]

[1]*Department of Physics and Chemistry, DGIST, Daegu 42988, Republic of Korea*

Quantum path interference between Floquet and Volkov states has recently emerged as a hallmark of time-resolved and angle-resolved photoemission spectroscopy (tr-ARPES), enabling precise access to laser-driven dynamics of the electronic structure. We theoretically identify an additional quantum path arising from the virtual interband excitation in tr-ARPES combined with the reconstruction of attosecond beating by interference of two-photon transitions (RABBIT). In particular, virtual interband excitation path is found to reveal topological information encoded in photoemission delays of the RABBIT sidebands. Our findings pave the way for attosecond spectroscopy of topological quantum phases beyond Floquet–Volkov dynamics in semiconductors.

Poster No.30

Hidden Origin of Strong Optical Absorption in h-TMDs: Obstruction-Driven Parity Inversion

Seungil Baek[1], Jun Jung[1], Yong-Hyun Kim[1,2,*]

[1]*Department of Physics, Korea Advanced Institute of Science and Technology, Republic of Korea.*

[2]*School of Physics, Institute of Science, Suranaree University of Technology, Thailand.*

Transitions between orbitals with the same parity are often suppressed by optical selection rules. However, hexagonal transition metal dichalcogenides (h-TMDs) exhibit strong optical absorption despite their band edges being derived from *d* orbitals. Although prior studies have focused on band nesting as the primary origin of large optical absorption, the origin of significant transition dipole moments has largely been overlooked. In this presentation, we elucidate a hidden parity inversion mechanism driven by obstructed atomic limit topology, which enables dipole-allowed optical transitions in h-TMDs. Our tight-binding analysis reveals that the dominance of intersite hopping over crystal-field splitting induces this parity inversion. Our study illuminates the origin of strong light-matter interactions in these materials, upon which many-body optical descriptions are built.

Poster No.31

Finding and Exploiting Compact Wave-Function Representations in Spin-Adapted Bases

Maru Song[1], Luca Bonfirraro[1], Ali Alavi[1,2], Ignacio Fdez. Gálvan[3], Roland Lindh[3], and Giovanni Li Manni[1]

[1]*Max Planck Institute for Solid State Research, Stuttgart, Germany*
[2]*University of Cambridge, Cambridge, United Kingdom*
[3]*Uppsala University, Uppsala, Sweden*

In addition to targeting specific spin states, the use of a spin-adapted basis can yield a compact wave function representation through the quasi-block-diagonal structure of the Hamiltonian matrix when an optimal orbital ordering is employed [1,2]. Sparse solvers, such as Full Configuration Interaction Quantum Monte Carlo (FCIQMC) [3], benefit from compact representations. We have developed a genetic algorithm [4] that efficiently identifies an optimal orbital ordering using an inexpensive fitness function that approximates wave function compactness. The presence of a highly single-reference character also motivated the development of a spin-adapted restricted open-shell Hartree–Fock method (CSF-ROHF). We further extended our CSF-ROHF implementation to incorporate missing charge-transfer effects [5] using the Stochastic SplitGAS method [6]. The resulting SSG-CSF-ROHF protocol efficiently captures both dynamic and static correlation.

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Poster No.32

Phonon renormalization and anharmonicity in PbTe

Sungmin Song and Seung-Hoon Jhi

Department of Physics, Pohang University of Science and Technology, Pohang 37673, Republic of Korea

Lead telluride (PbTe) is a benchmark thermoelectric material with high figure of merit. The coexistence of a narrow electronic band gap and pronounced lattice anharmonicity is considered as a key factor underlying the superior thermoelectric performance of PbTe. Despite extensive theoretical efforts, however, accurate first-principles description of its electronic and phononic properties remains challenging, as the low-energy states and their screening effects are highly sensitive to the choice of electron exchange-correlation functional and the treatment of spin–orbit coupling (SOC). In this study, we calculate the electronic structure and phonon dispersion of PbTe including both SOC and on-site Hubbard U correction. We investigate in particular the effects of SOC-driven orbital splitting and the U correction on electronic screening and phonon renormalization. We find significant modifications to transverse optical (TO) phonon self-energy and enhanced anharmonic effects in phonon linewidth, TO mode splitting, and lattice thermal conductivity.

Poster No.33

Electric-Field Control of Magnetic Anisotropy in Co/HfO_2: A First-Principles Study of Polarization-Driven Oxygen Diffusion

Jihoon Song[1], Sohee Park [2] and Young-Kyun Kwon*[1]

[1] *Department of Physics and Research Institute for Basic Sciences, Kyung Hee University, Seoul 02447, Korea*

[2] *Department of Physics, Kyung Hee University, Seoul 02447, Korea*

Multiferroic materials, which couple ferroelectric and ferromagnetic orders, exhibit strong magnetoelectric interactions that allow magnetic properties to be tuned by an electric field—a capability that makes them attractive for memory and logic devices and has driven extensive research. In the Co/HfO_2 system, recent experiments have shown that an applied electric field drives oxygen migration into the Co layer, producing an asymmetric modulation of the magnetic anisotropy energy (MAE). The microscopic origin of this asymmetry—in particular, how the ferroelectric polarization governs oxygen diffusion at the interface—remains to be clarified. Here, we use density functional theory (DFT) to compute the oxygen diffusion barrier at the Co/HfO_2 interface for opposite polarization states and to analyze the corresponding changes in MAE. Because structural imperfections form naturally at such interfaces, we also examine how cobalt vacancies modify the diffusion barrier. Feeding these barriers into random-walk simulations of oxygen migration, we quantify how the diffusion behavior differs between interfaces of opposite polarization. Together, these results provide a theoretical framework for understanding how ferroelectric polarization controls oxygen diffusion and, in turn, the MAE in Co/HfO_2 systems.

Poster No.34

First-principles Study of Electronic Structure of Hydrogenated 2D Electride Gd_2CH_x

Seungwoo Shin, Young Woo Choi

Department of Physics and Center for Nano Materials, Sogang University, Seoul, Korea

The two-dimensional electride Gd_2C hosts anionic electron states between its layers and at its surface. Recent experiments show that the 2D electride Gd_2C undergoes reversible magnetic and structural transitions upon hydrogenation, forming Gd_2CH_x phases with distinct stackings and magnetic orderings [1]. The electronic structure underlying these transitions, however, remains poorly understood. Here, we present a first-principles study of Gd_2CH_x as a function of hydrogen content, stacking, and magnetic ordering. Using density functional theory with and without Hubbard U corrections, we compute bulk magnetic phases and band structures across the relevant hydrogen concentrations, clarifying how interstitial electrons evolve as hydrogen occupies octahedral and tetrahedral sites. We further compute the surface electronic structure of Gd_2CH_x slabs to identify possible surface states. Our results provide a microscopic picture of hydrogenation-driven electronic reconstruction in 2D electrides.

[1] Lee et al., Nat. Commun. 14, 5469 (2023)]

Poster No.35

Benchmarking First-Principles DFT approaches for the electronic structure and magnetism of $SrFeO_3$

Hyoin Eo and Bongjae Kim

Department of Physics, Kyungpook National University, Daegu 41566, Korea

Despite its simple cubic structure, $SrFeO_3$ exhibits complex magnetic behaviors. The magnetic ground state of the system is characterized by helimagnetic order, which evolves into various multi-Q states under an applied magnetic field. However, accurate first-principles description of the electronic structure and magnetism of $SrFeO_3$ remains nontrivial.

In this study, we investigate the electronic structure and magnetic properties of $SrFeO_3$ using various density functional approaches. Adopting a ferromagnetic configuration as an approximation to the experimentally observed small-**q** ground state, we benchmark different exchange-correlation functionals, including LDA, GGA, meta-GGA, and hybrid schemes. In addition, we investigate Hubbard-corrected approach within the DFT+U and DFT+U+V frameworks. Our study emphasizes the importance of selecting an appropriate DFT scheme for an accurate description of the material properties of $SrFeO_3$.

Poster No.36

Quantifying Uncertainty of Admissible Solutions in Analytic Continuation

Kyungkyu Oh[1], Aaram J. Kim[2*], Hongkee Yoon[1*]

[1]Department of Physics, Kangwon National University, Chuncheon

[2]Department of Physics and Chemistry, DGIST, Daegu

Analytic continuation, the reconstruction of real-frequency spectral functions from imaginary-time Green's functions, is an inherently ill-posed inverse problem that is highly sensitive to statistical noise. Existing approaches, including the Maximum Entropy Method (MEM) [1], Padé approximation [2], stochastic analytic continuation (SAC) [3], the Nevanlinna method [4], projection, pole estimation, and semidefinite relaxation methods [5–8], and machine-learning approaches [9,10], can produce candidate spectra, but they do not generally characterize the admissible region of solutions consistent with the input data.

We propose a framework for quantitative uncertainty assessment in analytic continuation. By representing spectral functions using B-splines [11], which are smooth functions by definition, we use stochastic optimization to explore admissible spectra with systematically varied spectral features. The resulting error bars and error maps characterize the admissible region of solution space and allow uncertainty to be compared across spectra, noise levels, constraints, and methods. We benchmark this framework using the single-orbital Hubbard model [12] and systematically examine the admissible spectral region under controlled conditions.

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Poster No.37

Strong THz-driven Non-thermal Demagnetization in Ferromagnetic $LaMnO_3$

Jinseok Oh[1], Jeonghoon Kim[1], Jae-Woo Han[1], Chaeyoon Kim[2], Hyoung-Taek Lee[3], Noejung Park[1,], Fabian Rotermund[2], Changhee Sohn[1], Hyeong-Ryeol Park[1,**]*

[1]Department of Physics, Ulsan National Institute of Science and Technology, Ulsan 44919, Republic of Korea

[2]Department of Physics, Korea Advanced Institute of Science and Technology, Daejeon 34141, Republic of Korea

[3]Department of Mechanical Engineering, Pohang University of Science and Technology, Pohang 37673, Republic of Korea

** noejung@unist.ac.kr , ** nano@unist.ac.kr*

Intense THz time-domain spectroscopy measurements on Pr/Sr-doped $LaMnO_3$ (LPSMO) thin films show that the field-strength dependence of the THz transmittance spectrum closely resembles the temperature dependence observed across the ferromagnetic-to-paramagnetic transition. This similarity suggests that strong THz excitation drives the system toward a demagnetized state in a manner reminiscent of thermal heating, despite occurring on timescales where a conventional thermal picture, such as the three-temperature model (3TM), is not expected to fully apply.

To investigate this from a microscopic perspective, we performed real-time time-dependent density functional theory (rt-TDDFT) simulations. Since directly simulating the full LPSMO supercell is computationally demanding, we instead constructed a minimal model based on hole-doped $LaMnO_3$, obtained by tuning the Fermi level to reproduce a ferromagnetic ground state. A strong electric field was then applied to this system, and the resulting spin dynamics were tracked in real time.

Under this strong-field excitation, we observe rapid demagnetization within tens of femtoseconds, consistent with the sub-picosecond timescale reported experimentally. To clarify the role of the lattice in this process, we compared simulations performed with and without ionic dynamics, finding that the electronic channel dominates the demagnetization response while lattice motion plays only a secondary role on this timescale. These results suggest a non-thermal demagnetization pathway distinct from the picture assumed in the 3TM analysis and illustrate the utility of rt-TDDFT as a tool for examining strong-field-driven spin dynamics in correlated oxide systems beyond conventional thermal frameworks.

Poster No.38

-Mediated Phase Transformations in Titanium: A Machine Learning Force Field Study

Seungwoo Yoo, and Young-kyun Kwon

Department of Physics, Kyung Hee University, Seoul 02447, South Korea

Traditional approaches to understanding phase stability in transition metals rely primarily on conventional thermodynamic parameters like temperature and pressure. This study, however, establishes electronic charge as a crucial alternative variable that actively drives solid-state phase transformations. Our investigation centers on Titanium (Ti), a group 4 element characterized by a temperature-induced α→β phase transition.To probe these complex underlying mechanisms, we perform large-scale molecular dynamics (MD) simulations utilizing a machine learning force field (MLFF) trained on first-principles data. By integrating the Temperature-Dependent Effective Potential (TDEP) method, we precisely capture temperature-driven phonon dynamics and expand this methodology to charged environments to examine the synergistic effects of temperature and electron density. Our findings reveal that introducing excess electron density preferentially stabilizes the β phase, thereby significantly depressing the α→β transition temperature in Ti. These outcomes demonstrate that electronic charge serves as a potent regulatory dimension for phase control, breaking through traditional thermal limits. Ultimately, this MLFF-driven framework delivers a highly predictive and efficient computational tool for tailoring material phases via charge doping.

Poster No.39

Electronic Structures of β-(Ag,Ca)LaNb2O7 as a Transparent Conducting Oxide

DaGyeong Lee, JaeSeong Lee, SeYoung Park

Department of Physics and Origin of Matter and Evolution of Galaxies (OMEG) Institute, Soongsil University, Seoul, 06978, South Korea

We investigate the structural, electronic, and optical properties of β-AgLaNb2O7 (ALNO) using first-principles density functional theory. Similar to the n = 2 Ruddlesden–Popper phase, the atomic structure consists of corner-sharing oxygen octahedra surrounding Nb ions, forming a bilayer with La ions occupying the A-site position in the middle, sandwiched between Ag ions. We find that the material exhibits an insulating ground state where the occupied bands near the Fermi energy are mainly derived from O-p and Ag-d orbitals, and the low-lying unoccupied bands are from Nb-d orbitals. Due to the sufficiently large band gap of 2.63 eV relative to visible-light frequency and characteristics of the conduction bands, interband transitions are strongly suppressed upon electron doping, indicating its suitability as a transparent conductor. For electron doping of ALNO, Ca substitution at the Ag site is considered, in which the calculated dielectric function shows negligible absorption in the visible-light frequency range. Our work proposes ALNO as a candidate material and provides useful guidelines to identify materials suitable for transparent conductors.

Poster No.40

Computational insights into the stability, mobility, and doping of 3C-SiC using DFT and MLFF

Donggeon Lee[1], SeungYeop Lee[2], Sooran Kim[3] and Ji-Sang Park[1]

[1]*SKKU Advanced Institute of Nanotechnology (SAINT), Sungkyunkwan University, Suwon, South Korea*

[2]*Department of Nano Engineering, Sungkyunkwan University, Suwon, South Korea*

[3]*Department of Physics Education, Kyungpook National University, Daegu, South Korea*

In this work, we present a comprehensive computational analysis of the stability, electronic structures, and doping properties of silicon carbide (SiC) polytypes using density functional theory (DFT) and machine-learned force fields (MLFF). Although 4H-SiC is the industry standard, the 3C polytype offers superior electron mobility despite significant synthesis challenges. Structural benchmarks demonstrate that PBEsol and the MATPES-r2SCAN-0 MLFF accurately predict 3C-SiC lattice constants with minimal deviations. HSE06 calculations confirm that 3C-SiC exhibits superior carrier mobility among studied polytypes, regardless of its narrower band gap. Furthermore, tensile strain is found to thermodynamically stabilize the 3C phase over the 4H ground state, supporting its epitaxial growth on Si substrates. Finally, we identify Al_Si and N_C as the most promising shallow acceptor and donor dopants for 3C-SiC. This framework offers a computationally efficient approach for the design of high-performance SiC-based power electronics.

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Poster No.41

Stabilizing Li-Metal Anodes via Polysulfide Additives: A First-Principles Study

Moonwon Lee[1,2], Jinhong Lee[3], Kanghoon Yim[1*]

[1]*Energy AI & Computational Science Lab., Korea Institute of Energy Research, Republic of Korea*
[2]*Graduate School of Energy Science and Technology, Chungnam National University, Republic of Korea*
[3]*Energy Storage Research Department, Korea Institute of Energy Research, Republic of Korea*

Lithium–sulfur (Li–S) batteries are studied as next-generation energy storage systems due to their high theoretical energy density. However, their practical application is limited by capacity fading resulting from lithium dendrite growth and parasitic reactions at the Li-metal anode. In this study, lithium polysulfide species (Li_2S_4, Li_2S_6, and Li_2S_8) were introduced as electrolyte additives, which successfully suppressed localized Li corrosion and promoted the formation of a stable solid electrolyte interphase (SEI), experimentally demonstrating enhanced cycling stability of the Li-metal anode.

To elucidate the stabilization mechanism at the molecular level, we investigated the solvation behavior and polarity of these additives using density functional theory (DFT) calculations and *ab initio* molecular dynamics (AIMD) simulations. Specifically, the dynamic solvated structures were modeled using AIMD trajectories to quantitatively evaluate their solvation energies and dipole moments. The computational results show that the Li_2S_6 additive exhibits a relatively strong solvation energy and a low dipole moment. The strong solvation energy promotes the molecular stability and uniform dispersion of the additive within the electrolyte, while the low dipole moment establishes a low-polarity environment at the Li-anode surface that effectively mitigates excessive parasitic reactions. This synergistic effect leads to the formation of a thin, stable passivation layer and enhances overall electrochemical performance. Consequently, these computational insights are in excellent agreement with the experimental observations, confirming that regulating the solvation energy and polarity via polysulfide additives fundamentally contributes to the structural and electrochemical stabilization of the Li-metal anode.

Poster No.42

Tunable Electronic Transport in Pd/Pt-Based Delafossites via B-Site Engineering

YoungJun Lee[1], Sangmin Lee[2],Sangmoon Yoon[3,1], and Young-Kyun Kwon[1,4]

[1]*Department of Physics and Research Institute for Basic Sciences, Kyung Hee University, Seoul 02447, Korea*

[2] *Department of Materials Science and Engineering and Research Institute of Advanced Materials, Seoul National University, Seoul 08826, Republic of Korea*

[3]*Department of Physics and Semiconductor Science, Gachon University, Seongnam, Korea.*

[4]*Department of Information Display, Kyung Hee University, Seoul 02447, Korea*

As semiconductor devices continue to scale down, conventional Cu interconnects suffer from a rapid increase in resistivity caused by surface and grain-boundary scattering at nanoscale dimensions. Layered delafossites such as $PdCoO_2$ and $PtCoO_2$ have attracted attention as alternative interconnect materials because of their ultralow bulk resistivity and highly anisotropic transport properties. However, residual B-site d-orbital contributions near the Fermi level can interfere with the orbital–momentum locking mechanism that supports high conductivity.

Here, we propose B-site engineering as a strategy to optimize electronic transport in Pd- and Pt-based delafossites. Using first-principles calculations combined with Boltzmann transport theory, we investigate $PdBO_2$ and $PtBO_2$ compounds with B = Co, Al, Ga, and In. Replacing Co with group-13 elements suppresses B-site orbital contributions near the Fermi level, resulting in a cleaner Pd/Pt-derived conduction channel, enhanced band dispersion, and increased carrier velocity. While heavier substitutions such as Ga and In induce phonon softening and stronger electron–phonon scattering, Al substitution preserves favorable phonon characteristics while improving electronic transport.

Thickness-dependent resistivity calculations show that $PdAlO_2$ and $PtAlO_2$ are promising candidates for nanoscale interconnects. These results demonstrate that controlling orbital character, electron–phonon scattering, and transport anisotropy is a practical design principle for low-resistivity interconnect materials.

Poster No.43

Identification of the Shift Current Photovoltaic Materials Based on Materials Database:First-Principles Study

Jae Seong Lee[1], Jiwon Sun[2], Kyoungmin Min[2], Se Young Park[1]

[1]*Department of Physics and Origin of Matter and Evolution of Galaxies (OMEG) Institute, Soongsil University, Seoul, 06978, South Korea*

[2]*School of Mechanical Engineering, Soongsil University, Seoul, 06978, South Korea*

Based on the materials project database, we present a systematic way to identify materials with large shift current photovoltaic effects, which is a mechanism capable of increasing efficiency beyond the Shockley-Queisser limit. As a first step, we filter out the materials with space groups without inversion symmetry and band gaps in the visible light spectrum (1.1-3.1 eV), resulting in 235 candidates. We further narrow down the candidate materials with potentially high shift current responses and evaluate the light absorption. This is because the shift current is proportional to the product of the shift vector and square of the optical matrix element integrated over the Brillouin zone. Application of these criteria leads to a list of candidate materials, and the shift currents are evaluated with dense k-point mesh using the Wannier interpolation by constructing tight-binding Hamiltonian of frontier orbitals. We propose potential candidates exhibiting high shift currents and discuss the relation between the characteristics of the electronic structures and shift current responses. Our workflow enables efficient search strategy, involving materials screening criteria and high-throughput-capable optical conductivity calculations that are closely related to shift current, would be useful in identifying materials with large shift currents.

Poster No.44

First-principles study on the doping-dependent anomalous Hall conductivity in $La_{1-x}Sr_xCoO_3$

Joohyoung Lee[1], Chanul Kim[2], Young-Woo Son[2], Se Young Park[*1]

[1]*Department of physics, Soongsil University, Seoul, 06978, Korea*

[2]*School of Computational Sciences, Korea Institute for Advanced Study, Seoul 02455, Korea*

The perovskite $La_{1-x}Sr_xCoO_3$ (LSCO) alloy systems exhibit interesting magnetic and transport properties, such as the emergence of a large anomalous Hall conductivity (AHC), whose magnitude varies substantially with doping. So far, the microscopic origin of the doping-dependent change in AHC and its relation to the change in the electronic structures have not been fully understood. In this study, we investigate the doping-dependent evolution of magnetic properties and electronic structures in LSCO using first-principles density functional theory. Our results reveal a systematic increase in magnetization with increasing Sr doping. Moreover, the peak in the AHC at a specific doping concentration arises from the enhancement of Berry curvatures around the Fermi energy induced by the chemical potential shifts associated with the change in magnetization. By establishing a clear correlation between the source of the large AHC and band characteristics, this work provides an effective way to enhance AHC in ferromagnetic metals.

Poster No.45

Extended Linear Vibronic Coupling model for Nonadiabatic Quantum Dynamics: Accounting for bond dissociation

Chanyang Lee[1†], Seunghoon Lee[1*]

[1]Department of Chemistry, College of Natural Sciences, Seoul National University, 1 Gwanak-ro, Seoul 08826, Republic of Korea

[†]E-mail: jesuslee0110@snu.ac.kr; *E-mail: seunghoonlee@snu.ac.kr

Photoinduced bond dissociation, exemplified by Heme–CO photodynamics where ligand cleavage and spin-state transitions occur on ultrafast time scales, is a prototypical nonadiabatic process in which electronic state evolution and large-amplitude nuclear motion are strongly coupled. However, on-the-fly ab initio surface-hopping simulations remain computationally demanding for polyatomic systems because they require repeated electronic-structure calculations over many trajectories, electronic states, and nuclear degrees of freedom. The linear vibronic coupling (LVC) model offers an efficient alternative by representing the electronic Hamiltonian in a diabatic basis as a linear function of normal-mode displacements around a reference geometry, thereby enabling all-mode nuclear propagation at substantially reduced computational cost. Nevertheless, the standard LVC framework is intrinsically limited by its harmonic reference potential, making it inadequate for bond-breaking dynamics far from equilibrium. Here, we develop an extended linear vibronic coupling (ELVC) framework that removes this limitation while preserving the efficiency of the LVC model. The central methodological advance is the definition of a new dissociative coordinate that directly represents the relative motion of the bond-cleaving diatomic fragment, rather than relying solely on conventional normal modes. Along this coordinate, the harmonic approximation is replaced by a non-harmonic potential fitted to the dissociation pathway, whereas the remaining vibrational degrees of freedom are retained within the conventional LVC representation. We implemented the resulting ELVC Hamiltonian in a SHARC-based surface-hopping framework and evaluated its ability to reproduce both electronic population dynamics and bond-length evolution by comparison with reference SH/TDDFT simulations. This framework provides a practical and physically transparent route for simulating photoinduced bond dissociation in polyatomic molecules with model-Hamiltonian efficiency.

Poster No.46

Field-Responsive Equivariant Machine Learning Potentials with Long-Range Interactions

Jiwon Jeon[1,2], Soopil Kim[3] and JaeDong Lee[1,2,*]

[1]*Department of Physics and Chemistry, Daegu Gyeongbuk Institute of Science and Technology (DGIST), Daegu, 42988, Republic of Korea,*

[2]*InnoCORE AI-CRED Institute, Korea Advanced Institute of Science and Technology (KAIST), Daejeon, 34141, Republic of Korea,*

[3]*Division of Intelligent Robot, Daegu Gyeongbuk Institute of Science and Technology (DGIST), Daegu, 42988, Republic of Korea*

*E-mail: *jdlee@dgist.ac.kr*

Machine learning interatomic potentials (MLIPs) provide an alternative route to molecular dynamics simulations, extending the accessible length and time scales while maintaining near-quantum mechanical accuracy. Recently, equivariant message-passing neural networks have substantially improved the data efficiency and accuracy of interatomic potentials and have been extended to incorporate long-range interactions and electric-field responses. Although MLIPs have been increasingly extended to systems under external electric fields, developing MLIPs capable of both field response and long-range interactions has rarely been explored. Here, we introduce a field-responsive equivariant MLIP that uses classical electrostatic interaction energies of polarizable charges as a physical baseline and explicitly learns the differential structure of the potential energy surface with respect to an external electric field at zero field. This enables the proposed MLIP to represent potential energy surfaces responsive to external electric fields, even at large intermolecular separations beyond the cutoff radius of message-passing neural networks.

Poster No.47

Time-Reversal-Even and -Odd Control of Spin Hall Conductivity by Crystal and Magnetic Symmetry in Altermagnets

Dameul Jeong[1], Seoung-Hun Kang[3] and Young-Kyun Kwon*[1,2]

[1] *Department of Physics and Research Institute for Basic SciencesKyung Hee UniversitySeoul 02447, South Korea*

[2] *Department of Information DisplayKyung Hee UniversitySeoul 02447, South Korea*

[3]*Research Center for Technology CommercializationKorea Institute of Science and Technology Information (KISTI)Seoul 02456, South Korea*

Zero net magnetization coexists with symmetry-protected spin splitting in altermagnets, enabling unconventional spin transport without stray fields. To capture this physics systematically, we decompose the spin Hall conductivity (SHC) within the Kubo formalism into time-reversal-even ($\mathcal{T}$-even) and time-reversal-odd ($\mathcal{T}$-odd) contributions, building a unified symmetry-based framework for SHC. The $\mathcal{T}$-even SHC has a Fermi-sea Berry-curvature origin, and accordingly follows crystallographic selection rules identical to nonmagnetic systems. The $\mathcal{T}$-odd SHC, by contrast, is activated or suppressed component-by-component through antiunitary operations, since it is governed by magnetic symmetry rather than crystal symmetry alone. Applied to RuO_2, CrSb, and MnTe, this framework separates trivial unconventional SHC, a byproduct of structural tilting, from intrinsic unconventional SHC that originates in magnetic symmetry reduction. CrSb and MnTe in particular share the same crystal symmetry, yet generate distinct $\mathcal{T}$-odd tensor structures simply because their magnetic easy axes point in different directions. A practical symmetry guideline for designing spin Hall effects in zero-net-moment materials emerges from these results.

Poster No.48

Gauge-Field-Mediated Symmetry Breaking of Matter Under Electromagnetic Fields and Its Impact on Spin Dynamics

Uiseok Jeong[1], Esmaeil Taghizadeh Sisakht[1], Angel Rubio[2], Carsten A. Ullrich[3], Kyoung-Whan Kim[4], and Noejung Park[1,2,*]

[1]*Department of Physics, Ulsan National Institute of Science and Technology, 50, UNIST-gil, Ulju-gun, 44919, Ulsan, Republic of Korea*

[2]*Max Planck Institute for the Structure and Dynamics of Matter, Luruper Ch 149, 22607, Hamburg, Germany*

[3]*Department of Physics and Astronomy, University of Missouri, Columbia, 65211, Missouri, USA*

[4]*Department of Physics, Yonsei University, 50, Yonsei-ro, Seodaemun-gu, 03722, Seoul, Republic of Korea*

When a condensed-matter system is subjected to external electromagnetic fields, the gauge-invariant formulation of physical operators must explicitly incorporate the gauge-field contribution. However, in the context of spin–orbit coupling (SOC), this gauge-field term is often regarded as negligible or merely additive compared to the canonical SOC, which is typically localized near atomic cores. Here, we demonstrate that the symmetry breaking and consequent spin dynamics are governed by the gauge-field term, without which the spins remain symmetry-constrained. We perform real-time time-dependent density functional theory calculations to investigate spin–orbit dynamics, focusing on representative cases with mirror, glide, and screw-rotational symmetry. We demonstrate that when the gauge-field term in the time-dependent Hamiltonian perturbs the symmetry of the canonical term, a dynamical spin state gradually develops during the time evolution, beyond the symmetry-frozen states. We suggest that, for nonequilibrium spin–orbit dynamics, the gauge-invariant formulation of SOC is not only formally required but also quantitatively essential, even for a weak external field.

Poster No.49

Machine-Learning-Assisted Structural Identification of Catalytic Reaction Intermediates Towards Overpotential Calculation

Chanyeong Jeong, and Yong-Hyun Kim*

Department of Physics, Korea Advanced Institute of Science and Technology (KAIST), Daejeon 34141, Republic of Korea

The overpotential theory has become a standard framework for evaluating electrocatalytic activity, yet its practical application requires reliable Gibbs free energies of all adsorption intermediates along the reaction pathway. For complex catalytic systems such as dual atom catalysts (DACs), the large number of metastable adsorption configurations makes structural relaxation the most dominant computational bottleneck in constructing Gibbs free energy diagrams using density functional theory (DFT). Meanwhile, machine learning interatomic potential (MLIP) models have recently emerged as a promising tool to accelerate structure optimization; however, they are not yet reliable as standalone substitutes for DFT due to their limited physical rigor. Here, we propose an MLIP+DFT workflow that exploits the computational efficiency of MLIP while preserving the physical accuracy of DFT. In this approach, MLIP calculations with a loose force criterion are first employed to explore the configurational space and identify low-energy candidate structures, which are subsequently refined using DFT. By comparing runtimes and relaxed structures obtained from conventional DFT and the proposed MLIP+DFT workflow, we demonstrate a substantial reduction in computational cost without compromising structural fidelity. We further show that MLIP largely preserves the local minima of the DFT energy landscape, provided the force convergence criterion not being too strict. This work highlights a practical strategy for utilizing MLIP as a pre-conditioning tool for DFT-based catalysis studies and suggests a scalable pathway toward structure exploration in more complex catalytic systems, including triple atom catalysts (TACs).

Poster No.50

Native defects in CaO

Yunhwa Jo[1] and Minseok Choi[1,2*]

[1] *Department of Physics, Inha University, Incheon 22212, Korea,*

[2] *Institute of Quantum Science, Inha university, Incheon 22212, Korea*

Abstract:

Calcium oxide (CaO) is an emerging host for quantum defects owing to its large band gap, high dielectric constant, and long spin coherence time (34 ms) compared with other solid-state hosts such as diamond and SiC (typically a few ms) [1]. Recently, Davidsson *et al.* theoretically suggested several impurities-defect complexes in CaO that exhibit a two-level electronic structure analogous to that of the NV center in diamond [2]. Although several first-principles studies have investigated native defects in CaO [3-5], important aspects remain poorly understood. In particular, the migration barriers governing defect annealing, the stability and electronic properties of defect complexes, and the optical transitions associated with defects that may act as noise sources have not been systematically explored. In this work, we employ first-principles calculations using SCAN functional to investigate the formation energy, migration barrier, and optical properties of native defects and complexes in CaO, providing insights into their impact on the realization of defect-based quantum technologies.

Acknowledgement:
This work was supported by the government of the Republic of Korea (MSIT) and the National Research Foundation of Korea (RS-2024-00442710, RS-2025-25443942, RS-2025-16068832). We also acknowledge the National Supercomputing Center with supercomputing resources including technical support (KSC-2025-CRE-0596).

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Poster No.51

First-principles study of electron-phonon interaction in doped bulk 2H-WS_2: doping and temperature dependence

Min Chul Choi and Young Woo Choi*

Department of Physics and Center for Nano Materials, Sogang University, Seoul, Korea

Doped transition metal dichalcogenide semiconductors such as 2H-WS_2 host carriers in multiple inequivalent Brillouin-zone valleys (K and Q) and exhibit a variety of quantum phenomena under doping. Inter-valley electron-phonon (e-ph) coupling in such multivalley systems can strongly renormalize the quasiparticle spectrum and produce satellite features in the one-electron spectral function, yet a systematic first-principles understanding is still lacking. In this work, we compute the e-ph self-energy and spectral function of electron-doped bulk 2H-WS_2 from first principles as a function of doping concentration and temperature. We focus on satellite peaks and kinks induced by electron-phonon interactions and analyze dominant phonon modes that contribute to the coupling. A mode- and momentum-resolved decomposition identifies LA phonons near the M-point of the Q-valley as the dominant contribution. Our results provide a microscopic guideline for interpreting e-ph features in doped multivalley semiconductors.

Poster No.52

Pseudospin-selective polarimetric singularities in high harmonic generation of black phosphorus

Youngchan Choi, Gimin Bae, and J. D. Lee*

Department of Physics and Chemistry, DGIST, Daegu 42988, Republic of Korea.

Black phosphorus (BP) exhibits net opposite pseudospin polarizations for the electron and hole states. The pseudospin structure of BP causes a selectivity in the optical excitation engaging the symmetry between the optical pump polarization and the pseudospin state, which is confirmed in a simulation of the time-resolved angle-resolved photoemission spectroscopy (tr-ARPES). Further, the pseudospin selectivity is found to drive a unique polarimetric singularity in the high harmonic generation (HHG). Given the nth-order high harmonic signal, we reveal that the singularity arises predominantly through the multiphoton interband pathway and thereby becomes markedly substantial at $n\omega_{\mathrm{pump}} \gtrsim E_g$. ω_{pump} is the pump photon energy and E_g the energy gap of BP. This permits a coherent understanding of the pseudospin selectivity from tr-ARPES to HHG. In particular, the pseudospin-selective polarimetric singularity suggests a potential for the pseudospintronics to be integrated into the intrinsic dynamics due to the light-matter interaction in two-dimensional materials.

Poster No.53

Role of Many-Body Effects in Coverage-Dependent CO Adsorption on Cu(111)

Seungchang Han and Stefan Ringe

Department of Chemistry, Korea University, Seoul, Republic of Korea

Carbon monoxide (CO) adsorption on copper surfaces is a key elementary process governing catalytic pathways in electrochemical CO_2 reduction, as the distribution of adsorbed CO strongly influences reaction selectivity. Despite the widespread use of generalized-gradient approximation (GGA) density functional theory for modeling these systems, its apparent success often depends on fortuitous error cancellation, limiting confidence in predicted adsorption-site preferences and coverage-dependent energetics. In this study, we assess the impact of many-body electronic-structure effects on CO adsorption over Cu(111) using the random phase approximation (RPA). RPA calculations are performed for multiple adsorption sites and surface coverages to quantify how many-body interactions alter adsorption energetics relative to conventional semi-local DFT. We further examine how these corrections affect the energetic ordering of adsorption sites and their evolution as the CO coverage increases. Because direct RPA calculations over the full configurational space are computationally prohibitive, we adopt a multi-fidelity machine-learning approach that integrates low-fidelity DFT data with high-fidelity RPA calculations. The resulting surrogate model enables efficient prediction of adsorption energies across a broad range of surface configurations. These energetics are subsequently incorporated into Monte Carlo simulations to characterize equilibrium surface populations and coverage-dependent adsorption behavior under thermodynamic conditions. Finally, the predicted adsorption characteristics are compared with available experimental observations to evaluate the accuracy of the many-body-informed framework. This work clarifies the role of many-body electronic correlations in determining CO adsorption on Cu(111) and illustrates how combining high-level electronic-structure theory, machine learning, and statistical sampling provides an efficient strategy for modeling complex catalytic interfaces relevant to electrochemical CO_2 reduction.

Poster No.54-1

Computational studies of structural and vibrational properties in moiré materials

Dongsin Kim[1] and Young Woo Choi[1*]

1.Department of Physics and Center for Nano Materials, Sogang University, Seoul, Korea

Moiré materials, formed by stacking two-dimensional layers with a small twist angle, have emerged as a tunable platform for exploring exotic quantum phases such as superconductivity, strongly correlated states, and fractional quantum anomalous Hall (FQAH) states. However, understanding these phenomena from first principles remains computationally challenging because moiré supercells contain tens of thousands of atoms. To overcome this limitation, we employ a large-scale atomistic approach parametrized from density functional theory (DFT) that enables structural relaxation and phonon calculations of moiré supercells at DFT-level accuracy. We first apply our approach to twisted bilayer MoS_2, quantitatively reproducing the hexagonal-to-triangular moiré reconstruction observed in transmission electron microscopy (TEM) experiments. [1] We then calculate the Γ-point phonon modes of a twisted $MoTe_2/MoS_2$ heterobilayer and identify low-energy interlayer modes induced by the moiré reconstruction. These results demonstrate that our atomistic approach provides a framework for investigating structural and vibrational properties of moiré materials.

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Poster No.54-2

First-principles study of the charge density wave in 1T-$TiSe_2$ with DFT+*U* and DFT+*U*+*V*

Dongsin Kim[1] and Young Woo Choi[1*]

1. *Department of Physics and Center for Nano Materials, Sogang University, Seoul, Korea*

Charge density waves (CDWs) are correlated electronic phases characterized by periodic modulation of the electron density and the lattice. 1T-$TiSe_2$ is a prototype of CDW materials, which has been extensively studied for decades. However, the origin of the CDW phase in 1T-$TiSe_2$ is still under debate. In this work, we investigate the CDW phase of 1T-$TiSe_2$ using DFT+*U* and DFT+*U*+*V*, where *U* and *V* describe the on-site and inter-site Coulomb interactions respectively. We calculate the total energies of the normal and CDW phases as a function of the CDW amplitude and fit the resulting energy landscape to a Ginzburg-Landau free-energy functional to extract the microscopic parameters governing the CDW transition. The comparison between DFT+*U* and DFT+*U*+*V* reveals how inter-site Coulomb interaction *V* modifies the CDW energetics beyond on-site correlations alone. This work aims to provide new insight into the microscopic origin of the CDW phase in 1T-$TiSe_2$ and to assess the importance of extended Hubbard corrections for describing correlated CDW systems.

Poster No.55

A Scalable Configuration-Interaction Impurity Solver via Active Learning

Jeongmoo Lee and Ara Go*

Department of Physics, Chonnam National University, Gwangju 61186, Republic of Korea

*Email: arago@jnu.ac.kr

In dynamical mean-field theory (DMFT), quantum Monte Carlo solvers suffer from a severe sign problem for multiorbital interactions of the Kanamori type, where spin-flip and pair-hopping terms spoil the positivity of the sampling weights. Exact diagonalization (ED) is free of this issue and treats such interactions directly, but its reach is capped by the exponential growth of the Hilbert space with orbital count. Pushing back this exponential wall is therefore key to extending finite-Hamiltonian solvers to realistic multiorbital problems.

We address this with an active-learning configuration-interaction solver (AL-ATCI). A random-forest classifier, trained on configurations from earlier iterations, predicts which Slater determinants are important, and only that subset is diagonalized—so the cost tracks the relevant part of the wavefunction rather than the full combinatorial space, with the number of selected configurations setting the accuracy. We demonstrate the method on single-site DMFT for Sr_2RuO_4, a three-orbital t_{2g} system with the full rotationally invariant Kanamori interaction, where the dynamics converge systematically as the bath size is enlarged from 9 to 18 orbitals.

Poster No.56

Atomistic Insights into Anti-Reflective Polymer/Oxide Interfaces: A Combined DFT and MLIP Study

Suim Lim[1,2], Ji Seong Choi[2], Seong Min Kang[2*], Kanghoon Yim[1*]

[1]*Energy AI & Computational Science Laboratory, Korea Institute of Energy Research, Daejeon, Republic of Korea*

[2]*Department of Mechanical Engineering, Sogang University, Seoul, Republic of Korea*

Anti-reflective (AR) technologies are essential for maximizing the efficiency of next-generation optoelectronic devices by minimizing optical losses. While integrating polymer-based AR films with transparent conducting oxides is a promising strategy, natural reflection at the polymer/electrode interface intrinsically limits overall light transmittance. Traditionally, density functional theory (DFT) is used to investigate the structural and electronic properties of these interfaces; however, its high computational cost prohibits the simulation of realistic, large-scale systems comprising thousands of atoms. Although machine learning interatomic potentials (MLIP) offer a powerful solution to bridge this length-scale gap, comprehensive atomistic simulations targeting complex polymer-oxide interfaces remain exceptionally scarce.

In this study, we introduce an advanced multiscale simulation framework combining DFT and MLIP to model polymer/oxide interfaces across varying structural scales and concurrently evaluate their optical and mechanical properties. We initially validated our computational approach using the indium tin oxide (ITO) electrode system, simulating structures ranging from small-scale single-chain polymer models to large-scale interfacial systems. The calculated optical properteis and mechanical adhesion demonstrated excellent agreement with experimental data, confirming the reliability of our framework. Leveraging this validated methodology, we subsequently expanded our scope to predict the interfacial properties of indium zinc oxide (IZO) and aluminum zinc oxide (AZO) electrodes. Our predictive screening reveals that perfluoropolyether (PFPE)-based AR films exhibit substantially higher optical transmittance when interfaced with IZO and AZO compared to traditional ITO. Ultimately, this work provides the first atomistic insights into complex polymer/oxide interfaces, demonstrating that MLIP-driven multiscale simulations can significantly accelerate large-scale materials discovery and interface engineering.

Poster No.57

First-Principles analysis on the X-ray Spectroscopy of Time propagation Warm Dense Aluminum: Electron, Ion, and Lattice Effects from RPA, GW, and BSE

박춘기

GIST

Warm dense matter (WDM) is a state of matter located at the intersection of the solid, liquid, and plasma phases, characterized by strong quantum degeneracy and thermal effects. Because it is partially excited and partially degenerate, it requires simultaneous consideration of complex electron, ion contributions. This complexity primarily stems from three phenomena. First, the electronic structure changes due to thermal Fermi occupation, accompanied by a shift in density of state electron self-energy such as many-body perturbation. Second, the high-pressure state and volume expansion induced by the melting behavior of ions lead to changes in the Density of States (DOS) and symmetry breaking. Finally, electron-ion scattering becomes the dominant mechanism, driven by the altered screening environment of the warm dense state. When addressing the WDM formation process induced by laser irradiation, a hierarchical approach is required to clearly distinguish and analyze the time-dependent changes in physical properties, the individual effects of electrons and ions, and the dynamics of electron-ion interactions.

Accordingly, this study utilizes Ehrenfest dynamics based on Time-Dependent Density Functional Theory (TDDFT) to investigate the transition from a non-thermal electron distribution to a thermal occupation and the induction of ionic disorder over time. These processes are examined by comparing them with experimentally reported changes in the absorption spectra of the EUV region and L-edge of Warm Dense Aluminum. Furthermore, to interpret the dominant time-dependent changes in physical properties, we hierarchically consider electron, ion, electron-ion, and electron-hole interactions, thereby providing a theoretical framework for comparing and analyzing the experimentally measured absorbance in the EUV and L-edge

Poster No.58

Elucidating the Effects of Lattice Vacancies on Phase Transitions in Prussian Blue Analogues Using Machine Learning Interatomic Potentials

Sanghyeon Park[1], Wonjun Choi[1], Jaeeun Joo[1], Chan-Woo Lee[2*] and Jong Min Yuk[1*]

[1]*Department of Materials Science and Engineering, Korea Advanced Institute of Science and Technology (KAIST)*

[2]*Department of Energy and Materials Engineering, Dongguk University*

Prussian blue analogues (PBAs, $Na_2Fe[Fe(CN)_6]$) are promising cathode materials for sodium-ion batteries owing to their open framework structure, fast ion diffusion, low-cost synthesis, and excellent rate capability. However, their electrochemical performance and cycling stability are strongly affected by intrinsic $Fe(CN)_6$ vacancies and structural phase transitions during (de)sodiation. In particular, irreversible phase transitions can lead to capacity fading, yet the atomistic role of lattice vacancies in governing phase transition behavior remains unclear because systematic experimental control and conventional density functional theory (DFT) calculations are highly challenging for vacancy-containing PBAs.

Here, we employ a machine-learning interatomic potential (MLIP) fine-tuned using DFT-based molecular dynamics datasets to investigate the effect of $Fe(CN)_6$ vacancies on phase transitions. A structural search space was constructed by varying sodium content, vacancy concentration, and crystal phase, followed by MLIP-based molecular dynamics simulations and complementary DFT electronic structure analyses.

Our results reveal that phase transition behavior is governed by the local coordination environment between Na ions and cyanide groups. Increasing $Fe(CN)_6$ vacancy concentration suppresses the phase transition by reducing available cyanide coordination sites required for structural distortion. These findings provide atomistic insight into vacancy-mediated phase stability in PBAs and demonstrate the utility of MLIPs for exploring complex structural phenomena beyond conventional DFT limits.

Poster No.59

Tight-Binding Investigation of Electronic Structure Reconstruction in the HC 3×3 CDW Phase of 1H-$TaSe_2$

Sohee Park[1], Changwon Park[2], and Young-Kyun Kwon[1,*]

[1]Department of Physics and Research Institute for Basic Sciences,
Kyung Hee University, Seoul, 02447, Korea
[2]Department of Physics, Ewha Wonmans University, Seoul, 03760, Korea

We investigate the evolution of the electronic structure in the HC 3×3 charge density wave (CDW) phase of 1H-$TaSe_2$ using a Wannier-based tight-binding (TB) approach. Effective TB Hamiltonians are constructed for both the primitive (1×1) structure and the HC 3×3 CDW supercell, with and without spin–orbit coupling (SOC).

To isolate the effects of the CDW from those of Brillouin-zone folding, the TB band structure of the 3×3 supercell is compared with the folded bands obtained from the 1×1 Hamiltonian in the reduced Brillouin zone along the Γ–M–K–Γ path. This comparison enables the identification of band modifications arising from the CDW potential beyond simple zone-folding effects.

The evolution of the TB Hamiltonian is further analyzed through a quantitative comparison of onsite energies and hopping parameters between the two structural phases, providing insight into how lattice distortion modifies the effective electronic interactions. By incorporating SOC into both Hamiltonians, we also examine its influence on the reconstructed band structure and the lifting of band degeneracies in the CDW phase.

These results provide a quantitative tight-binding description of the HC 3×3 CDW phase and offer insight into the electronic structure evolution induced by the CDW in 1H-$TaSe_2$.

Poster No.60

Study of electrical conductivity of expanded Cu in warm dense matter regime using quantum molecular dynamics and DFT calculations

YOON Haesang[1],CHOI Jae won[1], LEE Nayoung[1], KIM Shinhui[1], CHI Hsiao-Chien[2], PARK Sungbin[2],
CHUNG Kyoung-Jae[2], CHO Jongweon[1,*]

[1]Department of Physics, Myongji University, Yongin 17058, Republic of Korea
[2]Department of Energy Systems Engineering, Seoul National University, Seoul 08826, Republic of Korea
**jwcho@mju.ac.kr*

Underwater electrical wire explosion experiments provide access to the density–temperature conditions of materials in the so-called warm dense matter (WDM) regime, where quantum mechanical effects may play substantial roles. However, a detailed understanding of the behavior of the electrical transport in the WDM regime remains rather elusive. In this work, we use first-principles Car–Parrinello molecular dynamics to simulate copper in the low-temperature WDM regime at various densities. We then compute the electrical conductivity via the Kubo–Greenwood formalism and examine the temperature and density dependent electrical conductivity in this system. Our results may provide microscopic insights into quantum mechanical transport phenomena under extreme conditions where experimental diagnostics are relatively limited.

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Poster No.61

Surface-normal photogalvanic effect in chiral materials

조예준, 신동빈*

Department of Physics and Photon Science, GIST

구조적 카이랄성은 원형이색성, 광갈바닉 효과, 스핀 전류과 같은 비전통적 광·수송 현상의 근원으로 작용한다. 본 연구에서는 기하학적 카이랄 물질의 표면에서 발생하는 out-of-plane 광전류가 단순한 표면 대칭성 깨짐만으로 설명되지 않으며, 표면 구속에 따른 광전이 선택성과 흡수 비대칭이 핵심적인 역할을 함을 이론적으로 제시한다. 대표적인 카이랄계인 1T-$TiSe_2$의 카이랄 전하밀도파 구조와 삼방정 Te 를 대상으로, 밀도범함수이론 기반 원형이색성 계산, Wannier 기반 광갈바닉 응답 계산, 실시간 시간의존 밀도범함수이론 및 시간의존 타이트바인딩 모형을 결합하여 표면 유도 광응답의 미시적 기원을 분석하였다. 벌크에서는 카이랄 구조에 의해 좌·우 원형편광에 대한 전이와 원형 광갈바닉 효과가 서로 반대 방향의 응답으로 나타나는 반면, 표면에서는 광 침투 깊이의 제한과 경계 조건으로 인해 브릴루앙 영역의 일부 상태가 선택적으로 여기된다. 이로 인해 원형편광에 대한 단순한 부호 반전이 아니라 크기 비대칭이 발생하며, 나아가 선편광만으로도 out-of-plane 방향의 유한한 광전류가 유도될 수 있음을 확인하였다. 또한 서로 다른 손성 또는 비카이랄 적층이 혼합된 구조에서는 국소적인 광전류 생성뿐 아니라 반대 표면에서 형성되는 반대방향 전류의 억제까지 함께 작용하여, 전체 순전류가 광 침투 깊이와 적층 계면의 위치에 민감하게 조절됨을 보였다. 이러한 결과는 표면이 단순히 벌크 대칭성을 깨는 경계가 아니라, 카이랄 물질의 광흡수 경로와 순 광전류를 능동적으로 제어하는 물리적 자유도임을 보여준다. 본 연구는 카이랄 기반 광전자 및 스핀트로닉스 소자에서 표면 설계와 적층 구조 제어를 통한 광전류 엔지니어링의 가능성을 제시한다.

Poster No.62

A Machine Learning Initialization Strategy for Nonlinear Bath Fitting in Hamiltonian-Diagonalization DMFT

Taeung Kim, Jeongmoo Lee and Ara Go*

*arago@jnu.ac.kr

Department of Physics, Chonnam National University, Gwangju 61186, South Korea

We present a machine-learning-assisted initialization scheme that addresses one of the principal computational bottlenecks in Hamiltonian-diagonalization-based dynamical mean-field theory (HD-DMFT): nonlinear bath fitting. In HD-DMFT, the continuous hybridization function is represented by a finite set of bath-site energies and hybridization amplitudes determined through the minimization of a highly non-convex multivariable objective function. As the bath size increases, this optimization becomes increasingly sensitive to the initial parameter guess and more susceptible to convergence toward suboptimal local minima, leading to slower and less reliable DMFT self-consistency.

To overcome this limitation, we formulate bath fitting as a supervised regression task and employ kernel ridge regression to predict high-quality initial bath parameters directly from the target Matsubara-axis hybridization function. Rather than relying on random parameter sampling, the training data are generated from tight-binding Hamiltonians of layered-perovskite-like ruthenate models with systematically distorted crystal structures, while the corresponding target bath parameters are obtained from fully converged conventional bath fitting. Time-reversal symmetry is incorporated explicitly into both the input features and output targets, reducing the effective parameter space and ensuring physically consistent predictions.

Benchmark calculations in the non-interacting limit demonstrate that the proposed initialization consistently lowers the initial fitting error, reduces the number of conjugate-gradient optimization steps, and enhances robustness against local minima over a broad range of bath sizes. We further validate the transferability of the approach in an interacting DMFT calculation for Sr_2RuO_4 using an adaptive-truncation impurity solver, where the machine-learning initialization achieves systematically faster convergence than a symmetry-preserving heuristic initialization while maintaining the same converged bath-fitting solution.

Poster No.63

Adaptive Temperature Ladder Optimization for Parallel Tempering on Frustrated Classical Heisenberg Lattices

MunjunJang and Ara Go

Department of Physics, Chonnam National University, Gwangju

Classical Heisenberg models on geometrically frustrated lattices exhibit rugged free-energy landscapes densely populated with metastable states, causing single-temperature Monte Carlo simulations to violate ergodicity. Parallel tempering mitigates this by coupling replicas across a temperature ladder, yet its effectiveness depends critically on the ladder spacing.

In this work, we examine the acceptance-rate method, which equalizes exchange probabilities between neighboring replica pairs using the overlap of energy histograms. We apply this method to the classical Heisenberg model on monolayer triangular lattices and confirm convergence of the phase diagram near the transition region through sufficiently long plain Monte Carlo simulations. As future work, we will compare this approach with the round-trip-time method and extend the study to multilayer triangular lattices to establish practical guidelines for selecting an optimal temperature ladder and the number of replicas in geometrically frustrated magnetic systems. These developments are expected to provide a robust simulation framework for investigating experimentally realized frustrated magnets such as $Na_2BaMn(PO_4)_2$.

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Poster No.64

DeepSCF: Recent Developments in Efficient and Physics-Informed Self-Consistent Electron Density Learning

Ryong-Gyu Lee, Minsu Jeong and Yong-Hoon Kim*

School of Electrical Engineering, Korea Advanced Institute of Science and Technology, 291 Daehak-ro, Yuseong-gu, Daejeon 34141, Korea

*(*Corresponding Author. Email: y.h.kim@kaist.ac.kr)*

The self-consistent field (SCF) generation of the three-dimensional (3D) electron density distribution (ρ) is a fundamental aspect of density functional theory (DFT) and related first-principles calculations, and how one can shorten or bypass the SCF loop represents a critical question in electronic structure theory from both practical and fundamental standpoints. Recently, a machine learning strategy DeepSCF, which learns the map between the SCF ρ and the initial guess density (ρ_0) based on 3D convolutional neural networks (CNNs), was developed. The high accuracy and transferability of DeepSCF were successfully demonstrated across various systems, ranging from molecular to infinitely extended DNA structures. Here, we present recent developments of DeepSCF, including the incorporation of three-dimensional depthwise separable convolutional layers, physics-informed descriptors, and optimization approaches. We also briefly present preliminary work related to various applications of the DeepSCF approach, including machine learning-based *ab-initio* molecular dynamics and quantum transport simulations. This work provides insights into new directions for the development of machine learning-based atomistic materials simulations.