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)

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Table of Content

Workshop Program

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

7월 9일 (목) — Day 1

09:20	**학회 시작 인사**
Session 1	**Machine Learning Applications** 좌장: 한승우 (서울대)
09:30 ~10:10	**이광렬** · KIST *Scientific communication in the future AI-Dominated era*
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*
11:30 ~13:00	🍱 점심식사
Session 2	**Correlated Oxide Materials** 좌장: 김흥식 (KENTECH)
13:00 ~13:40	**김충현** · 아주대 *From Jahn-Teller distortions to spin-orbital entanglement: pathways to Mott metal-insulator*
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*
17:00 ~20:00	🍽 **Poster Session & Dinner**

7월 10일 (금) — Day 2

Session 4	**New Methodology Developments** 좌장: 심은지 (연세대)
09:30 ~10:10	**김용훈** · KAIST *Machine learning and human learning of local chemical bonding characters*
10:10 ~10:50	**김인구** · 삼성전자 *Very-large-scale density functional theory on massively parallel GPUs*
10:50 ~11:20	☕ Coffee Break
Session 5	**Emergent Phenomena** 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 *The role of dynamical electron correlations on lattice dynamics*
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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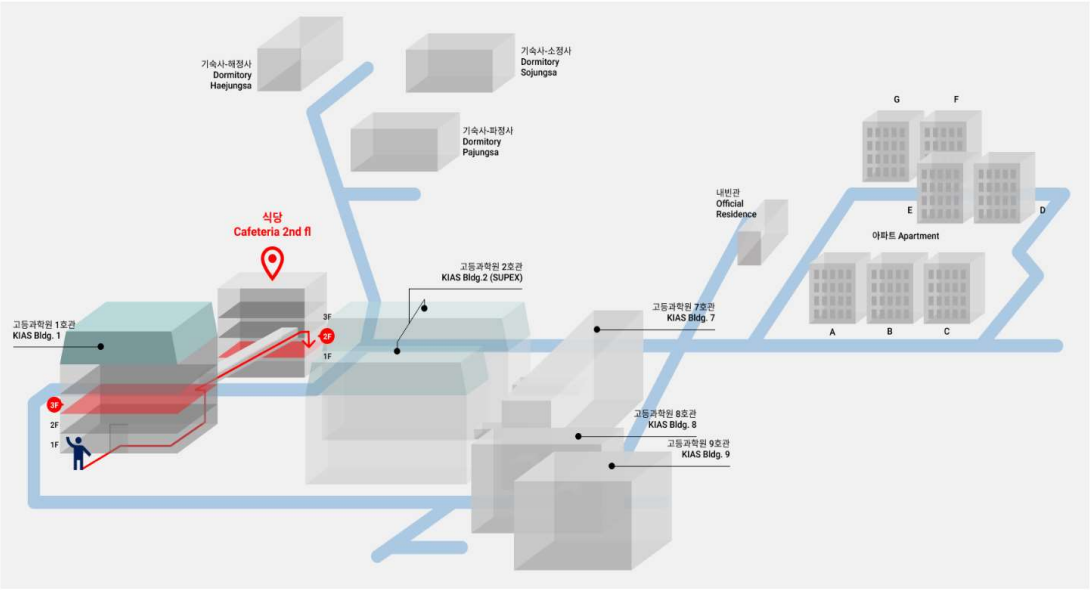
2. 포스터 발표자 이름, 포스터 제목
3. 포스터 발표자 이름, 포스터 제목
4. 포스터 발표자 이름, 포스터 제목

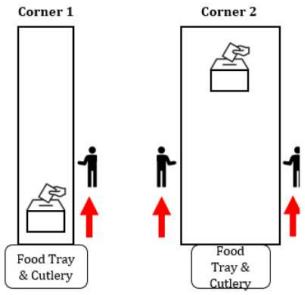
Bldg.1 to Cafeteria

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.

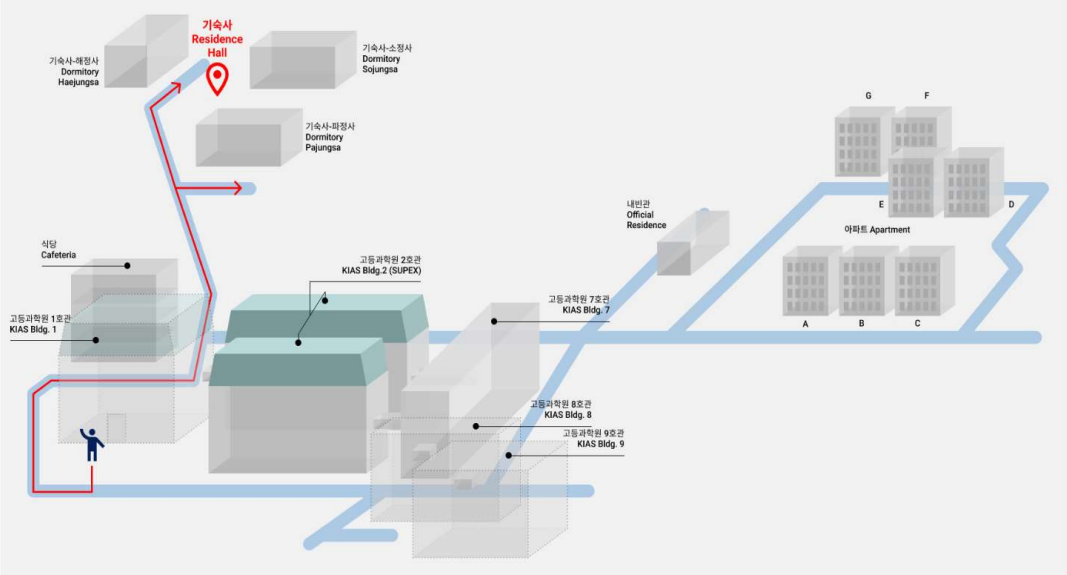


Lunch Coupon Usage

- 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

The role of dynamical electron correlations on lattice dynamics

Sun-Woo Kim

Department of Physics, Hanyang University

Strongly correlated materials have long been a central focus of condensed matter physics due to the rich and exotic phenomena they exhibit, including unconventional superconductivity and quantum magnetism. Decades of theoretical efforts have aimed at properly describing electron correlations on top of density functional theory (DFT), using methods such as DFT+U, which captures static correlations, and DFT+DMFT (dynamical mean-field theory), which accounts for dynamical correlations. Nevertheless, despite their well-established role in accurately describing electronic structures, the influence of electron correlations on lattice dynamics remains poorly understood, even in elemental correlated metals.

Here, we demonstrate that dynamical correlations are essential to quantitatively describe both electronic structures and phonon dispersions in elemental nickel and iron. Moreover, dynamical correlations can drive qualitatively opposite trends compared to static correlations in the dependence of phonon frequencies on correlation strength, a behavior that generalizes to more complex systems such as unconventional superconductors. We further show how dynamical correlations uniquely capture phonon phenomena, including novel spin-phonon coupling in the normal state of unconventional superconductors. These findings establish the fundamental role of dynamical correlations in lattice properties, providing a foundation for predictive modeling of strongly correlated materials.

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 hig h-accuracy many-body energy test that helps reduce the gap between experiment and stan dard theory, thereby making the RuO_2 analysis more consistent.

ABSTRACTS OF POSTERS