PROGRAM AND ABSTRACTS

제21회 고등과학원 전자구조계산학회

2025년 7월 10일(목) – 7월 11일(금)

고등과학원 1호관 대강당

초청연사

강창종 (충남대)
김흥식 (강원대)
박세영 (숭실대)
박진수 (포항공대)
박철환 (서울대)
박환열 (순천향대)
신민철 (한국과학기술원)
심은지 (연세대)
야나노세 구니히로 (고등과학원)
양우일 (고등과학원)
임성현 (울산대)
장석주 (CUNY)
장현주 (한국화학연구원)
진호섭 (울산과학기술원)
최영우 (서강대)
현상일 (한국세라믹기술원)
홍성민 (광주과학기술원)

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

김혜미 (고등과학원) 이메일: hmkim@kias.re.kr

TABLE OF CONTENTS

7월 10일(목)	
8:30 – 9:00 등록	
Session 1 **Machine Learning**	**09:00 ~ 09:40** **장현주 (KRICT)** Data~driven Materials Research with Experimental Research Data
	09:40 ~ 10:20 **현상일 (한국세라믹기술원)** AI~driven Real~Time Optimization using Multiscale and Multiphysics Simulation of Ceramic Sintering
10:20 ~ 10:50 Coffee Break	
Session 2 **Correlated and complex phenomena**	**10:50 ~ 11:30** **김흥식 (강원대)** Complex~time evolution of tensor networks for dynamics of correlated systems
	11:30 ~ 12:10 **박세영 (숭실대)** Ferroelectricity and inter~site Coulomb interactions
	12:10 ~ 12:50 **장석주 (CUNY)** Rate theories and computational modeling of transitions and nonradiative decay of electronic excited states of molecules
12:50 – 14:00 Lunch	
Session 3 **Device & Multiscale**	**14:00 ~ 14:40** **신민철 (KAIST)** DFT~based Multiscale Transport Calculation for IGZO Channel Devices
	14:40 ~ 15:20 **홍성민 (GIST)** Self~Consistency and Convergence Acceleration in Semiconductor Device Simulation
	15:20 ~ 16:00 **박환열 (순천향대)** Multiscale Computational Fluid Dynamics for Industrial Spatial Atomic Layer Deposition: Advanced Chamber Design and Process Strategy
16:00 ~ 16:30 Coffee Break	
Session 4 **Development of DFT methods**	**16:30 ~ 17:10** **심은지 (연세대)** Extending Density~Corrected DFT: From Molecular Systems to Solids
	17:10 ~ 17:50 **양우일 (KIAS)** Effects of spin-orbit coupling in extended Hubbard-corrected DFT
Poster Session	**18:10 ~ 20:00** **포스터 발표**

7월 11일(금)	
8:30 – 9:00 등록 및 준비	
Session 5 **Quantum and Nano**	**09:00 ~ 09:40** **최영우 (서강대)** One~dimensional van der Waals single~chain materials
	09:40 ~ 10:20 **야나노세 구니히로 (KIAS)** Large-scale electronic structure calculations of trilayer moiré-of-moiré systems
10:20 ~ 10:50 Coffee Break	
Session 6 **Phonon physics**	**10:50 ~ 11:30** **박철환 (서울대)** Plasmon~phonon hybridization in doped semiconductors and phonon linewidths due to phonon~dressed~electron coupling
	11:30 ~ 12:10 **박진수 (POSTECH)** Spin~phonon interaction and spin dynamics from first~principles
12:10 – 13:30 Lunch	
Session 7 **Magnetism**	**13:30 ~ 14:10** **임성현 (울산대)** Why Fe3GaTe2 has higher TC than Fe3GeTe2?
	14:10 ~ 14:50 **진호섭 (UNIST)** Odd~parity spin textures in compensated coplanar magnets
	14:50 ~ 15:30 강창종 (충남대) Electronic Structure of the Altermagnetic System MnTe and Symmetry Analysis of Its Physical Properties
Session 8 **시상 및 폐회**	**15:30 ~ 16:00** **우수 포스터 시상식 및 폐회**

시간표

7월 10일

08:30 ~ 09:00 등록

Session 1: Machine Learning

09:00 ~ 09:40 장현주 (KRICT) - Data-driven Materials Research with Experimental Research Data
09:40 ~ 10:20 현상일 (한국세라믹기술원) - AI-driven Real-Time Optimization using Multiscale and Multiphysics Simulation of Ceramic Sintering

10:20 ~ 10:50 휴식

Session 2: Correlated and complex phenomena

10:50 ~ 11:30 김흥식 (강원대) - Complex-time evolution of tensor networks for dynamics of correlated systems
11:30 ~ 12:10 박세영 (숭실대) - Ferroelectricity and inter-site Coulomb interactions
12:10 ~ 12:50 장석주 (CUNY) - Rate theories and computational modeling of transitions and nonradiative decay of electronic excited states of molecules

12:50 ~ 14:00 점심식사

Session 3: Device & Multiscale

14:00 ~ 14:40 신민철 (KAIST) - DFT-based Multiscale Transport Calculation for IGZO Channel Devices
14:40 ~ 15:20 홍성민 (GIST) - Self-Consistency and Convergence Acceleration in Semiconductor Device Simulation
15:20 ~ 16:00 박환열 (순천향대) - Multiscale Computational Fluid Dynamics for Industrial Spatial Atomic Layer Deposition: Advanced Chamber Design and Process Strategy

16:00 ~ 16:30 휴식

Session 4: Development of DFT methods

16:30 ~ 17:10 심은지 (연세대) - Extending Density-Corrected DFT: From Molecular Systems to Solids
17:10 ~ 17:50 양우일 (KIAS) - Effects of spin-orbit coupling in extended Hubbard-corrected DFT

18:10 ~ 20:00 포스터세션

7월 11일

08:30 ~ 09:00 등록및준비

Session 5: Quantum and Nano

09:00 ~ 09:40 최영우 (서강대) - One-dimensional van der Waals single-chain materials
09:40 ~ 10:20 야나노세 구니히로 (KIAS) - Large-scale electronic structure calculations of trilayer moiré-of-moiré systems

10:20 ~ 10:50 휴식

Session 6: Phonon physics

10:50 ~ 11:30 박철환 (서울대) - Plasmon-phonon hybridization in doped semiconductors and phonon linewidths due to phonon-dressed-electron coupling

11:30 ~ 12:10 박진수 (POSTECH) - Spin-phonon interaction and spin dynamics from first-principles

12:10 ~ 13:30 점심식사

Session 7: Magnetism

13:30 ~ 14:10 임성현 (울산대) -Why Fe_3GaTe_2 has higher T_C than Fe_3GeTe_2?
14:10 ~ 14:50 진호섭 (UNIST) - Odd-parity spin textures in compensated coplanar magnets
14:50 ~ 15:30 강창종 (충남대) Electronic Structure of the Altermagnetic System MnTe and Symmetry Analysis of Its Physical Properties

15:30 ~ 16:00 우수포스터시상식

ABSTRACTS OF TALKS

Talk No.1

Data-driven Materials Research with Experimental Research Data

Hyunju Chang

Korea Research Institute of Chemical Technology (KRICT)

Email: hjchang@krict.re.kr

Recently, numerous data-driven studies have been reported in materials science. These studies primarily utilize databases from first-principles calculations or the existing literature. However, based on computational data, machine learning prediction models often face limitations due to computational properties. Additionally, the literature provides limited champion data from experiments. Therefore, it is essential to build a machine-learning prediction model based on experimental research data, including the “dark results," to develop new materials efficiently. In this presentation, I will share our recent projects that gather experimental data throughout the entire material development cycle. To facilitate data collection, we have built web-based platforms and developed a machine-learning prediction model for various applications based on this data. I will cover the following topics as examples: [1] Perovskite Solar Cell Data Platform, [2] Development of SnSe-based thermoelectric materials, and [3] Closed-loop optimization of catalysts for oxidative propane dehydrogenation with CO2.

[1] https://solar.chemdx.org/
[2] Yea-Lee Lee et al., J. Am. Chem. Soc. 144, 13748 (2022) & APL Mater. 11, 041111 (2023)
[3] Jin-Soo Kim et al., Journal of CO2 Utilization, 78, 102620 (2023)

Talk No.2

AI-driven Real-Time Optimization using Multiscale and Multiphysics Simulation of Ceramic Sintering

Sangil Hyun

Korea Institute of Ceramic Engineering & Technology (KICET)

Ceramic sintering is a complex process influenced by thermal, mechanical, and diffusion-driven phenomena across multiple length and time scales. To address these challenges, we have developed a virtual engineering platform that integrates multiscale and multiphysics simulations with artificial intelligence (AI)-driven real-time optimization. This hierarchical modeling strategy incorporated continuum scale analysis with atomic scale simulation enables a comprehensive understanding of atomic-scale diffusion mechanisms, microstructural evolution, and macroscopic densification behavior. Furthermore, AI-based machine learning algorithms analyze simulation data to predict optimal processing conditions dynamically, enabling adaptive control of sintering parameters. By combining real-time optimization with physics-based simulations, the system minimizes defects, enhances material properties, and improves process efficiency. The simulation results are validated against experimental data, demonstrating the effectiveness of AI-enhanced scale-bridging modeling for optimizing ceramic sintering processes. This approach provides valuable insights for the intelligent manufacturing of advanced ceramics, enabling improved product quality and production efficiency.

Talk No.3

Complex-time evolution of tensor networks for dynamics of correlated systems

Heung-Sik Kim[1,2], Hyun-Yong Lee[3,4]

[1]Department of Semiconductor Physics and Institute for Quantum Convergence Technology, Kangwon National University, Chuncheon 24341, Korea
[2]Interdisciplinary Program in Earth Environmental System Science and Engineering, Kangwon National University, Chuncheon 24341, Republic of Korea
[3]Division of Semiconductor Physics, Korea University, Sejong 30019, Korea
[4]Department of Applied Physics, Graduate School, Korea University, Sejong 30019, Korea

Studying the real-time dynamics of strongly correlated systems poses significant challenges, which have recently become more manageable thanks to advances in density matrix renormalization group (DMRG) and tensor network methods. A notable development in this area is the introduction of a complex-time evolution scheme for tensor network states, originally suggested for solving Anderson impurity model and designed to suppress the growth of entanglement under time evolution. In this study, we employ the complex-time evolution scheme to investigate 1) the dynamics of one-dimensional spin systems and 2) the spectral properties of multi-orbital Anderson impurity models for application to the dynamical mean-field theory. In the spin model case, we study the dynamic critical exponent of the transverse-field Ising model and the dynamical structure factor of the XXZ model across the gapped and gapless phases. In the Anderson impurity model case, we employ a fork tensor network model and obtain self-energies directly in the real-frequency domain, which enables obtaining high-energy features in the spectral functions of several systems like $SrVO_3$ and CuV_2S_4. In both cases, complex-time evolution reproduces the results of real-time evolution while mitigating the rapid growth of quantum entanglement typically associated with the latter, providing a robust and efficient framework for studying the dynamics of correlated quantum systems.

Talk No.4

Ferroelectricity and inter-site Coulomb interactions

Se Young Park[1]

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

Ferroelectricity, showing switchable polarization emerging from spontaneous inversion symmetry breaking, has been actively investigated due to the wide range of applications such as high-fidelity memory devices, actuators/transducers, and high-K dielectrics. Various mechanisms that induce ferroelectricity are reported, ranging from the pseudo-Jahn-Teller effect for inducing polar distortions of conventional ferroelectrics to the correlation-induced charge transfer in electronic ferroelectrics. We focus on the role of the Coulomb interaction in stabilizing the polar phases, as it modulates the covalency and charge fluctuations. In the first part of the talk, we explore how Coulomb interactions influence the properties of conventional ferroelectrics. By utilizing the Agapito-Curtarolo-Buongiorno Nardelli pseudohybrid Hubbard functional (ACBN0) with on-site and inter-site interactions, we show the importance of the inter-site Coulomb interaction in reproducing correct band gap values and stabilizing the polar phases. In the second part, we discuss the role of the Coulomb interaction in charge-ordered ferroelectricity by investigating the one-dimensional Hubbard-Holstein model using the density-matrix renormalization group (DMRG) method. The phase diagram in terms of on-site and inter-site Coulomb interactions and polaronic coupling are obtained, showing that the inter-site Coulomb repulsion is crucial in stabilizing the polar charge-ordered phases. Our results stress the importance of the inter-site Coulomb interactions in describing both the stability and properties of a wide range of ferroelectric materials.

Talk No.5

Rate theories and computational modeling of transitions and nonradiative decay of electronic excited states of molecules

Seogjoo J. Jang[1,2]

[1]*Department of Chemistry and Biochemistry, Queens College, City University of New York, Queens, NY, USA;*
PhD Programs in Chemistry and Physics, Graduate Center, City University of New York, New York, NY, USA
[2]*School of Computational Sciences, Korea Institute for Advanced Study, Seoul, Korea*

The dynamics accompanying or ensuing the electronic excitation of molecular systems in complex environments occur over a broad range of time scales, entailing various microscopic mechanisms. Thus, it is important to treat those mechanisms carefully for proper characterization of the relaxation and decay of electronic excited states. For the past two decades, there have been significant advances in real time dynamics methods addressing relatively fast processes in electronic excited states. However, for slower and for more broad range of time scales, rate equation approaches remain proper or only available ways to address relatively slow processes that are important for the functionality of molecules and materials. While seminal rate theories addressing these issues have existed, many of them need further refinement and improvement in order to account for important molecular details that are revealed from modern experimental and computational studies. This talk provides an overview of our rate theories for resonance energy transfer and their applications to biological light harvesting complexes and organic dye molecules, and then describes a recent work on computational modeling of nonradiative decay of excited states due to non-adiabatic derivative couplings (NDCs). A general theory is also presented starting from the molecular Hamiltonian expressed in the basis of adiabatic electronic and nuclear position states, where a compact and complete expression for the NDC term is obtained. For a generic and widely used model where all nuclear degrees of freedom and environmental effects are represented as linearly coupled harmonic oscillators, the new formulation results in a closed-form rate expression that is easy to evaluate, while accounting for non-Condon effects due to the NDC terms. Model calculations highlight important non-Condon effects. Application of the theory to the nonradiative decay from the first excited singlet state of azulene illustrates the utility of the theory and challenges for quantitative modeling of nonradiative decay processes involving competing electronic pathways.

Talk No.6

DFT-based Multiscale Transport Calculation for IGZO Channel Devices

Mincheol Shin

School of Electrical Engineering
Korea Advanced Institute of Science and Technology, Daejeon 34141, Rep. of Korea

Indium gallium zinc oxide (IGZO) oxide semiconductor is currently the subject of significant research for future semiconductor applications due to its high mobility, low leakage current, and potential for 3D stackable DRAMs. In this work, we present a density functional theory (DFT)-based approach to evaluate the electrical properties of crystalline IGZO (c-IGZO) channel materials. By directly utilizing DFT-generated samples and their Hamiltonians, we compute the cation disorder-limited mobilities, obtaining results that are in good agreement with experimental data. To enable calculations for larger device structures, we develop a multiscale model Hamiltonian that faithfully reproduces atomistic results. Our method thus allows for a rigorous and efficient assessment of IGZO electrical properties across a wide composition space, from Zn-rich to In-rich cases. We also investigate the impact of dimensional confinement, revealing mobility enhancements in thin-body and nanowire structures. Furthermore, fully quantum-mechanical, non-equilibrium Green's function simulations of IGZO channel nanowire transistors incorporating cation disorder and phonon scattering effects are performed, which show disorder-induced threshold voltage variations and reduced ON-state currents.

Our multiscale framework, built on first-principles calculations, represents a significant advancement in transport modeling and simulations for c-IGZO devices. An innovative method is also developed that reduces computational cost by several orders of magnitude. Our approach can be extended to investigate the transport properties of amorphous IGZO channel devices as well as other oxide semiconductor channel devices.

Talk No.7

Self-Consistency and Convergence Acceleration in Semiconductor Device Simulation

Sung-Min Hong[1]

[1]*Semiconductor Device Simulation Laboratory, Department of Electrical Engineering and Computer Science, Gwangju Institute of Science and Technology*

Semiconductor device simulation is a kind of transport simulation that models the movement of charge carriers, such as electrons and holes, within semiconductor devices. Since these carriers are charged, they, along with the externally applied bias voltages, generate the electric field within the semiconductor device. The simulation must simultaneously satisfy both the transport equation and the Poisson equation. In order to obtain a self-consistent solution, the Newton-Raphson method is typically employed, but it requires a large number of iterations, making the process computationally expensive. The presence of external bias voltages further increases the computational burden.

In this work, we review recent efforts to accelerate the semiconductor device simulation by providing an approximate solution directly under non-equilibrium bias conditions.

One approach, proposed in [1], utilizes neural networks trained to learn the solution space. Once trained, these neural networks can predict approximate solutions. It has been shown that this approach can be applied to various devices. However, this method has limitations when applied to previously unseen device structures.

As an alternative way, in [2], the quasi-one-dimensional (quasi-1D) model is developed. This model simultaneously the 1D continuity equation and the compact charge model [3] simultaneously and efficiently. By using the cross-sectional quasi-Fermi potential, an approximate solution can be generated. Applications to nanosheet transistors have been demonstrated, showcasing its effectiveness.

After presenting these two approaches, we discuss potential future research directions.

Acknowledgement
This research was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (NRF-2023R1A2C2007417).

References
[1] S.-C. Han, J. Choi, and S.-M. Hong, *IEEE Transactions on Electron Devices*, **68**, 5483 (2021)
[2] K.-W. Lee and S.-M. Hong, *Solid-State Electronics*, **199**, 108527 (2023)
[3] K.-W. Lee and S.-M. Hong, *IEEE Transactions on Electron Devices*, **69**, 3014 (2022)

Talk No.8

Multiscale Computational Fluid Dynamics for Industrial Spatial Atomic Layer Deposition: Advanced Chamber Design and Process Strategy

Hwanyeol Park[1,2], Yunseok Kim[1,2], Seulwon Choi[1,2], Huichan Kang[1,2]

[1]*Department of Display Materials Engineering, Soonchunhyang University, Asan, Chungnam 31538, Republic of Korea*

[2]*Department of Electronic Materials, Devices, and Equipment Engineering, Soonchunhyang Uni-versity, Asan, Chungnam 31538, Republic of Korea*

Spatial atomic layer deposition (SALD) has emerged as an advanced variant of conventional ALD, offering precise atomic-scale control while significantly enhancing throughput. In this approach, a wafer traverses distinct precursor and purge gas zones within a single chamber, thereby enabling rapid layer-by-layer film growth. By fast ALD cycles through high-flow precursor and purging regions, SALD can reduce processing time to approximately 10 times compared to traditional methods. However, minimizing intermixing among the precursor gases requires careful engineering of reactor geometry and flow dynamics. To address these design challenges, we employed computational fluid dynamics (CFD) in combination with density functional theory (DFT) calculations, focusing on the temporal evolution of flow fields and surface reactions during Al_2O_3 deposition using trimethylaluminum (TMA) and water (H_2O). Our results indicate that reactor design—particularly purging strategy (top vs. bottom) and process pressure—strongly influences precursor distribution and film uniformity. Bottom purging under lower operating pressures (e.g., 10 Torr) effectively suppresses vortex formation and reduces CVD-like gas-phase reactions, in contrast to top purging. Moreover, the integrated CFD–DFT framework accurately captures the self-limiting, cycle-to-cycle growth rate (~1.3 Å/cycle), aligning closely with experimental observations. These findings highlight the advantages of combining reactor-scale fluid simulations with quantum-level chemical insights to optimize SALD reactor design and achieve fast and uniform deposition of high-quality thin films.

Talk No.9

Extending Density-Corrected DFT: From Molecular Systems to Solids

Eunji Sim[1]

[1]*Department of Chemistry, Yonsei University, Seoul 03722 KOREA*

Density-Corrected Density Functional Theory (DC-DFT) has emerged as a powerful approach for diagnosing and mitigating errors in electronic structure calculations. However, inconsistencies in the application of DC-DFT error decomposition can lead to misinterpretations. In this work, we critically examine the definition and implementation of DC-DFT error decomposition to ensure a more rigorous distinction between functional errors and density-driven errors, clarifying their respective roles in computational accuracy. Additionally, we extend this framework beyond small molecular systems to complex molecules and solid-state materials, demonstrating its robustness and broad applicability. By refining the methodology for error analysis, this study enhances the theoretical foundation of DC-DFT and expands its potential applications in computational chemistry and materials science.

Talk No.10

Effects of spin-orbit coupling in extended Hubbard-corrected DFT

Wooil Yang[1]

[1]*Korea Institute for Advanced Study, Seoul, Republic of Korea*

In this talk, we present an *ab initio* computational method correcting the conventional DFT by adding both on-site (U) and inter-site (V) Hubbard interactions (DFT+U+V) [1,2]. Recently, this approach has been generalized to a noncollinear spin framework to account for spin-orbit coupling [3]. A key feature of our method is the self-consistent determination of the Hubbard U and V parameters during each step of the self-consistent field cycle, rather than fixing them in advance. This on-the-fly calculation uses a Hartree–Fock-based formalism [4] to ensure local and non-local interactions are treated on equal footing [1,2]. By explicitly including spin-orbit coupling, our DFT+U+V calculations accurately predict spin-orbit splitting and hole effective masses in semiconductors. In low dimensional materials such as Bi_2Se_3 and Bi_2Te_3, we find that incorporating both U and V corrections significantly improves the reliability of predicted properties. Although the computational cost is moderately higher compared to conventional DFT, this method remains well-suited for large-scale systems with strong electron correlation and pronounced relativistic effects, for which more conventional approaches may struggle to maintain both accuracy and computational feasibility.

References

[1] S.-H. Lee and Y.-W. Son, Phys. Rev. Res. **2**, 043410 (2020).
[2] N. Tancogne-Dejean and A. Rubio, Phys. Rev. B **102**, 155117 (2020).
[3] W. Yang and Y.-W. Son, Phys. Rev. B **110**, 155133 (2024).
[4] L. A. Agaptio, et al., Phys. Rev. X **5**, 011006 (2015).

Talk No.11

One-dimensional van der Waals single-chain materials

Young Woo Choi[1]

[1]*Department of Physics and Center for Nanomaterials, Sogang University, Seoul, Korea 04107*

Low-dimensional materials offer exceptional platforms for exploring fundamental physics and enabling technological advancements. Although significant progress has been made with two-dimensional (2D) van der Waals materials, there has been recently growing interest in one-dimensional (1D) van der Waals single-chain systems. Specifically, encapsulating single-chain structures within nanotubes offers a controlled, protective environment, effectively shielding the fragile 1D chains from environmental degradation. Furthermore, this confinement stabilizes novel crystal structures unattainable in bulk or 2D structures. In this talk, we discuss our computational studies of 1D single-chain materials encapsulated within nanotubes. We focus on MX_3 (M = Cr, V; X = Cl, Br, I) magnetic single-chains [1], tetrahedral GeX_2 (X = S, Se) structures [2,3], and phosphorus-based nanostructures [4]. Through collaboration with experiments, our density functional theory (DFT) calculations reveal how structural confinement within nanotubes leads to unique atomic arrangements, such as face-sharing octahedra in MX_3 chains, modified tetrahedral connectivity in GeX_2 chains, and distinctive phosphorus nanorings and nanohelices. Our findings highlight the promise of 1D single-chain materials as platforms for exploring novel physics and potential technological applications in the single-chain limit.

[1] Y. Lee, Y. W. Choi, K. Lee, C. Song, P. Ercius, M. L. Cohen, K. Kim, and A. Zettl, Advanced Materials **35**, 2307942 (2023).
[2] Y. Lee, Y. W. Choi, K. Lee, C. Song, P. Ercius, M. L. Cohen, K. Kim, and A. Zettl, ACS Nano **17**, 8734 (2023).
[3] Y. Lee, Y. W. Choi, L. Li, W. Zhou, M. L. Cohen, K. Kim, and A. Zettl, ACS Nano **18**, 17882 (2024).
[4] Y. W. Choi, Y. Lee, K. Kim, A. Zettl, and M. L. Cohen, ACS Nano, *accepted* (2025).

Talk No.12

Large-scale electronic structure calculations of trilayer moiré-of-moiré systems

Kunihiro Yananose[1], Changwon Park[2], and Young-Woo Son[1]

[1]*Korea Institute for Advanced Study, Seoul 02455, Republic of Korea*
[2]*Department of Physics, Ewha Womans University, Seoul 03760, Republic of Korea*

Over the past decade, moiré materials such as twisted bilayer graphene have been extensively studied as novel platforms for emergent phenomena. Lattice reconstruction of the moiré superlattice can significantly modify its electronic structure. In trilayer moiré-of-moiré systems, the increased stacking possibility enriches diversity in the stacking order, thus offering higher tunability of electronic structure. To explore such possibilities, we developed new methodologies that can achieve a first-principles level of accuracy in calculating relaxed structures and electronic properties of moiré systems containing a few million atoms [1]. Using these methodologies, we investigated twisted trilayer graphenes (TTGs) [1] and twisted trilayer hexagonal boron nitrides (TTBNs) [2] in a very small twist angle regime (~0.1°). In the first part of this talk, we will discuss the unconventional stacking domain tessellations in these materials and their underlying physics [1]. The second part will present the electronic structure of TTG [1]. In the third part, we will discuss the electronic structure of TTBN, where we predict a well-ordered array of quantum dot states resembling quantum harmonic oscillators [2]. Notably, these quantum dot arrays are reconfigurable via an external electric field, which is impossible in the twisted bilayer systems. This tunability suggests their substantial potential for quantum applications, from array-based single-photon sources to scalable quantum processors.

[1] D. Park, C. Park, K. Yananose et al., *Nature* 641, 896 (2025).
[2] K. Yananose, C. Park, and Y.-W. Son, *arxiv*:2504.14925 (2025).

Talk No.13

Plasmon-phonon hybridization in doped semiconductors and phonon linewidths due to phonon-dressed-electron coupling

Cheol-Hwan Park[1,2]

[1]*Department of Physics and Astronomy, Seoul National University, Seoul 08826, Korea*
[2] *Center for Theoretical Physics, Seoul National University, Seoul 08826, Korea*

Interactions between electrons, phonons, and plasmons in solids give rise to many interesting phenomena. First-principles computational techniques have played an important role in the investigation of these phenomena. In this presentation, I will talk about first-principles methods to calculate the plasmon-phonon hybridization in doped semiconductors [1] and the non-adiabatic phonon self-energy due to coupling to electrons with finite linewidths [2].

References

[1] J.-M. Lihm and C.-H. Park, "Plasmon-Phonon Hybridization in Doped Semiconductors from First Principles." Phys. Rev. Lett. **133**, 116402 (2024).
[2] C.-H. Park, "Non-adiabatic phonon self-energy due to electrons with finite linewidths," arXiv:2411.12221v1.

Talk No.14

Spin-phonon interaction and spin dynamics from first-principles

Jinsoo Park[1]

[1]*Department of Physics, Pohang University of Science and Technology (POSTECH), Pohang 37673, Korea*

First-principles calculations enable accurate predictions of electronic interactions and dynamics. However, computing the electron spin dynamics remains challenging. The spin-orbit interaction causes various dynamical phenomena that couple with phonons, such as spin precession and spin-flip electron-phonon scattering, which are difficult to describe with current first-principles calculations. In this talk, I will present a rigorous framework to study phonon-induced spin relaxation and decoherence, by computing the spin-spin correlation function and its vertex corrections due to electron-phonon interactions. I will apply this approach to a model system and develop corresponding first-principles calculations of spin relaxation in GaAs. These calculations show that our vertex-correction formalism can capture the Elliott-Yafet, Dyakonov-Perel, and strong-precession mechanisms - three independent spin decoherence regimes with distinct physical origins - thereby unifying their theoretical treatment and calculation. Our method is general and enables quantitative studies of spin relaxation, decoherence, and transport in a wide range of materials and devices.

Talk No.15

Why Fe_3GaTe_2 has higher T_C than Fe_3GeTe_2?

Sonny H. Rhim[1], Bomin Kim[1], Tumentsereg Ochirkhuyag[2], Dorj Odkhuu[2]

[1] Department of Physics, University of Ulsan, Korea, [2] Department of Physics, Incheon National University, Korea

Physics of Fe_3GaTe_2 [1-3] having higher T_C than Fe_3GeTe_2 is explored theoretically in the framework of magnetic exchange interactions[4-6]. Fe_3GaTe_2, with just one less electron isostructural to Fe_3GeTe_2, has smaller J_1 and J_2, the first and second nearest neighbor exchange, which is against the common belief that larger J_1 or J_2 are essential for higher T_C. We show that higher order exchange coefficients, J_3 or higher, of Fe_3GaTe_2 are positive whereas those of Fe_3GeTe_2 are negative. As a consequence, total sum of all possible exchange coefficients in Fe_3GaTe_2 are larger than Fe_3GeTe_2, which accounts for higher T_C. To verify, T_C are evaluated using mean-field approach as well as Monte Carlo simulation. Indeed, the higher-order exchange coefficients with properly including number neighbors confirms Fe_3GaTe_2's higher T_C.

Reference

[1] D. Li, S. Haldar, T. Drevelow, and S. Heinze, Phys. Rev. B **107**,104428 (2023).

[2] W. Jin, G. Zhang, H. Wu, L. Yang, W. Zhang, and H. Chang, ACS Appl. Mater. Interfaces. **15**, 36519 (2023).

[3] C. Wang, J. Wang, W.-Q. Xie, G. Zhang, H. Wu, J. Zhou, X. Zhu, W. Ning, G. Wang, C. Tan, et al., Phys. Rev. B **107**, L140409 (2023).

[4] A. I. Liechtenstein, M. Katsnelson, V. Antropov, and V. Gubanov, J. Magn. Magn. Mater. **67**, 65 (1987). [5] H. Yoon, T. J. Kim, J.-H. Sim, S. W. Jang, T. Ozaki, and M. J. Han, Phys. Rev. B **97**, 125132 (2018).275

[6] H. Yoon, T. J. Kim, J.-H. Sim, and M. J. Han, Comput. Phys.Commun. **247**, 106927 (2020).

Talk No.16

Odd-parity spin textures in compensated coplanar magnets

Hosub Jin[1]

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

Altermagnetism is a new state of the compensated magnet where spin texture appears in momentum space. Besides the collinear altermagnets, odd-parity spin textures can be obtained from various compensated coplanar magnets. For example, helimagnetic ordering hosts a *p*-wave magnet, and √3×√3 spin ordering in triangular and Kagome lattices links to an *f*-wave magnet. In this talk, we discuss how the curved spin-space of the coplanar noncollinear spin ordering induces effective spin-dependent gauge fields to produce such an odd-parity spin texture. Furthermore, we show that compensated coplanar magnets can host more diverse spin textures.

Talk No.17

Electronic Structure of the Altermagnetic System MnTe and Symmetry Analysis of Its Physical Properties

Chang-Jong Kang[1]

[1]*Department of Physics, Chungnam National University, Daejeon 34134, Korea*

Altermagnetism is a recently identified fundamental form of magnetism characterized by vanishing net magnetization and a broken electronic structure with time-reversal symmetry. In this talk, we discuss the electronic structure and symmetry properties of the altermagnetic material MnTe. We reveal that the crystallographic symmetry groups of numerous magnetic materials with negligibly small relativistic spin-orbit coupling (SOC) are significantly larger than conventional magnetic groups. Consequently, a symmetry description incorporating partially decoupled spin and spatial rotations, termed the spin group, becomes essential. We establish classifications of spin groups that describe collinear magnetic structures, encompassing altermagnetic phases. Using MnTe as an example, we provide direct evidence of its altermagnetic nature and analyze the implications of its electronic structure on its physical properties.

ABSTRACTS OF POSTERS

Poster No.1

Quantum Computing Based Design of Multivariate Porous Materials

Shinyoung Kang, Jihan Kim*

Department of Chemical and Biomolecular Engineering, Korea Advanced Institute of Science and Technology 291 Daehak-ro, Yuseong-gu, Daejeon 34141, Republic of Korea

Multivariate (MTV) porous materials exhibit unique structural complexities based on their diverse spatial arrangements of multiple building block combinations. These materials possess potential synergistic functionalities that exceed the sum of their individual components. However, the exponentially increasing design complexity of these materials poses significant challenges for accurate ground-state configuration prediction and design. To address this, we propose a Hamiltonian model for quantum computing that integrates compositional, structural, and balance constraints directly into the Hamiltonian, enabling efficient optimization of the MTV configurations. The model employs a graph-based representation to encode linker types as qubits. Our framework leads to exponentially efficient exploration of a vast search space of the linkers to identify optimal configurations based on predefined design variables. To validate our model, a variational quantum circuit was constructed and executed using the Sampling VQE algorithm in the IBM Qiskit. Simulations on experimentally known MTV porous materials (e.g. Cu-THQ-HHTP, Py-MV-DBA-COF, MUF-7, and SIOC-COF2) successfully reproduced their ground-state configurations, demonstrating the validity of our model. Furthermore, VQE calculations were performed on a real IBM 127-qubit quantum hardware for validation purposes signaling a first step toward a practical quantum algorithm for the rational design of porous materials.

Poster No.2

Inverse Design of Metal-Organic Framework using Quantum Natural Language Processing

Shinyoung Kang, Jihan Kim*

Department of Chemical and Biomolecular Engineering, Korea Advanced Institute of Science and Technology 291 Daehak-ro, Yuseong-gu, Daejeon 34141, Republic of Korea

In this study, we explore the potential of using quantum natural language processing (QNLP) to inverse design metal-organic frameworks (MOFs) with targeted properties. Specifically, by analyzing 450 hypothetical MOF structures consisting of 3 topologies, 10 metal nodes and 15 organic ligands, we categorize these structures into four distinct classes for pore volume and CO_2 Henry's constant values. We then compare various QNLP models (i.e. the bag-of-words, DisCoCat (Distributional Compositional Categorical), and sequence-based models) to identify the most effective approach to process the MOF dataset. Using a classical simulator provided by the IBM Qiskit, the bag-of-words model is identified to be the optimum model, achieving validation accuracies of 88.6% and 78.0% for binary classification tasks on pore volume and CO_2 Henry's constant, respectively. Further, we developed multi-class classification models tailored to the probabilistic nature of quantum circuits, with average test accuracies of 92% and 80% across different classes for pore volume and CO_2 Henry's constant datasets. Finally, the performance of generating MOF with target properties showed accuracies of 93.5% for pore volume and 87% for CO_2 Henry's constant, respectively. Although our investigation covers only a fraction of the vast MOF search space, it marks a promising first step towards using quantum computing for materials design, offering a new perspective through which to explore the complex landscape of MOFs.

Poster No.3

THz 펄스를 활용한 2D SnTe 전기분극 조절 및 데이터 저장 시스템 구축

Daeheon Kim, Dongbin Shin

GIST

빛-물질 상호작용을 활용하면 물성을 조절할 수 있다는 측면에서 최근 많은 주목을 받았다. 특히, THz 주파수를 갖는 전기장을 이용해서 고체의 전기 분극을 조절하여 데이터를 저장 함에 있어 중요하다. 본 연구에서는 시간 의존적 밀도 범함수 이론 계산을 통해 2D SnTe 에의 전기 분극을 변화에 대하여 조사 하였다. 특히, THz 주파수를 갖는 전기장을 가할 때 전기장의 방향에 따라 SnTe 의 전기 분극을 원하는 대로 변화시킬 수 있음을 확인 했다. 또한, 강자성 도메인 형성에 대한 이해를 위하여 2D SnTe 의 포논 정보를 담고 있는 시간에 의존하지 않는 AIMD 결과를 이용해서 기계학습 역장 추출을 진행했다. 예를 들어, 기계 학습 역장을 통한 분자 동역학 계산에서 시간 의존적 전기장에 의해 2D SnTe 의 전기 분극 형성과 강자성 도메인 형성을 확인하였다. SnTe 가 x 방향 그리고 y 방향으로 네가지의 전기 분극을 가질 수 있기 때문에, 유한한 크기에서 외부 시간 의존적 전기장을 이용해 4개의 데이터를 저장하는 시스템을 구축 할 수 있을 것으로 기대된다.

Poster No.4

Structural and Electronic Properties of Oxygen-Deficient TaO_x (x=2~2.5) with γ~anatase and B~rutile Phases

Dohyun Kim[1,2], Taeyoung Jeong[1,2], Seungjae Yoon[1,2], Yunjae Kim[1,2] Cheol Seong Hwang[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

Tantalum oxide (Ta_2O_5) exhibits various polymorphs with comparable energies. While the low-temperature λ phase is better characterized, the high-temperature γ phase and high-pressure B phase remain less explored, despite their predicted energetic stabilities. Notably, γ- and B-Ta_2O_5 phases are known to be structurally related to the anatase- and rutile-TaO_2, respectively. By inserting additional oxygen layers into these TaO_2 frameworks, the corresponding Ta_2O_5 phases can be derived. This structural relationship enables the theoretical construction of oxygen-deficient TaO_x (x=2~2.5) suboxides by manipulating their stacking sequences. This study investigates the structural and electronic properties of these suboxides with γ~anatase and B~rutile phases. The two systems exhibit different capabilities to localize excess electrons originating from the oxygen deficiency. In particular, edge-sharing TaO_6 octahedra in the B~rutile phase allow neighboring Ta ions to approach closely, facilitating Ta–Ta bonding through 5d orbital overlap. In contrast, the γ~anatase phase lacks sufficient proximity between Ta ions, resulting in delocalized excess electrons occupying the shallow donor level. These findings provide fundamental insights into the interplay between oxygen deficiency, structural responses, and electronic properties of the tantalum oxide systems and potentially other transition metal oxides.

Poster No.5

Adatoms simulation in black phosphorus with DFT-informed adatom interaction

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

Departments of Physics, Kyung Hee University, Seoul, Korea

Liquid metals exhibit fascinating electronic properties—most notably, a pseudogap with a backward-bending band—that set them apart from conventional crystalline materials. Recent studies have investigated these disorder-induced effects by introducing disordered dopants on crystalline substrates. In particular, experiments involving alkali adatoms deposited on black phosphorus (BP) have revealed a range of disorder-driven phenomena. However, understanding how these effects depend on the spatial distribution of adatoms remains a significant challenge. The spatial arrangement of adatoms is governed not only by well-known interactions such as dipole–dipole forces and Friedel oscillations, but also by a previously uncharacterized deep interaction potential along the armchair direction. This deep potential, which is poorly explained in existing models, drives the formation of quasi one-dimensional chain-like structures and plays a critical role in shaping the global adatom distribution. To accurately capture these distribution-dependent effects, we develop a simulation framework that incorporates all relevant interaction mechanisms. Specifically, we employ simulated annealing on the effective potential energy landscape, incorporating theoretical Friedel oscillation terms to model dopant behavior on the BP surface. In addition, we perform density functional theory (DFT) calculations to evaluate total energies as functions of interatomic distance, dopant concentration, and species, enabling us to extract the deep interaction potential from first principles. 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-2D systems.

Poster No.6

Enhancing Adsorption Energies Predictions on Transition-Metal Surfaces with Density- and Dispersion-Corrected DFT

Sunwoo Kim[1], Youngsam Kim[1], and Eunji Sim[1]

[1]Department of Chemistry, Yonsei University, 50 Yonsei-ro, Seodaemun-gu, Seoul 03722, Korea
E-mail: esim@yonsei.ac.kr

Density functional theory (DFT) is widely used in catalytic reaction studies due to its balances cost and accuracy. However, estimating adsorbate binding strengths on transition-metal surfaces remains challenging. The QM/QM embedding approach, which combines low-level periodic boundary condition (PBC) calculations with high-level cluster-based methods, has improved adsorption energy predictions on transition metal surfaces.[1] Here, we apply density- and dispersion-corrected DFT (D^2C-DFT)[2] within QM/QM cluster models to enhance the adsorption energy accuracy. Leveraging the cluster models, we benchmark our results against reliable experimental data for both covalent and non-covalent adsorption and reveals that D^2C-DFT captures surface electron density more faithfully. These results highlight the benefit of combining explicit density corrections with dispersion treatments in solid-state catalysis and demonstrate applicability of D^2C-DFT to solid-state systems. Further studies will extend D^2C-DFT to more complex catalytic environments.

References

[1] Araujo R. B., Rodrigues G. L. S., dos Santos E. C., & Pettersson L. G. M., Adsorption Energies on Transition Metal Surfaces: towards an Accurate and Balanced Description. Nature Communications, 13, 6853 (2022)

[2] Lee, M., Kim, B., Sim, M., Sogal, M., Kim, Y., Yu, H., Burke, K., & Sim, E. Correcting Dispersion Corrections with Density-Corrected DFT. Journal of Chemical Theory and Computation, 20(16), 7155-7167 (2024)

Poster No.7

Band Gap Engineering of Graphene Kirigami Superlattice

Sungmin Kim1, Sungjong Woo1, Kyoung-Min Kim2,3*, Hee Chul Park1*

1Department of Physics, Pukyong National University, Busan, 48513, Korea
2Asia Pacific Center for Theoretical Physics, Pohang, Gyeongbuk, 37673, Republic of Korea
3Department of Physics, Pohang University of Science and Technology, Pohang, Gyeongbuk 37673, Korea
**Corresponding Author E-mail Address: kyoungmin.kim@apctp.org, hcpark@pknu.ac.kr*

We investigate the effects of graphene kirigami on its band structure and electrical properties by constructing a Graphene Kirigami Superlattice (GKS) using the tight-binding model. A periodic array of square holes is introduced, and we analyze how their size and arrangement influence the electronic structure. Our simulations show that the band structure of the GKS varies depending on the porous geometry, and that a bandgap can be induced or modulated by controlling the periodicity and size of holes. Furthermore, we examine the behavior of armchair-oriented graphene nanoribbons within the GKS. Finally, we expressed the network formed by the kirigami's ZZ edges in Hamiltonian form and demonstrated that the resulting effective tight-binding model effectively captures the Dirac-cone shift and gap opening investigated in our system.

Poster No.8

Analyzing Density-Driven Errors: Defining the Limits of Approximation

Sehun Kim, Youngsam Kim, Dokyeong Lee, Gyumin Kim, and Eunji Sim

Department of Chemistry, Yonsei University, 50 Yonsei-ro Seodaemun-gu, Seoul 03722, Korea

In density functional theory (DFT) computations, errors that emerge from producing and employing physically inaccurate electron densities are termed density-driven errors, which represent a core principle in density-corrected DFT (DC-DFT). While the ideal density-driven error would allow for density precision evaluation through energy calculations for any given density, its real-world application remains virtually unattainable since it necessitates the exact exchange-correlation. Consequently, prior research has utilized the practical density-driven error, which operates through approximated functionals. This investigation seeks to clarify the connections and circumstances under which the practical density-driven error can replicate the ideal density-driven error, while also offering warnings about possible misunderstandings that could occur when applying practical density-driven error to explain DC-DFT fundamentals outside these validated conditions.

Poster No.9

Pressure-Induced Magnetic and Spin-State Transitions in the 2D vdW Material CrSBr

Seulbi Kim[1], Resta A. Susilo[2] and Bo Gyu Jang[1]

[1]*Department of Materials Science and Engineering, Kyung Hee University, Yongin 17104, Korea*
[2]*Department of Physics, Pohang University of Science and Technology, Pohang, Korea.*

Two-dimensional (2D) van der Waals (vdW) magnets have attracted significant attention due to their unique low-dimensional properties and potential applications in high-performance spintronic and next-generation computing devices. Among them, CrSBr has recently gained attention as an antiferromagnetic 2D vdW semiconductor exhibiting strong magnetic anisotropy. While CrSBr has a layered structure, the strong intralayer Cr–S coupling results in a ferromagnetic alignment within each layer, whereas the interlayer coupling leads to an antiferromagnetic ordering, forming an A-type antiferromagnetic structure. Band structure calculations using density functional theory (DFT) confirm a strong anisotropy along a specific crystallographic axis. In this study, we perform DFT calculations to investigate the structural and electronic properties of CrSBr under high pressure. We particularly focus on identifying pressure-induced magnetic and spin-state transitions, offering insights into the evolution of magnetic and electronic characteristics in low-dimensional systems under external perturbation.

Poster No.10

Reducing Basis Set Errors in Density- and Dispersion-Corrected Density Functional Theory

Youngsam Kim and Eunji Sim*

Department of Chemistry, Yonsei University, 50 Yonsei-ro Seodaemun-gu, Seoul 03722, Korea
E-mail: esim@yonsei.ac.kr

Understanding electronic structure problems has become of great importance to interpret experimental results and develop predictive models. Among various electronic structure methods, density functional theory (DFT) is the preferred choice due to its balance between accuracy and computational efficiency. Under periodic boundary conditions, plane-wave codes are commonly utilized, but exact exchange calculations in Hartree-Fock and hybrid DFT are the most time-consuming, making them unsuitable for routine calculations. On the other hand, the Fritz Haber Institute ab initio molecular simulations (FHI-aims) code employs numeric atom-centered orbital basis sets and provides a more efficient approach for exact exchange calculations. In this study, we benchmark the results from the widely utilized plane-wave code (VASP) and FHI-aims with particular focus on basis set errors. Furthermore, this study aims to minimize basis set errors in density- and dispersion-corrected DFT (D^2C-DFT) calculations and assess the reliability of D^2C-DFT.

Poster No.11

Comparison of Switching Mechanisms in Ferroelectric Wurtzite AlN

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

[1]*Electronic and Hybrid Materials Research Center, Korea Institute of Science and Technology, Korea*
[2]*Department of Materials Science and Engineering and Inter-University Semiconductor Research Center, Seoul National University, Korea*

Ferroelectric materials are promising candidates for next-generation semiconductor devices due to their reversible polarization under an electric field. Polarization switching in ferroelectrics is generally classified into two mechanisms: homogeneous switching and inhomogeneous switching. In homogeneous switching, atoms move collectively, whereas in inhomogeneous switching, the atoms move sequentially along the switching path through the domain wall motion. Wurtzite AlScN, a representative hard ferroelectric material, transitions from homogeneous to inhomogeneous switching as the Sc concentration increases, indicating that pure AlN typically follows a homogeneous switching mechanism with a high switching barrier. However, previous studies have overlooked the role of domain wall energy generated during ferroelectric switching, but only considered the nudged elastic band for uniform bulk structures. This work evaluates the inhomogeneous switching barrier in wurtzite AlN by explicitly considering the domain wall energy associated with sequential switching events. The inhomogeneous barrier is compared with its homogeneous counterpart, providing a more comprehensive understanding of the switching behavior in wurtzite AlN. This work highlights the importance of domain wall contributions in modeling ferroelectric switching mechanisms.

Poster No.12

Machine Learning-Based Bath Initialization for Dynamical Mean-Field Theory in Layered Perovskite Structures

Taeung Kim*, Ara Go**

Department of Physics, Chonnam National University, Gwangju 61186, South Korea
**taeung98@jnu.ac.kr, **arago@jnu.ac.kr*

Dynamical mean-field theory (DMFT) is a powerful tool for probing strongly correlated electron systems. When Hamiltonian-based impurity solvers—such as exact diagonalization (ED), configuration-interaction (CI) methods, or Hilbert-space truncation methods based on adaptive sampling, such as the Adaptive Sampling Configuration Interaction (ASCI) approach —are employed, the continuous hybridization function must be represented by a finite set of bath parameters. Optimizing these parameters to satisfy DMFT self-consistency yields a highly non-convex cost function; as the number of bath sites grows, innumerable local minima emerge and the converged solution becomes sensitive to the initial bath configuration.

To mitigate this difficulty, we propose a machine-learning approach that supplies physically motivated initial bath parameters. Training data are generated by constructing Hamiltonians that respect the crystal symmetries of layered perovskite structures and performing standard ED-DMFT calculations to obtain optimized baths. An independent test set was employed to assess the model's capability to generate good initial bath configurations. We expect that machine-learning-based initial configuration will not only alleviate conventional challenges of bath fitting but also broaden the scope of research on strongly correlated systems by eliminating the reliance on heuristic, physical intuition-based initial guesses.

Poster No.13

Simulating IR-induced Ferroelectricity in $SrTiO_3$ and $EuTiO_3$

Kim Hanbyul, Shin Dongbin

Department of Physics and Photon Sciences, GIST

Ultrafast laser pulses can uniquely manipulate material properties by driving strong light-matter interactions, leading to emergent phenomena such as chirality control, ferroelectricity, and unconventional magnetism [1-6]. Recent studies have demonstrated that mid-infrared (IR) pulses can selectively excite specific optical phonon modes, enabling the dynamical stabilization of non-equilibrium states through nonlinear phonon coupling [4,5]. In particular, it is experimentally demonstrated that IR excitation in $SrTiO_3$ can induce a long-lived ferroelectric phase, with polarization persisting for hours after the pulse has ended [4]. However, the fundamental microscopic mechanisms underlying this effect remain an open question. Here, we investigate how IR-driven phonon dynamics play a critical role in stabilizing the metastable ferroelectricity. We solve the time-dependent Schrödinger equation based on first-principles calculations [7]. Our results suggest that IR pulse-excited phonon modes, which has strong non-linear phonon interaction, induce strain along the c-axis, facilitating the emergence of a ferroelectric phase after IR phonon mode has dissipated. Building on this, we aim to induce ferroelectricity in the multiferroic material $EuTiO_3$ to control its magnetic orientation as desired. This mechanism provides a pathway for optically controlling ferroelectricity and its coupling to magnetism, which could be leveraged in future memory and spintronic devices [8].

[1] Z. Zeng et al., Science 387, 431-436 (2025).
[2] X. Li, T. Qiu, J. Zhang, E. Baldini, J. Lu, A. M. Rappe, and K. A. Nelson, Science 364, 1079 (2019).
[3] Basini, M., Pancaldi, M., Wehinger, B. et al. Nature 628, 534–539 (2024).
[4] T. F. Nova, A. S. Disa, M. Fechner, and A. Cavalleri, Science 364, 1075 (2019).
[5] Afanasiev, D., Hortensius, J.R., Ivanov, B.A. et al., Nat. Mater. 20, 607–611 (2021).
[6] Fechner, M., Först, M., Orenstein, G. et al. Nat. Mater. 23, 363–368 (2024).
[7] D. Shin, S. Latini, C. Schafer, S. A. Sato, E. Baldini, U. De Giovannini, H. Hubener, and A. Rubio, Phys. Rev. Lett. 129, 167401 (2022).
[8] Narayan, A., Cano, A., Balatsky, A.V. et al. Nature Mater 18, 223–228 (2019).

Poster No.14

Generalized First-Principles Evaluation of Dzyaloshinskii–Moriya Interaction in Self-Intercalated $Cr_{1+\delta}Te_2$

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

Department of Physics, Kyung Hee University, Seoul

Non-collinear spin textures, such as skyrmions, have garnered increasing attention for their potential applications in nanoscale spintronic devices. A central mechanism underlying these textures is the Dzyaloshinskii–Moriya interaction (DMI), a relativistic effect that promotes spin canting in magnetic systems. Although several computational methods have been developed to evaluate DMI, many are limited to specific crystal structures, which constrains their general applicability. In this study, we propose a generalized approach for evaluating DMI that extends beyond a single structural configuration. Using first-principles density functional theory (DFT) calculations, we analyze spin configuration–dependent energies across varying compositions of self-intercalated $Cr_{1+\delta}Te_2$. From these results, we extract a unified set of global DMI parameters that effectively characterize the CrTe material system. This generalized DMI framework facilitates predictive modeling of DMI in other members of the CrTe family and supports more accurate simulations of their non-collinear spin textures.

Poster No.15

Thermoelectric-driven triboelectric charge transfer

Ji-Ho Mun, Eui-Cheol Shin, Jaeuk Seo and Yong-Hyun Kim*

Department of Physics, Korea Advanced Institute of Science and Technology (KAIST), Daejeon 34141, Republic of Korea.
*Correspondence to: yong.hyun.kim@kaist.ac.kr

Although friction-induced static electricity has been the subject of extensive research and holds considerable practical importance, a rigorous quantitative theory describing triboelectric charge transfer remains elusive. Here, we present the detailed dynamics of triboelectric charge transfer driven by an interfacial thermoelectric bias that satisfies a steady state at the interface. We demonstrate that, in a steady state, triboelectric charge exhibits a delta-like spatial distribution. We propose that the transferred triboelectric charge is equal to half of the difference between the thermoelectrically induced surface charges. Furthermore, we discuss a quantitative approach to electrostatic adhesion and static discharge, which are governed by transferred charges, and we highlight the role of surface charge non-uniformity. These insights have significant implications for the control of static electricity and the development of advanced energy-harvesting technologies.

Poster No.16

First-Principles Study of Proximity-Induced Spin Effects from Carbon-Related Defects in Graphene/hBN Heterostructures

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

1) Department of Physics, Kyung Hee University, Seoul, South Korea
2) Department of Information Display and Research Institute for Basic Sciences,
Kyung Hee University, Seoul, South Korea

Spin-related proximity effects in graphene have traditionally been explored through magnetic substrates. Recently, however, atomic-scale spin defects have emerged as a promising alternative for inducing spin splitting without relying on long-range magnetic order. In this study, we investigate proximity-induced spin phenomena in graphene/hBN heterostructures mediated by carbon-related defects, using first-principles density functional theory (DFT) calculations. We focus on defect configurations where carbon atoms substitute boron (C_B) or nitrogen (C_N) atoms in hBN, both of which are known to host localized spin-polarized states. When these spin defects are placed in proximity to graphene, their states hybridize with graphene's Dirac bands, resulting in spin splitting without the need for external magnetic fields or magnetic substrates. Furthermore, we demonstrate that the magnitude—and even the nature—of the induced spin splitting can be tuned by varying the defect concentration and applying out-of-plane electric fields. Our findings suggest a defect-engineered, tunable platform for inducing spin textures in graphene, paving the way for 2D spintronic applications based on van der Waals heterostructures.

Poster No.17

Anisotropic Multi-centered Polarons in $BiVO_4$

Seyeon Park[1], Yajing Zhang[1, 2], Bongjae Kim[1]

[1]*Department of Physics, Kyungpook National University, Daegu 41566, Korea*
[2]*MPPC-CPM, Max Planck POSTECH/Korea Research, Pohang, 37363, Korea*

Polarons are localized quasiparticles formed through charge-lattice coupling in solids. As they often create localized in-gap states from excess charge carriers, the description of polarons is critical for explaining key materials properties such as optical, spectroscopic, and transport behaviors. $BiVO_4$, a representative photocatalyst for water splitting applications, has been intensively investigated, and polarons in this system are known to significantly affect its efficiency. However, the exact nature of these polarons and related experimental measurements remain not coherently understood. In this study, employing first-principles calculations, we show the possible existence of multi-centered polarons, a striking departure from conventionally reported single-centered configurations. We further demonstrate the anisotropic character of electron polaron compared to the hole counterpart, showing how lattice distortions and electron-phonon coupling distinctively drive the formation of anisotropic multi-centered polaron states. These theorical results are directly compared with optical and spectroscopic experiments, providing evidence for the presence of an anisotropic multi-centered polaron in $BiVO_4$. [1]

[1] A. Chaudhuri *et al.*, Phys. Rev. B **97**(19), 195150 (2018).

Poster No.18

Generalized Momentum Sum Rule as the Origin of Multiple Charge Density Wave Transitions

Sohee Park,[1] Changwon Park[*,2] and Young-Kyun Kwon[*,1,3]

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

[2] School of Computational Sciences,

KoreaInstitute for Advanced Study, Seoul 130-722, Korea

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

E-mail: cwparksnu@gmail.com and ykkwon@khu.ac.kr

Charge density wave (CDW) transitions in low-dimensional materials, particularly in transition metal dichalcogenides (TMDCs), often exhibit multiple first-order phase transitions and complex modulation patterns. While phenomenological theories offer qualitative insights, the microscopic origin of such transitions remains elusive. In this work, we identify a universal principle underlying CDW transitions: a generalized momentum sum rule that governs the anharmonic coupling between low-energy phonon modes. Using a highly accurate interatomic potential trained on first-principles calculations, we reproduce the full sequence of CDW transitions in 2H-TaSe$_2$, including commensurate, incommensurate, and symmetry-broken intermediate phases. We construct a variational model in which CDW phases emerge from interacting phonon eigenmodes constrained by specific momentum sum rules. These rules dictate that nonlinear phonon interactions occur only when their wavevectors satisfy quantized momentum conditions (e.g., $\boldsymbol{k}_1 + \boldsymbol{k}_2 + \boldsymbol{k}_3 = 0$ or $\mathbf{G}$). We demonstrate that such momentum constraints determine the energetic hierarchy of competing CDW configurations and predict universal features, such as the stabilization of unidirectional order in square lattices and spontaneous symmetry breaking in triangular lattices. Our results provide a broadly applicable and physically grounded framework for constructing CDW phase diagrams from a minimal set of microscopic parameters.

Poster No.19

Three band understanding of strain-driven direct-to-indirect band gap transition in MoS_2

Seungil Baek, Jun Jung, and Yong-Hyun Kim*

Department of Physics, Korea Advanced Institute of Science and Technology (KAIST), Daejeon 34141, Republic of Korea.
*Correspondence to: yong.hyun.kim@kaist.ac.kr

Two-dimensional hexagonal transition metal dichalcogenides offer a honeycomb lattice with a direct band gap, attracting significant interest in both physics and materials science. Recently, sp^2-like hybridization of three d orbitals (d_{z^2},d_{xy}, and $d_{x^2-y^2}$) revealed an electronic breathing kagome lattice near the Fermi level of h-TMDs, leading to the discovery of their nontrivial topology. Here, we investigate biaxial-strain-induced direct-to-indirect band gap transition in monolayer MoS_2 from the perspective of the hybrid d-orbital basis. Using first-principles calculations and maximally localized Wannier functions (MLWFs), we traced the strain dependence of the band structure and hopping parameters. First, we revealed that the seemingly high-order hoppings in the breathing kagome view effectively collapse onto nearest-neighbor Mo-Mo interactions, lifting the Γ-point valence band to near degeneracy with the K-point valence band maximum. Second, we found evolution of hopping generally follows the sign of the corresponding overlap integral. Finally, the weakening of breathing strength under strain, combined with the elevated Γ-point valence band, drives the direct-to-indirect band gap transition. This study highlights the hybrid d-orbital framework as an insightful perspective for understanding the unique electronic structure of h-TMDs and their strain responses.

[1] J. Jung, and Y.-H. Kim, *Hidden breathing kagome topology in hexagonal transition metal dichalcogenides*, Phys. Rev. B **105**, 085138 (2022).

Poster No.20

First-Principles Study of Polarization-Modulated Oxygen Diffusion and Magnetic Anisotropy at the Co/HfO$_2$ Interface

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

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

Multiferroic heterostructures that combine ferroelectric and ferromagnetic components enable electric-field control of magnetic properties through magnetoelectric coupling, making them promising candidates for next-generation memory and logic devices. Recent studies have shown that electric fields applied to Co/HfO$_2$ systems can drive oxygen migration into the Co layer, leading to asymmetric modulation of the magnetic anisotropy energy (MAE). In this study, we employ density functional theory (DFT) to investigate oxygen diffusion across the Co/HfO$_2$ interface under different ferroelectric polarization states, and we evaluate the corresponding changes in MAE. To account for structural imperfections commonly present at interfaces, we also examine the influence of cobalt vacancies on oxygen diffusion. Our calculations reveal that the presence of vacancies significantly lowers the diffusion barrier, and the associated diffusion coefficients are estimated using Monte Carlo simulations. These results demonstrate that oxygen diffusion behavior is strongly modulated by polarization direction, providing microscopic insight into electric-field-driven control of interfacial magnetism. Our findings offer a theoretical foundation for the design of magnetoelectric devices with electrically tunable magnetic functionalities.

Poster No.21

Flexible Hofmann-Type Metal-Organic Frameworks for Xe Storage: Machine Learning Potential-Based Molecular Dynamics Approach

Dong Yun Shin[a], Hyojin Kim[b], Chang Seop Hong[b], and Jung-Hoon Lee[a,c]*

[a]Computational Science Research Center, Korea Institute of Science and Technology (KIST), Seoul 02792, Republic of Korea
[b]Department of Chemistry, Korea University, Seoul 02841, Republic of Korea
[c]KU-KIST Graduate School of Converging Science and Technology, Korea University, Seoul 02841, Republic of Korea.

Flexible metal organic frameworks (MOFs) exhibit various dynamic behaviors including framework expansion/shrinkage and pore opening/closing, providing exceptional potential for gas storage and separation applications. In particular, the sigmoidal adsorption behavior enables superior storage and separation performance. In this study, we investigate Xe adsorption behavior in three flexible Hofmann-type MOFs (CoNi-Pipe, NiNi-Pipe, and CoPd-Pipe) by developing machine learning potentials (MLPs) for molecular dynamics (MD) simulations. Our MLPs reach DFT-level accuracy and enable large-scale, long-timescale MD simulations, achieving root mean square errors (RMSEs) of 0.004 eV/atom, 0.001 eV/atom, and 0.009 eV/atom for energy, and 0.059 eV/Å, 0.018 eV/Å, and 0.056 eV/Å for force, in Xe-adsorbed CoNi-Pipe, NiNi-Pipe, and CoPd-Pipe, respectively. According to our MLP-based MD simulations, CoNi-Pipe shows the highest Xe mobility, followed by CoPd-Pipe and NiNi-Pipe despite their comparable Xe adsorption energies. Thus, CoNi-Pipe achieves the highest Xe uptake among the three MOFs. We find that framework flexibility plays a crucial role in Xe diffusion: CoNi-Pipe exhibits the highest flexibility, followed by CoPd-Pipe and NiNi-Pipe. This trend is consistent with the order of maximum Xe uptake. We further find that for CoPd-Pipe, Xe diffusion is limited at low Xe loadings but significantly improves at higher loadings due to enhanced framework flexibility. These findings provide a clear explanation for the sigmoidal adsorption behavior observed in CoPd-Pipe. This study highlights a new strategy for understanding the structural dynamics of flexible frameworks during gas adsorption and expands the scope of computational approaches for studying stimuli-responsive materials.

Poster No.22

Extending HF-DFT to Dipole Moments of Linear Molecules

Jiye Shin[1], YoungSam Kim [1], and *Eunji Sim*[1]

f[1]Department of Chemistry, Yonsei University, 50 Yonsei-ro, Seodaemun-gu, Seoul, 03722, Republic of Korea

Density Functional Theory with Hartree-Fock density(HF-DFT), a practical framework of density-corrected density functional theory(DC-DFT), has been demonstrated to significantly improve energies and energy differences in a variety of chemical reactions by correcting for density-driven errors in DFT. Dipole moments also come out of the response of the energy to a constant electric field, indicate a molecule's polarity, and are relevant to long-range electrostatics in force field parametrization. At the dipole moment, the HF density has quite different behavior than the self-consisent density.[1] In addition, HF-DFT also has a small overall RMS error, so it can be used to get closer to CCSD(T) in systems where DFT has a large error.[2] It is necessary to present a general analysis of the HF DFT in the dipole moment calculations and to make some cautions. RHF-DFT in a closed shell should be used to calculate the dipole moment. UHF-DFT in closed shells has been shown to have large errors due to spin contamination. RHF/ROHF-DFT performed better than SC-DFT in the Halogen Group and post-transition/Transition Metal Group.

Poster No.23

Flat Mid-Gap States at Domain Walls of 3D Stiefel–Whitney Insulators

Hongsik Shin, Sungkyun Ahn, Youngkuk Kim

Department of Physics, Sungkyunkwan University

Flat-band systems have garnered much interest as a platform for strongly correlated phases, with quantum geometric structures reminiscent of Landau levels. In this work, we investigate a class of topological phases that generically host flat bands by stacking Su–Schrieffer–Heeger (SSH) chains into three dimensions. Specifically, we identify a parameter regime in which three-dimensional Stiefel–Whitney insulators (3DSWIs) and Dirac nodal-line semimetals (DNLSs) emerge and undergo topological phase transitions. We construct a tight-binding model by stacking SSH chains and introducing centrosymmetry-preserving deformations, enabling exploration of a four-dimensional parameter space relevant to PT-symmetric topological phases. We demonstrate that domain walls between distinct 3DSWI phases can host mid-gap interface states, which may serve as a robust platform for realizing flat bands. Our results provide a general theoretical framework for engineering topological boundary states and interface flat bands in three-dimensional systems.

Poster No.24

First-principles study on small polaron and Li diffusion in layered $LiCoO_2$

Seryung Ahn, Jiyeon Kim, Bongjae, Sooran Kim

Kyungpook National University

Li-ion conductivity is one of the essential properties that influences the performance of cathode materials for Li-ion batteries. Here, using density functional theory, we investigate the polaron stability and its effect on the Li-ion diffusion in layered $LiCoO_2$ with various magnetic orderings. We show that the local magnetism promotes the localized Co^{4+} polaron with the Li-diffusion barrier of ~0.34 eV. While the Li-ion diffuses, the polaron migrates in the opposite direction to the Li movement. In the non-magnetic structure, on the other hand, the polaron does not form, and the Li diffusion barrier is lowered to 0.21 eV. Although the presence of the polaron raises the diffusion barrier, the magnetically ordered structures are energetically more stable during the migration than the non-magnetic case. Thus, our work advocates the hole polaron migration scenario for Li-ion diffusion. We further demonstrate that the strong electron correlation of Co ions plays an essential role in stabilizing the Co^{4+} polaron.

Poster No.25

Ab Initio Thermodynamic Investigation of Charge-Dependent Transition Temperature in Titanium

Seungwoo yoo, Howook Choi, Heung Nam Han, and Young-kyun Kwon

1 Department of Materials Science and Engineering, Seoul National University, Seoul, Republic of Korea
2 Department of Physics, Kyunghee University, Seoul, Republic of Korea

The phase stability of metals is fundamentally governed by thermodynamic state variables such as temperature, pressure, and composition. Titanium is a representative metal that undergoes a solid-state phase transition from the α-phase (hcp structure) to the β-phase (bcc structure) at elevated temperatures. While this α→β transformation has been theoretically attributed to specific phonon modes and supported by various experimental and computational studies, direct quantitative validation at the level of thermodynamic free energy using ab initio methods remains scarce. In this study, we employ the temperature-dependent effective potential (TDEP) method based on ab initio molecular dynamics simulations to capture the temperature-dependent dynamical behavior of titanium. Using this approach, we calculate the phonon free energies of both the α and β phases at high temperatures. Our results demonstrate that the β phase becomes thermodynamically favorable as temperature increases, thereby quantitatively confirming the phonon-driven transformation mechanism at the density functional theory (DFT) level. Furthermore, we extend the TDEP framework to charged systems and find that increasing the charge density reduces the free energy difference between the α and β phases, indicating a thermodynamic destabilization of the α phase. These findings not only validate the theoretical understanding of solid-state phase transitions but also provide a predictive framework for evaluating phase stability under external stimuli such as charge doping.

Poster No.26

Multi-fidelity Training Strategies for Enhancing the Cross-Domain Applicability of Machine-Learning Interatomic Potentials

Jinmu You[1], Jaesun Kim[1], Yutack Park[1], Haekwan Jeon[1], Suyeon Ju[1],
and Seungwu Han[1,2]

[1]*Department of Materials Science and Engineering, Seoul National University, Seoul 08826, Korea.*
[2]*Korea Institute for Advanced Study, Seoul 02455, Korea.*

Universal machine-learning interatomic potentials (MLIPs) promise chemically generalizable and data-efficient atomistic simulations across diverse material systems. However, most existing approaches are limited to narrow chemical domains—such as inorganic crystals or organic molecules—restricting their applicability to hybrid systems like molecule–surface interactions. A key challenge to achieving universal MLIPs lies in the heterogeneity across *ab initio* datasets, which vary not only in chemical composition but also in computational fidelity (e.g., generalized gradient approximation vs. hybrid functionals), hindering seamless integration.

To address this, we apply a multi-fidelity learning framework based on the Scalable EquiVariance-Enabled Neural NETwork (SevenNet) architecture. This approach enables joint training on chemically and computationally diverse datasets along with fidelity information. Furthermore, L2 regularization on metadata parameters and the use of domain-bridging configurations promote cross-fidelity knowledge transfer among different fidelities. Trained on over 230 M structures from datasets such as the Materials Project, Open Molecules 2025, and Open Catalyst 2020, the trained model SevenNet-Omni demonstrates strong cross-domain generalization. On complex systems requiring accurate description on both organic and inorganic components, our model outperforms state-of-the-art single-domain models such as eSEN and ORB-v3, as well as unregularized multi-fidelity approaches including UMA. These results underscore the effectiveness of regularization and domain-bridging schemes in fidelity-aware training for developing robust and transferable MLIPs, paving the way for reliable simulations across increasingly complex and chemically diverse domains.

Poster No.27

Semimetallic Transition Metal Telluride Contacts for p-type Te-Channel Thin Film Transistors

Seungjae Yoon[1,2], Wonho Choi[2], Byongwoo Park[2], Taeyoung Jeong [1,2], Dohyun Kim[1,2], Yunjae Kim[1,2], Cheol Seong Hwang[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

As thin film transistor (TFT) channel lengths continue to scale down, minimizing contact resistance becomes increasingly vital to maintain the device performance. Decreasing the Schottky barrier height (SBH) at the channel/contact interface is essential but often hindered by Fermi level pinning (FLP) caused by metal-induced gap states (MIGS). Tellurium (Te), composed of one-dimensional helical chains featuring high hole mobility along the c-axis, has attracted interest as a p-type TFT channel material. Nevertheless, strong FLP at conventional metal-Te contacts necessitates improved contact engineering. While semimetal contacts with chalcogenides like MoS_2 have shown FLP suppression and reduced SBH, similar studies on Te remain underexplored. Therefore, this study systematically investigates the SBH using the projected density of states, enabling analysis of MIGS at Te interfaces to assess the extent of FLP. High work function metals (Ni, Pd, Pt) and their corresponding semimetallic transition metal telluride (TMT) compounds ($NiTe_2$, $PdTe_2$, $PtTe_2$) were investigated as contact materials. Metal contacts (Ni-Te, Pd-Te, Pt-Te) exhibited interfacial reconstruction forming $NiTe_x$, $PdTe_x$, and $PtTe_x$, with large MIGS indicating stronger FLP. Ni-Te had the Fermi level pinned near mid-gap with high hole SBH (~ 0.2 eV), while others had their Fermi levels pinned near the valence band maximum with low hole SBHs (< 0.1 eV). In contrast, semimetallic TMT contacts ($NiTe_2$-Te, $PdTe_2$-Te, $PtTe_2$-Te) retained clean interfaces without reconstruction and suppressed MIGS, leading to suppressed FLP and lower SBH following the Schottky-Mott limit. Notably, $NiTe_2$ and $PdTe_2$ achieved near-zero hole SBHs owing to their higher work functions (4.9 and 5.0 eV), establishing them as promising ohmic contacts for p-type Te-based transistors. On the other hand, Pt-Te exhibited a smaller hole SBH than $PtTe_2$-Te, which was contrary to expectation, due to the substantial work function difference between Pt and $PtTe_2$.

Poster No.28

Density Functional Theory understanding of intrinsic defects and acceptor dopants in NiO

Na-Young Lee and Ji-Sang Park

[1]*SKKU Advanced Institute of Nanotechnology (SAINT), Sungkyunkwan University, Suwon 16419, South Korea*

NiO is widely used as a hole transport layer in perovskite solar cells due to its wide band gap, low cost, and stability. However, as a p-type material, NiO has low hole mobility due to non-stoichiometry and Ni vacancy defects when used alone. In this study, we use density functional theory to find suitable p-type dopants for NiO, considering alkali metals, transition metals, and group 15 elements. Our PBE+U calculation shows that the carrier concentration can be generated more easily by doping Li and K than by Ni vacancy. The configurational coordinate diagrams of the dopants and the vacancy defect were calculated by using the hybrid density functional theory to determine whether the defects can emit visible light. Nickel vacancy was able to emit violet lights, but the dopants do not emit visible lights.

Poster No.29

Tuning Self-Assembled Monolayers for Trap-Free Exciton Dissociation in Tungsten Diselenide Bilayers

Noki Lee[1], Jeongwon Lee[2], Sehoon Oh[1], Ryong-Gyu Lee[2], Hyeonwoo Yeo[2],
Yong-Hoon Kim[2], Jaichan Lee[1]*

1 School of Advanced Materials Science and Engineering, Sungkyunkwan University (SKKU),
Suwon 16419, Republic of Korea
2 School of Electrical Engineering, Korea Advanced Institute of Science and Technology (KAIST),
291 Daehak-ro, Yuseong-gu, Daejeon 34141, Republic of Korea

Transition metal dichalcogenides are promising materials for next-generation self-powered photodetectors due to their strong light-matter interactions and outstanding optoelectronic properties. However, their high exciton binding energies present a challenge for efficient exciton dissociation, limiting practical device applications. In this study, we present a computational approach using first-principles density functional theory and nonadiabatic molecular dynamics to design self-assembled monolayers for effective, trap-free exciton dissociation in bilayer tungsten diselenide. Our design features two different self-assembled monolayers separately enclosing each side of the bilayer, modified with electron-donating and electron-withdrawing groups. We demonstrate that the surface work function of the self-assembled monolayers is a key macroscopic parameter for optimizing band alignment and eliminating trap states. By tuning this work function across a broad range, we achieve a substantial built-in electric field, enabling type-II band alignment with offsets exceeding the exciton binding energy for dissociation. Nonadiabatic molecular dynamics simulations confirm ultrafast electron transfer under field-driven conditions. These computational results provide design guidelines for two-dimensional self-powered photodetectors and establish a universal strategy for interface engineering in quantum material systems.

Poster No.30

Prediction of accurate enough *k*-point samplings using machine learning

Jinyoung Byun[1], Donggeon Lee[2,3], Euyheon Hwang[3], Sooran Kim[2], and Ji-Sang Park[3]

[1]*Department of Nano Engineering, Sungkyunkwan University, Suwon, 16419, South Korea*
[2]*Department of Physics, Kyungpook National University, Daegu, 41566, South Korea*
[3]*SKKU Advanced Institute of Nanotechnology (SAINT), Sungkyunkwan University (SKKU), Suwon, 16419, South Korea*

Accurate sampling of the reciprocal space is essential for reliable high-throughput DFT simulations, yet performing convergence tests for every material is computationally expensive. To address this, we trained regression models using DFT-derived features—such as the nonlinearity of the band structure, electronic band gap, and the number of atoms—and elemental descriptors. The linear regression model using DFT features achieved an R^2 of 0.803, providing interpretable insights into the physical factors affecting convergence. More notably, a model trained solely on elemental features, without requiring prior DFT calculations, achieved an R^2 of 0.880. This approach enables rapid and accurate estimation of *k*-point convergence behavior, offering a scalable solution for efficient high-throughput screening of materials.

[1] J. Byun, D. Lee, E. Hwang, S. Kim, and J.-S. Park, J. Phys. Chem. A 129, 367–372 (2025).

Poster No.31

DeepSCF: Deep Convolutional Network Learning of Self-consistent Electron Density

Ryong-Gyu Lee 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. Herein, we present further developments of DeepSCF by introducing physics-informed descriptors and applying them to the molecular dataset. We briefly present preliminary work related to various applications of the DeepSCF approach, including machine learning-based *ab-initio* molecular dynamics and exchange-correlation functionals. This work provides insights into new directions for the development of machine learning-based atomistic materials simulations.

Poster No.32

Molecular Dynamics Simulation of Sodium Deposition on Carbon-based Hosts Using Machine-learned Potentials

Moonwon Lee[1,2], Hana Yoon[3], Kanghoon Yim[1*]

[1]*Energy AI & Computational Science Lab., Korea Institute of Energy Research,*
Daejeon, 34129, Republic of Korea
[2]*Graduate School of Energy Science and Technology, Chungnam National University,*
Daejeon, 34134, Republic of Korea
[3]*Energy Storage Research Department, Korea Institute of Energy Research,*
Daejeon, 34129, Republic of Korea

Sodium-ion batteries (SIBs) are gaining interest as a cost-effective alternative to lithium-ion batteries due to the abundance of sodium and its similar electrochemical behavior to lithium. However, like their lithium counterparts, SIBs suffer from safety concerns associated with dendritic growth, which can result in internal short circuits and thermal runaway. To overcome these issues, anode-free sodium all-solid-state batteries have been investigated as a promising strategy, since solid electrolytes enhance non-flammability and battery safety, while anode-free systems maximize energy density. However, these systems often experience non-uniform sodium metal deposition on the current collector, leading to dendrite formation and degraded cycling performance.

In this study, to improve interfacial contact with the solid electrolyte and promote uniform sodium deposition, we introduce a three-dimensional (3D) carbon-based laser-induced graphene host structure onto the metal current collector. This 3D host structure can accommodate volume changes during plating and stripping processes, effectively suppressing dendrite formation. Using density functional theory (DFT)-based machine learning potentials, we predict sodium deposition growth patterns within the 3D carbon-based hosts. Specifically, we focus on elucidating differences in sodium deposition behavior between graphene oxide (GO) and reduced graphene oxide (rGO) by combining DFT calculations with machine learning-based molecular dynamics (MD) simulations.

\

Poster No.33

Automated Active Region Selection in Multi-level Calculations Using Density Sensitivity

Soohyeon Lee and Eunji Sim

Department of Chemistry, Yonsei University

As chemical systems of interest grow increasingly complex, there is a growing demand for electronic structure calculation methods that can scale efficiently without compromising accuracy. However, the steep computational cost of high-level methods poses a challenge. Embedding theory offers a promising approach by partitioning a system into active and inactive regions, applying expensive, high-accuracy methods only to the active region. A challenge in this approach is the identification of chemically important regions that strongly influence properties such as total or reaction energy. In this study, we propose a quantitative and automated method for selecting active regions based on density sensitivity. We define density sensitivity as the energy difference resulting from variations in electron density obtained from different methods. Atoms with high density sensitivity are assumed to have a large impact on the system's total electronic energy. To validate our method, we performed a series of embedding calculations by sequentially adding atoms to the active region in order of decreasing density sensitivity. We observed that the total energy of the system rapidly approaches the reference energy obtained from a full high-level calculation when atoms with the highest density sensitivity are included early in the embedding process. This shows density sensitivity serves as a meaningful indicator for active region selection, ultimately improving both the accuracy and efficiency of multiscale quantum chemical simulations.

Poster No.34

Comparison Study of SiC Polymorphs Using Density Functional Theory

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

[1]Department of Nano Engineering, Sungkyunkwan University, Suwon, 440-746 Korea
[2]Department of Physics, Sungkyunkwan University, Suwon, 440-746 Korea
[3]SKKU Advanced Institute of Nanotechnology (SAINT), Sungkyunkwan University, Suwon, 440-746 Korea

Silicon carbide (SiC) is widely regarded as a leading material for power semiconductor devices due to its wide band gap, high breakdown field, and excellent thermal conductivity. In this study, we compared the structural, electronic, and transport properties of the 2H, 3C, and 4H polytypes using density functional theory (DFT). Lattice constants calculated with the PBEsol functional show good agreement with experiment. Phonon and free energy analyses confirm 4H-SiC as the ground state structure at low temperatures, while 3C becomes more stable at high temperatures or under tensile strain. Transport calculations indicate that 3C-SiC has the highest carrier mobility, although effective mass alone does not fully account for the trend.

Poster No.35

Momentum-resolved modeling of size-dependent resistivity in anisotropic metallic thin films

Youngjun Lee[1], Jin Soo Lee[1], Seungjun Lee[2],
Seoung-Hun Kang[1], and Young-Kyun Kwon[1,3]
[1]*Department of Physics, Kyung Hee University, Korea*
[2]*Department of Electrical and Computer Engineering, University of Minnesota, USA*
[3]*Department of Information Display, Kyung Hee University, Korea*

As interconnect thickness in advanced CMOS technologies continues to shrink, increasing electrical resistivity in metal lines—primarily caused by enhanced surface, interface, and grain boundary scattering—poses a critical challenge to device performance. Conventional models, often relying on isotropic mean free path approximations, fall short in capturing the anisotropic and quantum mechanical nature of electron transport at nanometer scales. In this work, we present a momentum-resolved relaxation-time framework that integrates ab initio electron-phonon interactions with a direction-dependent mean free path model within the Boltzmann transport equation. This method captures both the spatial and directional variation of scattering processes in confined metallic films, allowing accurate predictions of size-dependent resistivity without relying on empirical fitting parameters. We apply our approach to both isotropic metals (Cu, Ag, Au) and anisotropic systems, including tungsten and MAX-phase compounds such as Ti_2GeC. Our results show excellent agreement with experimental trends and emphasize the critical role of crystallographic anisotropy in determining electron transport. Notably, layered anisotropic materials emerge as promising candidates for next-generation interconnects due to their favorable transport characteristics in ultra-thin geometries. This study offers a physically rigorous and computationally tractable methodology for evaluating and designing low-resistance interconnect materials at the nanoscale.

Poster No.36

Active Learning Configuration Interaction Approach for Multiorbital Impurity Systems

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), the quantum Monte Carlo solver encounters a severe sign problem when applied to multiorbital Hamiltonians such as the Kanamori Hamiltonian, due to the presence of spin-flip and pair-hopping terms. In contrast, the exact diagonalization (ED) solver does not suffer from a sign problem and is suitable for treating multiorbital interactions, although the rapid growth of the Hilbert space with the number of orbitals imposes a strict limit on the accessible system size.

Therefore, it is necessary to develop methods to mitigate this exponential wall as much as possible. To this end, we employ the active learning configuration interaction method as an impurity solver. This method uses a trained classifier to sort out the most relevant configurations for Hamiltonian diagonalization.

We demonstrate the effectiveness of our approach on a benchmark multiorbital single-site DMFT model with a cubic lattice structure and degenerate d orbitals, using $SrRu_2O_4$ as a representative system.

Poster No.37

Density Functional Effective Mass Approximation Calculations of 2D Halide Perovskite Nanoplatelets

Jeongwon Lee, Hyeonwoo Yeo, and Yong-Hoon Kim*

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

Two-dimensional (2D) halide perovskites are attractive candidates for optoelectronic applications, owing particularly to their tunable photoluminescence and bandgap properties enabled by compositional and layer-number modulation. [1,2] First-principles density functional theory (DFT) and DFT-based many-body calculations can, in principle, offer valuable insights into the electronic structure and excitonic properties of 2D halide perovskites and corresponding 1D nanoribbons and 0D nanoplatelets, thus enabling the rational design of novel halide perovskite nanostructures. However, realistic simulations of these systems are often computationally prohibitive, especially for nanoplatelets where periodic boundary conditions are not applicable. To address the limitation, we herein further develop and apply our multi-scale simulation framework that combines DFT and effective mass approximation (EMA) calculations (Fig 1). [3] We first perform DFT calculations on bulk-like 2D halide perovskites to extract effective masses and potential profiles along the lateral and vertical directions, respectively. For nanoplatelets, these parameters are then used to construct a DFT-informed EMA Hamiltonian, which is solved on a real-space grid to obtain their electron and hole states and corresponding exciton binding energies. The computational results show excellent agreement with experimental data (Fig 2), demonstrating the accuracy and efficiency of our DFT-EMA multi-scale simulation scheme in modeling low-dimensional halide perovskite nanostructures.

References [1] Y. Bekenstein, *J. Am. Chem. Soc.*, 137, 16008-16011. (2015). [2] Y. Liao, *J. Am. Chem. Soc.*, 139, 6693-6699. (2017) [3] H. Yeo, et al., *J. Phys. Mater.* 3, 034012 (2020).

Poster No.38

Strain-direction selectivity of electronic and magnetic phases in $La_{0.75}Ca_{0.25}MnO_3$

Juhyeon Lee[1], Beom Hyun Kim[2] and Bongjae Kim[1*]

[1]Department of Physics, Kyungpook National University, Daegu 41566, Republic of Korea
[2]Department of Physics & Astronomy, Seoul National University, Seoul 08826, Republic of Korea

Doped $LaMnO_3$ has gained significant interests from the solid state physics community due to its exhibition of diverse magnetic and electronic phase transitions upon varying physical parameters. Epitaxial strain is an important tool to impose external perturbations of the system, which offers viable route to tune its material properties. Recent successful achievement of applying extreme tensile strain up to 8% have further expanded opportunities for this system, revealing unprecedent electronic and magnetic phase transitions in Ca-doped LaMnO3 (LCMO)[1].

Inspired by such experimental advances in strain engineering, here, we investigate the electronic structures and magnetic properties of LCMO under the diverse epitaxial strain conditions: uniaxial strains along (100), (010), and (110) as well as biaxial strains. We report that spin, orbital, and charge phases, which are interconnected with Jahn-Teller distortion, show high selectivity to the direction of applied epitaxial strains. Our study demonstrates additional dimension in the epitaxial engineering in complex oxides.

[1] S. S. Hong et al. Science 368, 6486 (2020)

Poster No.39

Strain-Driven Higher-Order Topological Dirac Semimetal in Noncentrosymmetric γ-GeSe

Churlhi Lyi and Youngkuk Kim

SUNGKYUNKWAN UNIVERSITY

Strain-engineered topological phases in noncentrosymmetric materials provide a promising route to realizing exotic quantum states, though experimental validation remains limited. In this study, first-principles calculations reveal that the van der Waals material γ-GeSe undergoes a series of strain-driven topological phase transitions, including the emergence of a higher-order topological Dirac semimetal. Applying in-plane biaxial tensile strain leads to a rich sequence of phases—ranging from nodal-line semimetals and Dirac semimetals to a higher-order topological Dirac semimetal. This unique phase features Dirac points on the $k_z = 0$ plane coexisting with higher-order topological insulating states, supported by the quantization of the mirror-resolved Zak phase. These findings establish γ-GeSe as an experimentally accessible platform for exploring strain-driven topological effects specific to noncentrosymmetric systems.

Poster No.40

The effect of pressure on the physical properties of NV center in diamond

Hyungwoo Lee[1], Junghyun Lee[2], Chris G. Van de Walle[3] and Minseok Choi[1*]

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

[2]*Center of Quantum Information, Korea Institute of Science and Technology, Seoul 02792, Korea,*

[3]*Materials department, University of California, Santa Babara, California 93106, United states*

The negatively charged nitrogen-vacancy (NV^-) center in diamond, with long spin lifetimes (~6 ms) at room temperature, coherence time (~few ms) and high sensitivity, is promising for quantum information science including quantum computing, quantum sensing and quantum communication. Recently, efforts have been made to utilize the NV^- center for probing pressure-induced properties of materials under extreme conditions. However, despite its potential, a comprehensive understanding of the physical properties of the NV^- center under pressure remains limited, which is crucial for its successful application. In this work, we perform first-principles density functional theory (DFT) calculations to investigate key quantities of the NV^- center such as the ionization potential, zero-filed splitting, and zero-phonon line under pressure. The exchange-correlation functional constructed by Strongly Constrained and Appropriately Normed family of meta-generalized gradient approximation was used, and to simulate the excited states, delta self-consistent field method, allowing for full atomic relaxation in a constrained-occupation DFT approach, was employed. Our findings offer valuable insights into the pressure-induced properties of the NV^- center in diamond, with potential applications in quantum information science.

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-2024-00466625) and Basic Science Research Program funded by the Ministry of Education (RS-2022-NR070869). We also acknowledge the National Supercomputing Center with supercomputing resources including technical support (KSC-2024-CRE-0395).

Poster No.41

Unveiling the effects of Alkali Defects at the CIGS/Buffer Layer via First-Principles Study

Suim Lim[1,2], Ara Cho[1], Chanwon Jung[3], Kihwan Kim[1], and Kanghoon Yim[1*]

[1] *Korea Institute of Energy Research, Republic of Korea*
[2] *Sogang University, Republic of Korea*
[3] *Pukyong National University, Republic of Korea*
E-mail address: khyim@kier.re.kr

$Cu(In,Ga)Se_2$ (CIGS) thin-film solar cells have attracted significant attention due to their lower production costs, tunable direct bandgap, high absorption coefficient, high conversion efficiency, and long-term stability. Buffer layers such as CdS and $Zn_{1-x}Mg_xO$ (ZMO) are crucial for optimizing charge transport and reducing recombination losses by modifying the conduction band alignment. Furthermore, alkali doping has been widely employed to enhance device performance with elements such as Na, K, Rb, and Cs, improving open-circuit voltage and charge collection efficiency.[1,2] In previous research, Kim *et al.*[3] have shown that how alkali doping can compensate for structural defects in CIGS solar cells, providing both experimental and theoretical evidence.

In this study, we investigate the effects of alkali doping and atomic diffusion between the buffer layer and the CIGS layer on solar cell performance. First, we calculate the formation energies of alkali defect and intrinsic chemical diffusion from the CIGS and buffer layers on each surface structures through first-principles calculations. Additionally, we calculate the barrier energies for atomic diffusion along both depth and surface on each surface. Our results indicate that Na atoms diffuse into the bulk more easily than Rb atoms and that the ZMO layer is more stable against interdiffusion compared to CdS. These theoretical results are consistent with the experimental observations, especially from the atom probe tomography (APT) analysis. By analyzing the role of the alkali incorporation at CIGS/buffer layer interfaces, this study contributes to the design of CIGS solar cells with advanced efficiency.

References

1. A. Chirilă, P. Reinhard, F. Pianezzi, P. Bloesch, A. R. Uhl, C. Fella, L. Kranz, D. Keller, C. Gretener, H. Hagendorfer, D. Jaeger, R. Erni, S. Nishiwaki, S. Buecheler, A. N. Tiwari, *Nature mater*, 12, 1107-1111 **(2013)**
2. Hsu, C.-H., Ho, W.-H., Wei, S.-Y., Lai, C.-H. *Adv. Energy Mater*. 7, 1602571 **(2017)**
3. Kim, K., Jung, C., Yim, K., Jeong, I., Shin, D., Hwang, I., Song, S., Ahn, S. K., Eo, Y.-J., Cho, A., Cho, J.-S., Park, J. H., Choi, P.-P., Yun, J. H., Gwak, *J. ACS Appl. Mater. Interfaces* 14, 52825–52837 **(2022)**

Poster No.42

Resolving Theory-Experiment Discrepancies in Bismuth's Topology and Optical Properties via an Extended Hubbard Model

Dameul Jeong[1] and Young-Kyun Kwon[1,2]

[1] Department of Physics and Research Institute for Basic Sciences, Kyung Hee University, Seoul, 02447, Korea
[2] Department of Information Display, Kyung Hee University, Seoul, 02447, Korea.

Bismuth (Bi) is well known for its strong spin–orbit coupling and intriguing electronic properties. However, its topological classification—whether trivial or nontrivial—has remained contentious due to persistent discrepancies between theoretical predictions and experimental observations. In this study, we address this issue by employing an extended Hubbard model that incorporates both on-site Coulomb repulsion (U) and intersite Coulomb interactions (V). By fitting the model parameters to experimentally measured lattice constants and band gaps, we accurately reproduce the spin–orbit–induced band inversion at the L point, thereby resolving the longstanding mismatch between theory and experiment. Using this same framework, we further compute the optical conductivity of Bi and demonstrate that the sub–1 eV absorption peaks originate from interband transitions between nearly flat bands near the T and W points—contradicting earlier assignments to the Γ point. Our results clarify the electronic and topological nature of bismuth and establish a unified theoretical framework that can guide future studies of Bi-based spintronic and quantum devices.

Poster No.43

First-principles study of asymmetric electrical characteristics in graphene-based molecular junction

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

School of Electrical Engineering, Korea Advanced Institute of Science and Technology,
Rep. of Korea
**E-mail: y.h.kim@kaist.ac.kr*

Single-molecule diodes, as fundamental components of molecular electronics, have long been pursued for their potential to exhibit robust and high-performance rectification. In addition, utilizing graphene electrodes, studies have explored gating effects through ionic liquid gating in molecular devices [1]. Among them, Graphene-based ferrocene junctions have emerged as promising molecular rectifiers, primarily owing to their large rectification ratios. [2]. However, existing theoretical approaches have limitations in providing atomic-level insights, particularly concerning the electronic structure of graphene electrode [3,4]. In this study, based on multi-space constrained search density functional theory (MS-DFT) we have recently developed [5,6], we carry out first-principles non-equilibrium quantum transport. Using MS-DFT, we first study the asymmetric current-voltage characteristics and rectifying property of the junctions coming from the bias-dependent electronic structure change. Next, by introducing the gate electrode, we investigate the effect of the gate bias on rectification behavior of the device. We obtain NDR properties characterized by high peak-to-valley current ratios (PVRs, up to ~ 212) under the negative gate bias. It will be emphasized that these NDR characteristics originate from the quantum hybridization NDR mechanism [7,8].

References [1] Jia, C. *et al.*, *Sci Adv* **4**, eaat8237 (2018) [2] Chen, X. *et al.*, *Nat Nanotechnol* **12**, 797-803 (2017) [3] Jia, C. *et al.*, *Chem* **6**, 1172-1182 (2020) [4] Trasobares, J. *et al.*, *Nat Commun* **14**, 1381 (2023) [5] Lee, J., Kim, H. S. & Kim, Y.-H., *Adv. Sci.* **7**, 2001038 (2020) [6] Kim, Y.-H. & Lee, R.-G., *IEEE Nanotechnology Magazine* **18**, 4-10 (2024) [7] Kim, T. H., Lee, J., Lee, R.-G. & Kim, Y.-H., *npj Computational Materials* **8**(2022) [8] Son, H. *et al.*, *Appl. Surf. Sci.* **581**(2022).

Poster No.44

Automated Atomistic Simulations by Multi Agent System

Yeonwoo Chung[1], Yutack Park[1], Jinmu You[1], and Seungwu Han[1,2] *

[1]Department of Materials Science and Engineering, Seoul National University, Seoul, 08826, Korea
[2]AI Center, Korea Institute of Advanced Study, Seoul, 02455, Korea
E-mail address: hansw@snu.ac.kr

Recent advances in artificial intelligence have ushered in a new era of agentic systems built upon large language models (LLMs), enabling autonomous workflows that extend far beyond text generation. More recently, the emergence of reasoning LLMs has further enhanced the decision-making and planning abilities, broadening the reach of agentic systems to scientific environments such as autonomous laboratories. However, developing accurate molecular models and defining simulation protocols that guarantee physically reliable results still remains a significant barrier, confining atomistic molecular dynamics (MD) to expert practitioners. Here, we introduce Paimon, a multi-agent system designed to perform end-to-end atomistic MD simulations that utilizes (i) expert knowledge extracted from literature such as calculation conditions and (ii) low-level technical knowledge for execution of specific tools like LAMMPS or Python ASE modules. Given a user query, Paimon generates a complete computational workflow and activates sub-agents to perform each calculation step, enabling high-level automation. We demonstrate capabilities of Paimon by calculating densities of liquid electrolytes mainly used in lithium-ion batteries.

Poster No.45

Octahedral Features and Their Impact on Photovoltaic Properties in Thin-Film Inorganic Solar Absorber

Wonzee Jung[1,2], Suim Lim[2,3], Kihwan Kim[4], Joo Hyung Park[4], Kanghoon Yim[*2]

[1]*Departmen of Physics, Chungnam National University, Daejeon , South Korea*
[2]*Energy AI & Computational Science Laboratory, Korea Institute of Energy Research, Daejeon 34129, South Korea.*
[3]*Department of Mechanical Engineering, Sogang University, Seoul, South Korea*
[4]*Photovoltaics Research Department, Korea Institute of Energy Research, Daejeon , South Korea*

In recent years, inorganic perovskite solar cells have been extensively studied to address the stability issues associated with organic–inorganic hybrid perovskites (OIHPs). However, achieving both high photovoltaic performance and long-term stability with fully inorganic perovskite absorbers remains a challenge. Motivated by the outstanding photovoltaic properties of perovskite-structured materials, we systematically screened octahedral inorganic compounds from crystal structure databases using high-throughput density functional theory (DFT) calculations, focusing on their octahedral features. As a first step, we targeted ABX_3 stoichiometry and confirmed that our screening reproduces previously reported promising perovskite materials. Beyond perovskite materials, our screening also covers perovskite-inspired structures, enabling a broader investigation of octahedral geometry and its impact on photovoltaic properties. By analyzing photovoltaic properties in relation to structural features, we identified key influences of octahedral characteristics—such as interconnection types, local regularity of individual octahedra, and the presences of residual valence states of cations within octahedra—on photovoltaic performance. Interestingly, we found that chalcogenides exhibit greater tolerance to structural deviations compared to halides. As a next step toward discovering novel solar-cell absorbers, we are extending our research to all ternary compounds. We also discuss theoretical considerations for searching thin-film solar cell absorbers based on light absorption and charge recombination mechanism.

Poster No.46

Current-driven symmetry breakings and consequent spin-orbit polarizations of screw-symmetric chiral wire

Uiseok Jeong[1], Daniel Hill[2], Angel Rubio[3], Binghai Yan[4], Carsten A Ullrich[2*],
Noejung Park[1,3*]

1Department of physics, Ulsan National Institute of Science and Technology(UNIST), UNIST-gil 50, Ulju-gun, 44919, Ulsan, Republic of Korea.
2Department of Physics and Astronomy, University of Missouri, Street, Columbia, 65211, Missouri, USA.
3Max Planck Institute for the Structure and Dynamics of Matter, Luruper Ch 149, 22607, Hamburg, Germany.
4Department of Physics, Pennsylvania State University, 201 Old Main, 16802, Pennsylvania, USA.

The spin states of electrons propagating through a chiral wire have attracted significant interest and debate, particularly over whether geometric chirality intrinsically induces spin polarization or merely acts as a spin filter. Using ab-initio real-time time-dependent density functional theory calculations, we systematically investigate how charge current leads to spin and orbital polarization beyond the constraint imposed by time-reversal symmetry. We investigate the space group symmetries and time-reversal symmetry of the Hamiltonian, focusing on how symmetry breaking influences the spin–orbital textures of individual eigenstates and their Kramers' pairings. When the current exceeds a critical threshold, the constraints imposed by time-reversal symmetry on spin and orbital configurations are lifted, independent of the underlying Hamiltonian structure. We interpret the resulting emergence of rotational dynamics---in both spin and orbital degrees of freedom---as a consequence of sacrificing the translational (linear) momentum carried by the current.

Poster No.47

A Halogen-Based Dataset for Building Chemical Reaction Foundation Model

Jinyoung Jeong, Minhyeok Lee and Eunji Sim*

Department of Chemistry, Yonsei University, 50 Yonsei-ro Seodaemun-gu, Seoul 03722, Korea
E-mail: *esim@yonsei.ac.kr*

Machine Learning Interatomic Potentials (MLIPs) have emerged as powerful tools for achieving quantum-level accuracy calculations at the computational cost of a classical force fields. However, the performance of MLIPs heavily depends on the quality and diversity of the training data. Existing datasets predominantly consist of equilibrium or near-equilibrium molecular configurations and are mostly limited to molecules composed of C, H, N, and O elements. To address this limitation, we present a new dataset that includes both equilibrium and non-equilibrium structures of halogen-containing molecules, systematically sampled along diverse reaction pathways[1]. By incorporating molecules with F, Cl, and Br atoms, the dataset significantly broadens chemical coverage, enabling MLIPs to accurately model a wide range of organic reactions, including those relevant to chemical hazards. The dataset comprises over 21 million molecular structures with reference energies and atomic forces. This method offers a good balance between accuracy and computational efficiency by incorporating dispersion corrections and an adequate basis set. Structural and reaction space analysis demonstrates that our dataset captures a diverse and chemically relevant portion of chemical space. Furthermore, a graph neural network–based feature vector analysis with dimensionality reduction reveals the extensive coverage of local atomic environments within the dataset. Designed for training reactive MLIPs, this dataset can be readily extended to accommodate new chemical reactions while maintaining computational efficiency.

Poster No.48

First-principles Study on the Kondo Resonance of a Self-assembled Ni-HHTP on Au(111)

Chanyeong Jeong,[1] Seungil Baek,[1] Min Hui Chang,[2] Sejong Kahng,[2] and Yong-Hyun Kim[1,*]

[1] *Department of Physics, Korea Advanced Institute of Science and Technology (KAIST),*
Daejeon 34141, Republic of Korea;
[1] *Department of Physics, Korea University, Seoul 02841, Republic of Korea;*
* *yong.hyun.kim@kaist.ac.kr*

Two-dimensional metal-organic frameworks (MOFs) are gaining recognition as versatile platforms for quantum spin liquids and qubit architectures. MOFs are highly advantageous owing to their ability to self-assemble into diverse and tunable structures. In this work, we present a theoretical study of the Ni-HHTP (2,3,6,7,10,11-hexahydroxytriphenylene) complex on the Au(111) surface. Using density functional theory (DFT) calculations, we examined how the electronic structure and oxidation states of Ni are modulated by different adsorption sites, exploring the Ni-substrate interaction. Our electronic structure analysis reveals that unpaired electrons on the Ni atoms give rise to magnetic impurities, providing a plausible explanation for the observed Kondo resonance. These results deepen our understanding of spin behavior in 2D MOFs and underscore their potential for quantum informatics and spintronics applications.

Poster No.49

Effective Parameter Extraction for Vacancy-mediated Diffusion from *Ab Initio* Molecular Dynamics

Taeyoung Jeong[1,2], Kun Hee Ye[1,2], Seungjae Yoon[1,2], Dohyun Kim[1,2], Yunjae Kim[1,2],
Cheol Seong Hwang[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*

Multiscale modeling, incorporating atomic-scale insights into continuum-scale models, provides a robust framework for optimizing semiconductor devices. However, modeling mass transport poses a central challenge: *ab initio* methods yield diffusion parameters specific to individual migration pathways, whereas continuum-scale models require a single set of effective parameters that capture the overall transport behavior. To bridge this gap, this work presents *VacHopPy*, an open-source Python package for extracting effective parameters for vacancy-mediated diffusion based on ab initio molecular dynamics (AIMD). The extracted parameters include effective values for hopping distance, migration barrier, coordination number, attempt frequency, and correlation factor. These parameters are determined by statistically integrating energetic, kinetic, and geometric contributions across all migration paths. They are provided in a material-independent, simplified form for seamless integration into continuum-scale models. The capability of *VacHopPy* is demonstrated in two representative materials: rutile TiO_2 and monoclinic HfO_2. In rutile TiO_2, both isolated charged oxygen vacancies (mono-V_O^{2+}) and neutral di-vacancies (di-V_O^0) are considered. The results reveal that defect-defect interactions can induce significant correlations between diffusion events, altering the overall diffusion landscape. In monoclinic HfO_2, diffusion of mono-V_O^{2+} is examined. The findings highlight the critical role of anisotropy in thermal vibrations, an often-overlooked factor, in accurately extracting effective diffusion parameters. The extracted effective parameters feasibly reproduce temperature-dependent diffusion behavior and agree highly with experimental data. *VacHopPy* establishes a robust bridge between atomic- and continuum-scale models, enabling accurate and transferable multiscale simulations.

Poster No.50

First-principles calculation of native point defects in CaO

Yunhwa Jo[1], Hyungwoo Lee[1], Inseo Kim[1], Minseok Choi*[1]

[1]*Department of Physics, Inha University*

Simple alkaline-earth metal oxides have attracted interest due to their ultrawide bandgaps, which can host well-isolated in-gap defect levels [1,2]. This property makes them promising candidates for quantum defect applications in quantum information technologies. Recently, CaO has gained particular attention, as it exhibits nuclear spin-limited coherence times at least ten times longer than those measured in naturally abundant diamond and SiC [3]. Indeed, several candidates are reported. For example, two complexes, negatively charged X (X=Sb, Bi) on Ca site with the O vacancy and positively charged I on Ca site with the O vacancy, show similarities to the NV^- center in diamond [4]. However, fundamental understanding of native point defects in CaO remains limited. In this study, we investigated the charge-state transition level and formation energy of native defects in CaO using the SCAN functional.

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-2024-00466625) and Basic Science Research Program funded by the Ministry of Education (RS-2022-NR070869). We also acknowledge the National Supercomputing Center with supercomputing resources including technical support (KSC-2024-CRE-0395).

References

[1] L. Gordon *et al.,* MRS Bull. **38**, 802 (2013).
[2] Y. Chen, M. E. Turiansky, and C. G. Van de Walle, Phys. Rev. B **106**, 174113 (2022).
[3] S. Kanai *et al*., Proc. Natl. Acad. Sci. **119**, e2121808119 (2022).
[4] J. Davidsson *et al.,* Nat. Commun. **15**, 4812 (2024).

Poster No.51

Revealing H Diffusion Mechanism in IGZO System through Machine Learning Interatomic Potential

Hyunsung Cho,[a] Seungwu Han,[ab] and Youngho Kang[c]

[a] *Department of Materials Science and Engineering and Research Institute of Advanced Materials, Seoul National University, Seoul 08826, Republic of Korea.*
[b] *Korea Institute for Advanced Study, Seoul 02455, Republic of Korea.*
[c] *Department of Materials Science and Engineering, Incheon National University, Incheon 22012, Republic of Korea.*

Understanding hydrogen diffusion mechanisms in amorphous indium gallium zinc oxide (*a*-IGZO) is essential for elucidating the nature of instability in oxide semiconductor devices. However, density functional theory (DFT)-based simulations are inherently limited in timescale, making it difficult to access the slow diffusion behavior of hydrogen, especially in amorphous systems where the highly disordered atomic structure further complicates the identification of diffusion pathways. In this study, we develop a fine-tuned machine learning interatomic potential (MLIP), derived from the pretrained SevenNet-0 model[1], to accurately model hydrogen-related energetics and dynamics in *a*-IGZO and crystalline CAAC-IGZO. The MLIP is trained on a carefully curated dataset of hydrogen defect structures and validated against DFT in terms of energy, force, defect formation energies, and migration barriers. Using long-timescale MLIP molecular dynamics simulations, we identify distinct hydrogen diffusion mechanisms in the two systems. In *a*-IGZO, hydrogen exhibits ring-confined inner-ring hopping and ring-to-ring flipping, with the latter playing a dominant role in long-range transport. In contrast, CAAC-IGZO enables fast in-plane diffusion via Ga/Zn-O nearest neighbor hopping, while out-of-plane diffusion is strongly suppressed due to the high barrier imposed by In-O layers. These findings not only clarify the origin of hydrogen mobility in oxide semiconductors but also offer a mechanistic explanation for the superior bias stability observed in CAAC-IGZO devices.

References:

1. Park, Yutack, et al. "Scalable Parallel Algorithm for Graph Neural Network Interatomic Potentials in Molecular Dynamics Simulations." J. Chem. Theory Comput. (2024).

Poster No.52

Water effect on CO2 capture and diffusion in bare and functionalized Mg-MOF-74 analogs, using Machine Learning Potential.

Joharimanitra Randrianandraina, Jung-Hoon Lee

Korea Institute of Science and Technology, Republic of Korea
E-mail address: jhlee84@kist.re.kr

This study investigates the adsorption and diffusion of carbon dioxide (CO_2) and water (H2O) in pristine and diamine-functionalized metal-organic frameworks (MOFs), specifically Mg-MOF-74 and its derivatives, Mg2(dobpdc). The research explores MOF modifications using various diamines with different chain lengths, including N-N'-methylethylenediamine (m-2), N,N′-dimethylethylenediamine (m-2-m), N-ethylethylenediamine (e-2), and N, N'-diethylethylenediamine (e-2-e).

To elucidate water's impact on CO_2 capture and diffusion dynamics, machine-learning (ML) interatomic potentials were developed for both CO_2 and H_2O adsorption in pristine and functionalized MOFs. These potentials enable molecular dynamics (MD) simulations with density functional theory (DFT)-level accuracy at a computationally feasible cost for MD-scale investigations.

The ML potential-based MD simulations reveal that H_2O predominantly occupies adsorption sites, especially in open metal site structures, with higher diffusion rates for CO_2 compared to H_2O. The transition from dobdc to dobpdc linkers enhances the mobility of both CO_2 and H_2O in the channels, further amplified by diamine functionalization. However, H_2O maintains a lower diffusivity than CO_2 due to its higher affinity with the diamines.

This research enhances the accuracy of analyses and provides deep insights into the complex interplay between MOF structure, dynamics, and functionality. The findings contribute to a more comprehensive understanding of CO_2 capture mechanisms in the presence of water, which is crucial for developing more effective carbon capture technologies. The study's outcomes have significant implications for optimizing MOF design and improving the efficiency of carbon capture systems in real-world applications.

Poster No.53

First principles study of dielectric properties of ferroelectric perovskite oxides with extended Hubbard interactions

Min Chul Choi[1], Wooil Yang[2,*], Young-Woo Son[2,*], and Se Young Park[1,3,*]

[1]Department of Physics and Integrative Institute of Basic Sciences, Soongsil University, Seoul, 06978, Korea
[2]Korea Institute for Advanced Study, Seoul 02455, Korea
[3]Origin of Matter and Evolution of Galaxies (OMEG) Institute, Soongsil University, Seoul, 06978, Korea
[*]yspacefirst@kias.re.kr, [*]hand@kias.re.kr, and [*]sp2829@ssu.ac.kr

We investigate the atomic and electronic structures of ferroelectric perovskite oxides, $BaTiO_3$, $PbTiO_3$, $LiNbO_3$, and $BiFeO_3$ using ab initio extended Hubbard functionals (DFT+U+V), where on-site and inter-site Hubbard parameters are self-consistently determined via a pseudohybrid density functional by Agapito–Curtarolo–Buongiorno Nardelli. We compute band structures, ferroelectric distortions, polarization, Born effective charges, and switching barriers, compared with local density approximation, generalized gradient approximation (GGA), meta-GGA, and hybrid (HSE06) functionals. Results from DFT+U+V closely match experimental data, with the inter-site Hubbard terms significantly increasing band gaps, making closer alignment with *GW* results. The crucial role of the inter-site Coulomb interactions, restoring polar distortions suppressed by on-site U is discussed. Our approach yields accuracy comparable to HSE06 at over an order-of-magnitude lower computational cost. This combination of accuracy and efficiency makes DFT+U+V well suited for high-throughput calculations and properties such as bulk photovoltaic effect and band alignments of ferroelectric heterostructures.

Poster No.54

Phase transition of CoPS3 under pressure

CHOI Seong Jae, KIM Heung-Sik

Department of Physics, Kangwon National University

Trichalcogenide (MPX3) exhibits significant structural changes under pressure. This study aims to predict the orbital characteristics of cobalt (Co) in CoPS3 under various pressures and identify two distinct states within a single pressure condition. The first-principles electronic structure calculations revealed the following findings: First, when the characteristics at each pressure were measured, it was experimentally confirmed that the material transitions from an insulator to a metal at approximately 8 GPa. The calculations show that the bandgap closes at around 6 GPa. Structural changes include the overlap of phosphorus (P) orbitals between layers at 12 GPa. Additionally, magnetization per Co atom becomes zero at 16 GPa. Second, differences were found between increasing and decreasing pressure. When the P-31m structure is calculated under increasing pressure, it is stable at 8 GPa. However, upon decreasing pressure, the structure transitions to C2/m, accompanied by lower enthalpy and magnetization. Finally, dynamic mean-field theory (DMFT) was applied to track the orbital distribution of CoPS3, revealing the unique characteristics of each state. To investigate additional phase transitions experimentally observed in CoPS3, the analysis was repeated for various space groups, uncovering further phase transitions.

Poster No.55

Thermodynamic analysis of the Ti-O-H System based on DFT calculations for oxygen control in Titanium

Changjoong Kim[1], Junyoung Choi[1], and Jiwoong Kim[1,2,†]

1 Department of Materials Science and Engineering, Soongsil University, Seoul 06978, Republic of Korea
2 Department of Green Chemistry and Materials Engineering, Soongsil University, Seoul 06978, Republic of Korea

Titanium (Ti) exhibits excellent mechanical properties, corrosion resistance, and biocompatibility, driving growing demand for titanium in high-performance aerospace, biomedical, and automotive applications. However, conventional manufacturing processes predominantly yield Ti products with high O content, which degrades mechanical properties such as tensile strength and toughness. Recent studies have demonstrated that addition of H on Ti lattice increases chemical potential of O and facilitates deoxidation. We performed density functional theory (DFT) calculations to compute the formation energy in the Ti-O-H system to predict the equilibrium partial pressures of H_2 and O_2. These results show that thermodynamic calculations through computational simulations can make practical predictions of experimental parameters and contribute to the efficiency of materials research.

Poster No.56

Altermagnetism in orthorhombic $NaOsO_3$

Hong-Suk Choi[1], Kyo-Hoon Ahn[2], and Kwan-Woo Lee[1,3]

[1] *Department of Applied Physics, Graduate School, Korea University, Sejong 30019, Korea*
[2] *Institute of Physics, Czech Academy of Sciences, Cukrovarnick´a 10, 162 00 Praha 6, Czechia*
[3] *Division of Semiconductor Physics, Korea University, Sejong 30019, Korea*

Altermagnetism (AM) is a newly identified magnetic phase characterized by spin-split electronic bands, despite having a zero net magnetic moment. This arises since its magnetic sublattices are related by rotational symmetry, in contrast to conventional antiferromagnets, where sublattices are typically connected by translational or inversion symmetry. Interestingly, AM enables spin-dependent transport and gives rise to unconventional forms of the anomalous Hall and spin Hall effects, even in the absence of net magnetization.

In this work, we investigate the orthorhombic perovskite antiferromagnet $NaOsO_3$, which exhibits a high Néel temperature above 410 K and a narrow gap of approximately 70 meV, using *ab initio* calculations. This system has been proposed as the first example of a Slater metal-insulator transition (MIT), in which antiferromagnetic ordering drives the gap opening without any accompanying structural distortion. Consistent with the Slater picture, its most physical quantities evolve continuously across the MIT. However, a discontinuity emerges in the magnetic susceptibility, along with the appearance of a weak magnetic moment of $0.005\mu_B$ at low temperatures.

Through a comprehensive symmetry analysis of the magnetic space group and detailed *ab initio* calculations, we identify the origin of this weak magnetism. Additionally, our results also reveal characteristic signatures of AM in both spin dynamics and transport properties. In the magnon spectra, we observe chiral splittings in both the acoustic and optical branches. Furthermore, the anomalous Hall conductivity exhibits a relatively large magnitude near the Fermi energy. In this presentation, we will discuss these findings in detail.

[Acknowledgements] We acknowledge W. E. Pickett and Myung-Chul Jung for collaborations of this research that is supported by National Research Foundation of Korea (NRF) grants (RS-2024-00392493)

Poster No.57

Discovering Oxide Solid Electrolytes with Corner-sharing Framework Using Crystal Structure Prediction

Seungwoo Hwang[1,*], Jiho Lee[1], Seungwu Han[1], Youngho Kang[2], and Sungwoo Kang[3]

[1] Department of Material Science and Engineering, Seoul National University, Seoul, Korea
[2] Department of Material Science and Engineering, Incheon National University, Incheon, Korea
[3]Korea Institute of Science and Technology, Seoul, Korea

Discovering new oxide solid electrolytes with high lithium-ion conductivity is critical for advancing all-solid-state battery technology. Computational screening offers a time- and cost-efficient alternative to purely experimental approaches, already resulting in several promising electrolyte candidates identified from the Inorganic Crystal Structure Database (ICSD). Yet, extensive chemical space remains unexplored, raising uncertainty about potential materials yet to be synthesized. Crystal structure prediction (CSP), especially methods employing optimization algorithms such as evolutionary algorithms, can explore diverse configurations independently of existing prototypes. Integrating machine learning interatomic potentials (MLIPs) greatly accelerates CSP process even for complex materials with approximately 50 atoms per unit cell. Nevertheless, many oxide electrolytes are notably more complex, typically featuring over four elements and more than 100 atoms per cell.

To mitigate complexity, we exploit a common structural motif among high-conductivity oxide electrolytes: corner-sharing networks consisting of MO_6 and TO_4 polyhedra, described by formulas like $Li_x(MO_{6/2})_m(TO_{4/2})_n$. Restricting CSP searches exclusively to these corner-sharing frameworks significantly simplifies computational complexity. This study introduces the targeted CSP framework called TOPIC (TOpology-based crystal structure Prediction of Inorganic solid electrolytes with Corner-sharing frameworks), explicitly designed to investigate unexplored quaternary oxide systems. Initially, the lithium-free host framework structures are predicted. By leveraging the structural rule that anions reside between two cations within corner-sharing networks, we significantly reduce anion positional degree of freedom, transforming a complex quaternary CSP into a simpler binary problem with fewer than 50 atoms. Our approach employs reverse process: cation positions are randomly assigned, and oxygen atoms are subsequently inserted between cation pairs, forming initial structures. These configurations are first relaxed via classical potentials, followed by refinement using MLIPs. Lithium sites are then determined through Voronoi tessellation, and stable lithium configurations are obtained using Monte Carlo simulations with MLIPs.

Applying TOPIC successfully reproduces known quaternary electrolytes like NASICON and $LiTa_2PO_8$, and also identifies previously undiscovered quaternary oxide solid electrolytes. We find lithium concentration significantly impacts the thermodynamic stability of these corner-sharing frameworks. Using the pretrained SevenNet-0 potential, we systematically screen candidate structures for thermodynamic stability, electronic bandgap, and ionic conductivity, evaluating their effectiveness as potential solid electrolytes.

Poster No.58

Magnetostriction and spin polarization properties in superperiodic Janus twisted bilayer graphenes

G.T. Oyeniyi[1], Iu.A. Melchakova[2], L.A. Chernozatonskii[3], P.V. Avramov[4], Bongjae Kim[1]

[1] *Department of Physics, Kyungpook National University, 80 Daehak-ro, Daegu 41566, Republic Korea*
[2] *School of Physics and Engineering, ITMO University, St. Petersburg 197101, Russian Federation*
[3] *Emanuel Institute of Biochemical Physics, Russian Academy of Sciences, 4 Kosigin St., Moscow 119334, Russian Federation*
[4] *Department of Chemistry, Kyungpook National University, 80 Daehak-ro, Daegu 41566, Republic Korea*

This study presents a comprehensive theoretical investigation of novel superperiodic vertical Janus-type heterostructures based on doped twisted bilayer graphene (TBG), using electronic structure calculations to explore their atomic and electronic properties. Periodic sublattices of oppositely charged fluorine and aluminum adatoms were introduced to induce structural charge polarization and generate uncompensated spin moments of up to $1.05\,\mu$B per unit cell. These effects originate from intense local transverse electric fields arising from ferromagnetically aligned spin polarization across the graphene layers. The spin polarization is primarily governed by electronic states of carbon and fluorine near the Fermi level, while the aluminum superlattices modulate the degree of charge polarization, symmetry breaking, and the strength of the internal electric fields, which can reach up to -0.018 e^2/Å. The proposed heterostructures exhibit spin-resolved electronic features, entanglement potential, and magnetostriction—indicating strong promise for spintronic and quantum applications. The tunability of magnetic and electronic properties through twist angle, adatom patterning, and doping offers a versatile platform for designing multifunctional 2D materials. The interplay between lattice symmetry, charge distribution, and spin ordering enables external control over spin dynamics and transport characteristics. These findings provide a theoretical foundation for future experimental synthesis and pave the way toward innovative devices in nanoelectronics, spin-based logic, and quantum sensing technologies.

Poster No.59

First principles study of flat electronic bands in 2D Silicate Monolayers

Haleem Ud Din[1], Nojoon Myoung[1]

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

The emergence of flat electronic bands in two-dimensional (2D) materials presents a compelling platform for exploring exotic quantum phenomena driven by strong electron-electron correlations, including ferromagnetism, superconductivity, and Wigner crystal formation. Here, we present a comprehensive first-principles study to investigate the electronic properties of a novel 2D silicate monolayer, demonstrating the presence of remarkably flat electronic bands. Our calculations reveal that the unique hexagonal arrangement of silicon-oxygen tetrahedra within the monolayer geometry leads to highly localized electronic states, thereby suppressing kinetic energy dispersion and resulting in an isolated flat band near the Fermi level. We analyze the orbital contributions and real-space localization of these flat band states, elucidating the underlying quantum geometric frustration responsible for their formation. Furthermore, we investigate the stability of this 2D silicate monolayer and discuss the potential for experimental synthesis. These findings highlight 2D silicate monolayers as a promising new class of materials for realizing tunable flat band physics, opening avenues for future research into strong correlation phenomena and novel electronic device applications based on earthabundant elements.

Poster No.60

A comparative analysis of methods for calculating Hubbard parameters using cRPA

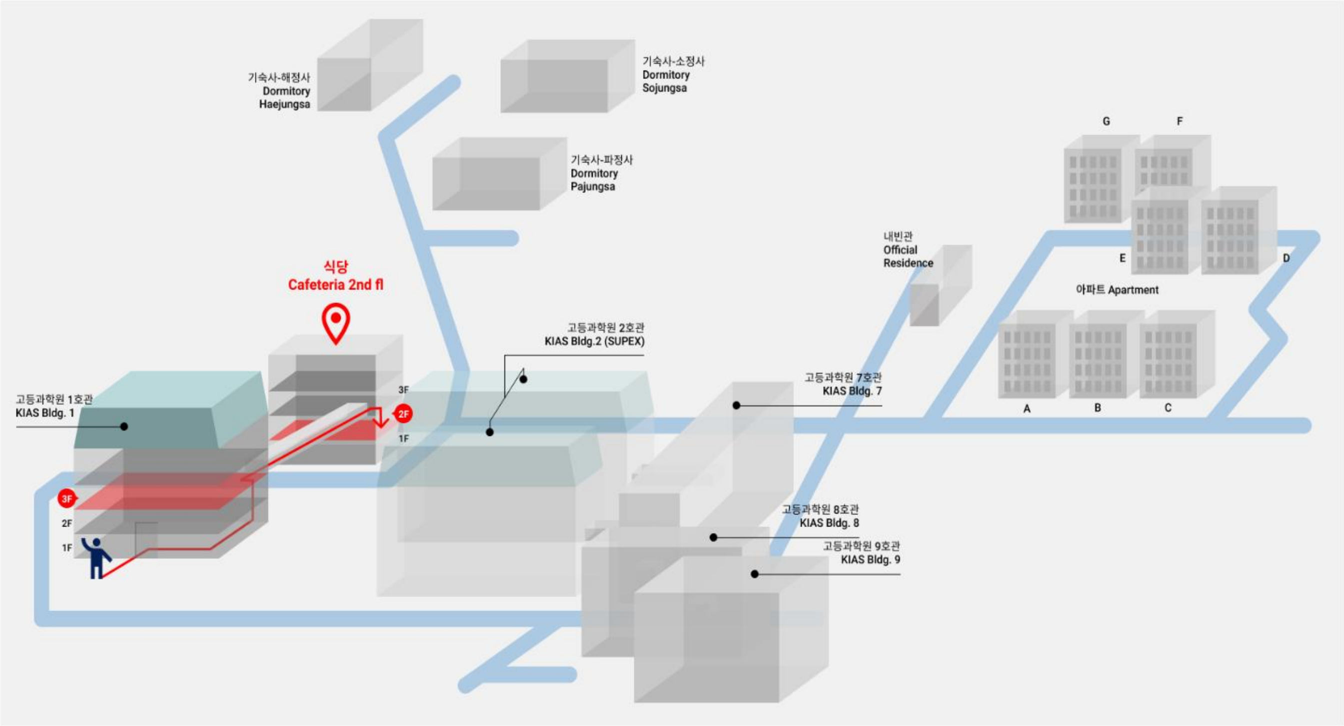
Indukuru Ramesh Reddy[1], M. Kaltak[2], and Bongjae Kim[1,*]

[1]*Department of Physics, Kyungpook National University, Daegu 41566, Republic of Korea*
[2]*VASP Software GmbH, Berggasse 21/14, 1090 Vienna, Austria*
* bongjae@knu.ac.kr

We present a systematic investigation of the calculation of Coulomb interaction parameters, specifically focusing on the Hubbard U, using the constrained random-phase approximation (cRPA). The complexity arises from the different ways of defining the correlated space and performing projections, particularly in systems with entangled bands, where different projection schemes from hybridized bands to the target space can yield varying sizes of interaction parameters. We systematically evaluate different approaches to construct the Wannier basis for extracting the correlated subspace from Kohn-Sham orbitals, addressing the challenges associated with defining the correlated basis. We then examine the dependence of U on different projection schemes within cRPA methods. Finally, we compare the values of U obtained from various cRPA approaches, highlighting their distinct advantages as well as challenges related to screening accuracy and consistency. To illustrate these effects, we study two representative family of d-orbital oxides: $\mathrm{Li}M\mathrm{O_2}$ (M = V - Ni) as examples of systems with isolated d-bands, and $\mathrm{Sr}M\mathrm{O3}$ (M = Mn, Fe, and Co) as cases of entangled d-bands. Through this systematic comparison, we provide a detailed analysis of different cRPA methodologies for computing the Hubbard parameters.

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)