PROGRAM AND ABSTRACTS

제20회 고등과학원 전자구조계산학회

2024년 7월 11일(목) - 7월 12일(금)

고등과학원 1호관 대강당

초청연사

강성우 (KIST)

김　건 (세종대 물리천문학과)

류　훈 (KISTI)

박철홍 (부산대 물리학과)

이건도 (서울대 재료공학부)

이성훈 (경희대 응용물리학과)

이승훈 (서울대 화학부)

윤홍기 (강원대 물리학과)

장보규 (경희대 정보전자신소재학과)

정우석 (KIER)

정유성 (서울대 화학생물공학부)

진경환 (전북대 물리학과)

최덕현 (삼성종기원)

최운이 (삼성종기원)

한명준 (KAIST 물리학과)

자문위원회

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

조직위원회

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

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9:10 ~ 9:20 개회 인사

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9:20 ~ 10:00 박철홍 (부산대)
Negligible bowing effect of bandgap in perovskite halide alloy

10:00 ~ 10:40 최덕현 (SAIT)
Ferroelectric HfO_2: from physics to industry

10:40 ~ 11:00 커피 및 다과

Session II: Interactions and magnetisms 좌장 김흥식 (강원대)

11:00 ~ 11:40 한명준 (KAIST)
Recent Progress of 'Jx' code for magnetic force linear response theory and its applications

11:40 ~ 12:20 장보규 (경희대)
The Role of Intersite Coulomb Interaction in mixed-valence compounds

12:20 ~ 14:00 점심식사

Session III: Charge density waves 좌장 박창원 (고등과학원)

14:00 ~ 14:40 이성훈 (경희대)
1T-TaS_2: Mott Insulator or Band Insulator?

14:40 ~ 15:20 진경환 (전북대)
Emerging quantum phenomena in 1T-transition metal dichalcogenides with noncentrosymmetric charge-density wave

15:20 ~ 16:00 커피 및 다과

Session IV: ML potentials 좌장 박지상 (성균관대)

16:00 ~ 16:40 강성우 (KIST)
Pushing the limit of crystal structure prediction using machine-learned potentials

16:40 ~ 17:20 윤홍기 (강원대)
Accelerating Atomic-Scale Simulations through Machine Learning Potentials and Diffusion Models

17:20 ~ 20:00 포스터 좌장: 김세중 (UST)

7 월 12 일 (금요일)

8:30~9:20 등록

Session V: AI and materials 좌장 신동빈 (GIST)

9:20~10:00 정유성 (서울대)
Materials Generation and Synthetic Predictions Enabled by AI

10:00~10:40 정우석 (KIER)
Active Learning Configuration Interaction for Excited State Calculations of Aromatic Systems

10:40 ~ 11:00 커피 및 다과

Session VI: Low dimensional systems 좌장 김아람 (DGIST)

11:00 ~ 11:40 김건 (세종대)
First-principles investigations of two-dimensional electrides

11:40 ~ 12:20 이건도 (서울대)
Thermal Decoupling: Origin of Strange Metal Phase in Unconventional High-Tc Superconductors

12:20 ~ 13:40 점심식사

Session VII Quantum Dots and Defects 좌장 김한슬 (충북대)

13:40 ~ 14:20 이승훈 (서울대)
Simulating Ground-State Electronic Structure and X-ray Spectra of Transition Metal Clusters

14:20 ~ 15:00 최운이 (삼성전자)
Novel charge trap mechanism in amorphous silicon nitride

15:00 ~ 15:40 류훈 (KISTI)
Development of a Virtual Quantum Computer based on Multi-scale Simulations of Si Quantum Dot Structures

15:40 ~ 16:00 시상 및 폐회

ABSTRACTS OF TALKS

Talk No 1.

Negligible bowing effect of bandgap in perovskite halide alloy

Chul Hong Park[1,2], M. S. Kim[2], S. Lee[3], and Y. W. Heo[3]

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[2]*Quantum Matter Core-Facility and Research Center of Dielectric and Advanced Matter Physics, Pusan National University, Korea*

[3]*School of Materials Science & Engineering, Kyungpook National University, Daegu 41566, Korea*

Halide perovskites have broad bandgap tunability, making them suitable for diverse applications in optoelectronics and photovoltaics. The optical bandgap of halide perovskites varies almost linearly with the halide ionic size, and therefore, it can be controlled through compositional engineering. However, the mechanism underlying this low-bandgap variation is not yet fully understood. Thus, this study comprehensively investigates the bandgap bowing of cesium–lead mixed-halide perovskites using compositional engineering and demonstrates that bandgap bowing is extremely small in a variety of compositions including Cl, Br, and I. Subsequently, through density functional theory calculations, it is suggested that the antibonding character of the valence band maximum, tilt distortion of halide ions, and entropy effect leading to equal participation of various halide ions around Pb are collectively responsible for the small bandgap bowing.

Ref) Adv. Optical Mater. 11, 2300682 (2023)

Talk No 2.

Ferroelectric HfO_2: from physics to industry

Duk-Hyun Choe[1]

[1] *Device Research Center, Samsung Advanced Institute of Technology (SAIT), Suwon, Korea*

Over the past decade, there has been a resurgence of interest in ferroelectric (FE) devices in the fields of materials science and electrical engineering. This interest is driven by the discovery of ferroelectricity in a simple binary oxide, HfO_2. FE HfO_2 exhibits ultra-scalable ferroelectricity that is compatible with Si electronics, presenting compelling opportunities for the use of FEs in advanced memory and logic devices. Recent studies further reveal some unconventional aspects of its FE properties compared to traditional perovskite counterparts, highlighting the need for more fundamental investigations into the physics of ferroelectricity in HfO_2.

In this talk, I will briefly review the status of the field [1,2], and present our theoretical and experimental approaches for utilizing FE HfO_2 for industrial applications. Starting from the basics, I will first revisit the modern theory of polarization to accurately define the multi-valued polarization in FE HfO_2 [3]. We then introduce unconventional polarization switching scenarios by leveraging the unique structural topology of FE HfO_2 [3]. Finally, I will share some of our recent experimental efforts on applying ferroelectric hafnia to negative capacitance FETs (NCFETs) [4] and FEFETs [5-7]. If time allows, I will also discuss my role as a physicist in industry research.

[1] {J. Y. Park, D.-H. Choe, D. H. Lee} et al., *Adv. Mater.* **2023,** 2214970 (2022)
[2] José P. B. Silva et al. *APL Mater.* **11,** 089201 (2023)
[3] D.-H. Choe et al., *Mater. Today* **50,** 8 (2021)
[4] {S. Jo, H. Lee} et al., *Nat. Electron.* **6,** 390 (2023)
[5] S. Yoo et al., *Appl. Phys. Lett.* 123, 222902 (2023)
[6] H. J. Lee et al., *IEEE-TED* **71,** 2411 (2024)
[7] S. Yoo et al., *VLSI Symposium* accepted (2024)

Talk No 3.

Recent Progress of 'Jx' code for magnetic force linear response theory and its applications

Myung Joon Han [1]

[1]*Department of Physics, KAIST*

In this talk, I will report our recent progress of 'Jx' code [1, 2] for calculating magnetic interactions in molecules and solids based on magnetic force theorem (MFT). Originally started from a 'OpenMX' subroutine [3, 4], 'Jx' has been separated and re-written in Julia to foster more active developments. In the first part of this presentation, I will try to introduce the basic idea of MFT formalism with a particular emphasis on the less-known features [5]. 'Jx' has been successfully combined with more advanced schemes of self-energy computations including QSGW (quasi-particle self-consistent GW) [6] and single-site DMFT (dynamical mean-field theory) [7]. For the former, this implementation can be particularly useful because the total energy is typically not accessible. Last couple of years efforts have focused on the spin-orbit coupled case whose Hamiltonian includes such terms as Dzyaloshinskii-Moriya and Kitaev-Gamma [8]. After a brief introduction to this extended formalism, I will present some results of real material examples.

[1] H. Yoon, T. J. Kim, J. -H. Sim, M. J. Han, Comp. Phys. Comm. 247, 106927 (2020).
[2] https://kaist-elst.github.io/Jx.jl/
[3] M. J. Han, T. Ozaki and J. Yu, Phys. Rev. B 70, 184421 (2004).
[4] https://openmx-square.org/
[5] H. Yoon, T. J. Kim, J. -H. Sim, S. W. Jang, T. Ozaki, M. J. Han, Phys. Rev. B 97, 125132 (2018).
[6] H. Yoon, S. W. Jang, J. -H. Sim, T. Kotani, M. J. Han, J. Phys.: Condens. Matter 31 405503 (2019).
[7] H. J. Lee et al., (in preparation)
[8] D. H. Kiem et al., (in preparation)

Talk No 4.

The Role of Intersite Coulomb Interaction in mixed-valence compounds

Bo Gyu Jang[1], Sang-Hoon Lee[2], Wooil Yang[2], Minjae Kim[2], and Young-Woo Son[2]

[1] *Department of Advanced Materials Engineering for Information & Electronics, Kyung Hee University, Yongin 17104, Republic of Korea*

[2]*Korea Institute for Advanced Study, Seoul 02455, Republic of Korea*

In this presentation, I will discuss the DFT+*U*+*V* (*U*: onsite Coulomb interaction, *V*: intersite Coulomb interaction) study of mixed valence compounds [1, 2]. Firstly, I will examine the prototypical charge-ordered material $BaBiO_3$, where the charge-ordered state can be suppressed by substituting Ba with K, leading to superconductivity. However, the conventional DFT method fails to describe its physical properties. Our study reveals that the intersite Coulomb interaction *V* is essential to describe all their doping-dependent experimental features such as breathing instabilities and electron-phonon matrix element [4]. Secondly, I will discuss $LiCu_2O_2$ which contains Cu(II) (d^9) and Cu(I) (d^{10}) ions in its crystal structure. This material exhibits an unprecedented 250 % broadening of the bandwidth compared to the DFT prediction [3]. However, DFT+*U*+*V* successfully describes the experimental bandwidth, indicating the significance of inter-site Coulomb interaction in this system.

[1] S.-H. Lee and Y.-W. Son, Phys. Rev. Res. **2**, 043410 (2020).

[2] B. G. Jang, M. Kim, S.-H. Lee, W. Yang, S.-H. Ji, and Y.-W. Son, Phys. Rev. Lett. **130**, 136401 (2023).

[3] M. Moser et al., Phys. Rev. Lett. **118**, 176404 (2017).

Talk No 5.

1T-TaS_2: Mott Insulator or Band Insulator?

Sung-Hoon Lee[1]

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

1T-TaS_2, a transition metal dichalcogenide, comprises stacked layers of triangular lattices of Ta ions in the d1 electronic configuration. Upon cooling below 180 K, this material undergoes a transformation into a charge density wave (CDW) state, characterized by a $(\sqrt{13} \times \sqrt{13})$ "Star of David" distortion, which changes the material from metallic to insulating. The precise nature of this insulating phase has triggered considerable debate, particularly concerning whether it acts as a Mott insulator or an interlayer-hybridized band insulator. In this talk, we present the key physical ideas underlying the insulating phase of 1T-TaS_2 and then discuss the latest findings concerning its surface properties.

Talk No 6.

Emerging quantum phenomena in 1T-transition metal dichalcogenides with noncentrosymmetric charge-density wave

Kyung-Hwan Jin[1]

[1] *Department of Physics, Jeonbuk National University, Jeonju, 54896, Republic of Korea*

1T-transition metal dichalcogenides (TMD) have been an exciting platform for exploring the intertwinement of charge density waves and strong correlation phenomena. While the David star structure has been conventionally considered as the underlying charge order in the literature, recent scanning tunneling probe experiments on several monolayer 1T-TMD materials have motivated a new, alternative structure, namely the anion-centered David star structure. In this talk, I'll show that this novel anion-centered David star structure manifestly breaks inversion symmetry, resulting in flat bands with pronounced Rashba spin-orbit couplings. These distinctive features unlock novel possibilities and functionalities for 1T-TMDs, including the giant spin Hall effect, the emergence of Chern bands, and spin liquid that spontaneously breaks crystalline rotational symmetry. Our findings establish promising avenues for exploring emerging quantum phenomena of monolayer 1T-TMDs with this novel noncentrosymmetric structure.

Talk No 7.

Pushing the limit of crystal structure prediction using machine-learned potentials

Sungwoo Kang

Computational Science Research Center, Korea Institute of Science and Technology (KIST)

Crystal structure prediction (CSP) is a computational method for determining the crystal structures of inorganic compounds based on their composition, essential for material discovery in uncharted chemical spaces. Typically, CSP involves sampling configurational spaces using density-functional theory (DFT) combined with either random sampling or optimization methods like genetic algorithms. However, the extensive computational demands of DFT calculations restrict the ability to perform high-throughput material discovery. An alternative CSP approach utilizes informatics to leverage the structural frameworks of known inorganic compounds from existing databases, though this method falls short in discovering materials with entirely new structural prototypes. In this presentation, I will discuss our latest advancements in developing a direct-search CSP method accelerated by machine-learned potentials (MLPs). Initially, I will outline our MLP training method using disordered structures, which allows for efficient training set sampling without prior knowledge of the target compound [1]. Following this, I will introduce SPINNER, a CSP workflow that effectively integrates MLPs with optimization algorithms [2]. Our findings indicate that SPINNER achieves an 80% success rate (with a maximum error of 36 meV/atom) for complex ternary materials. We also find that SPINNER surpasses conventional CSP codes such as USPEX, and CALYPSO. Leveraging SPINNER's high accuracy and speed, we explored all potential elemental combinations of unknown ternary metal oxides, resulting in the discovery of 45 novel, and synthesizable compositions [3]. To conclude, I will briefly introduce recent developments in AI-based methods, such as generative model, and offer perspectives on future directions in this field.

[1] C. Hong et al. Training machine-learning potentials for crystal structure prediction using disordered structures. *Phys. Rev. B* **102**, 224104 (2020).
[2] S. Kang et al. Accelerated identification of equilibrium structures of multicomponent inorganic crystals using machine learning potentials. *npj Comput. Mater.* **8**, 108 (2022).
[3] S. Hwang et al. Stability and equilibrium structures of unknown ternary metal oxides explored by machine-learned potentials. *J. Am. Chem. Soc.* **145**, 19378 (2023).

Talk No 8.

Accelerating Atomic-Scale Simulations through Machine Learning Potentials and Diffusion Models

Hongkee Yoon[1,2]

[1]*Kangwon National University*

[2]*KIAS Center for Artificial Intelligence and Natural Sciences*

In this talk, we present our recent advancements in accelerating atomic-scale simulations by developing and applying machine learning potentials and diffusion models. Machine learning has emerged as a powerful tool, enhancing the efficiency of calculations to unprecedented levels. We have addressed the stability issues of machine learning potentials by incorporating regularization techniques and data augmentation strategies, enhancing their robustness and transferability. Furthermore, we introduce a novel transformer-based model that efficiently represents atomic environments, significantly improving these potentials' accuracy and computational efficiency. This advancement enables large-scale simulations that were previously intractable. Additionally, we demonstrate our work on diffusion models for generating stable molecular structures. We guide the diffusion model to generate energetically favorable and physically plausible molecular configurations by integrating physical ideas and constraints into the learning process. This integration includes the application of energy-based constraints and symmetry considerations, which helps to generate more stable structures. These advancements in machine learning potentials and diffusion models would provide a robust framework for accelerating atomic-scale simulations and unlocking new insights into material properties and design.

Talk No 9.

Materials Generation and Synthetic Predictions Enabled by AI

Yousung Jung[1]

[1]*Department of Chemical and Biological Engineering, Seoul National University*

Materials informatics utilizes data to establish relationships between the structures and properties of materials, enabling the exploration of the vastness of the materials space through the use of models. Generative model, in particular, can serve as an inverse design tool, mapping from property to materials space. Trained on diverse datasets, these generative models can unlock the potential for predicting novel materials with tailored properties. While the key advantage of generative models is a potential to produce novel materials, often times they may be “too novel” and cannot be synthesized. In order to minimize the time and resources for experimental synthesis attempts, models that can predict the synthesizability (and, if synthesizable, synthesis recipes as well) would be immensely helpful. Thus, in this talk, I will delve into two important aspects of materials design: generation and synthesis prediction based on data and machine learning. These will complement the traditional electronic structure theory-based high-throughput virtual screening.

Talk No 10.

Active Learning Configuration Interaction for Excited State Calculations of Aromatic Systems

WooSeok Jeong[1]

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Understanding the excited states of aromatic organic molecules is crucial for the development of materials for optoelectronics, photocatalysis and photovoltaics. Time-dependent density functional theory (TD-DFT) is one of the most widely used methods for excited state calculations. However, it is well known that TD-DFT is highly sensitive to functionals and cannot describe strongly correlated systems well because it is based on a single reference scheme. To overcome this limitation, multiconfigurational quantum chemistry methods have been developed, but they are limited to relatively small systems because they require huge computational resources. In this talk, I will introduce the active learning based configuration interaction (ALCI) method. This method is based on the Selected Configuration Interaction (SCI) theory, which is conceptually simple compared to other multiconfiguration methods, combined with a machine learning (ML) model. In SCI theory, reliable results are only possible if all or most of the energetically important electronic configurations are used to construct the wave function. In our scheme, we adopted a binary classification ML model to identify important configurations and designed an iterative procedure in which the performance of the ML model is improved during the iterations based on active learning. The ALCI method has been shown to successfully predict the lowest singlet-singlet and lowest singlet-triplet vertical excitation energies for small and medium-sized aromatic compounds compared to complete active space CI (CASCI) results. In addition, our method can handle larger systems with very large active spaces, which cannot be handled by conventional multireference methods.

Talk No 11.

First-principles investigations of two-dimensional electrides

Gunn Kim

(*Department of Physics and HMC, Sejong University, Seoul 05006, Korea*)

Electrides, characterized by electrons acting as anions within a cationic framework, demonstrate unique behaviors when formed into ultrathin layers. In this study, we have examined various physical properties of two-dimensional (2D) electrides, focusing on layered structures such as Gd_2C, Ca_2N, and Y_2C, using first-principles calculations.

For Gd_2C, we examined how its surface anionic electrons, which make up about 25% of the electrons in the interlayer region, increase under an external electric field, suggesting applications in spintronics due to the spin-polarized electronic gas in the material. The manipulation of Ca_2N and Y_2C bilayers through translation, rotation, and compression alters their electronic and magnetic properties, with significant effects observed from interlayer electron localization and symmetry changes in bilayer sliding. Besides, the creation of Moiré patterns in twisted bilayers indicates potential uses in straintronics and twistronics. Further, we analyzed the impact of structural defects in Ca_2N bilayers on electron distribution and visualized these effects using scanning tunneling microscopy, showing the sensitivity of electrides to atomic configuration changes. Finally, the study of the dielectric functions and optical conductivity of Ca_2N, using pseudoatomic orbital basis sets, reveals distinct interband transitions. This work will contribute to understanding the optical behavior of 2D electrides and pave the way for future technological applications. Our approach highlights the versatility and profound potential of 2D electrides in advanced material science.

Talk No 12.

Thermal Decoupling: Origin of Strange Metal Phase in Unconventional High-T_c Superconductors

Gun-Do Lee[1,2]

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[2] *Institute of Advanced Materials, Seoul National University*

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Although many years have passed since the discovery of high-critical temperature (high-T_c) superconducting materials, the underlying mechanism is still unknown. In particular, the intricate interplay between non-ergodic bad metals and strange metals in high-T_c superconductors has remained enigmatic. Intriguingly, most of these unconventional high-T_c superconductors have layered structures. Using ab initio molecular dynamics (AIMD) simulations coupled with the temperature-dependent effective potential (TDEP) method, we recently discovered an interlayer thermal decoupling in YBCO, a representative material of unconventional high-T_c layered superconductors. It is found that the thermal decoupling is driven by Ba atoms in YBCO. Surprisingly, we found that the thermal decoupling solves the linear-T resistivity in the strange metal phase, which has been a major mystery in unconventional high-T_c superconductors. It is revealed that the thermal decoupling can also explain the Uemura relation, another mystery in high-temperature superconductivity, rigorously and quantitatively. The strange metal and Uemura relation are tightly coupled by thermal decoupling. The thermal decoupling is also a key factor in understanding the relationship between the superconductivity and flat bands found in magic-angle twisted bilayer graphene. The relation between thermal decoupling and quantum geometry will be mentioned. Our discoveries will offer a revolutionary perspective on high-T_c superconductivity, suggesting the potential for a transformative shift in our comprehension.

Talk No 13.

Simulating Ground-State Electronic Structure and X-ray Spectra of Transition Metal Clusters

Seunghoon Lee

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Transition-metal clusters, ubiquitous in the active sites of biological enzymes, serve as remarkable catalysts. A notable example is the FeMo-cofactor in the nitrogenase enzyme of bacteria. This cofactor catalyzes the conversion of nitrogen gas into ammonia even at room temperature and atmospheric pressure. The key to its impressive functionality is believed to lie in its complex and strongly correlated electronic structure.

To explore the relation between the catalytic activity and the strongly correlated nature, we have performed the ground-state electronic-structure simulation of the cluster, using the active space model. Employing the density-matrix renormalization group (DMRG) algorithm, along with the matrix-product-state (MPS) representation of the active-space wavefunction, has yielded insightful findings. Notably, we have observed extremely large multi-reference character in the ground state. [1] Intriguingly, our simulation suggests that the Mo atom in the cluster could function as an electron pump, pushing electrons to the Fe atoms, potentially enhancing nitrogen gas binding.

Validating the theoretical active-space model can be achieved through X-ray spectra simulations. We considered L-edge X-ray absorption spectroscopy (XAS) and 2p3d resonant inelastic X-ray scattering (RIXS) spectroscopy. These spectroscopies provide high-intensity and high-resolution spectra, capturing the complex phenomena of electron correlation, ligand-field splitting, and multiplet splitting, spin-orbit splitting, etc. We have developed a novel approach to simulate the spectra of transition metal clusters, which overcomes several challenges using the correction vector formulation and MPSs. [2] We achieved the first successful spectra simulation for transition metal clusters. This breakthrough enables the correction of a previously misassigned experimental RIXS band, highlighting the significant role of ligand-to-metal charge transfer (LMCT) in the cluster. Moreover, the analysis of similarities and differences between experimental and theoretical spectra allows us to rigorously validate the strength and the limitation of the active space model. We believe these novel techniques will advance our understanding of the electronic structures of transition metal clusters.

[1] S. Lee, J. Lee, H. Zhai, Y. Tong, A. M. Dalzell, A. Kumar, P. Helms, J. Gray, Z.-H. Cui, W. Liu, M. Kastoryano, R. Babbush, J. Preskill, D. R. Reichman, E. T. Campbell, E. F. Valeev, L. Lin, G. K. Chan, *Nat. Commun.*, 14, 1952 (2023)
[2] S. Lee, H. Zhai, and G. K. Chan, *J. Chem. Theory Comput.*, 19, 7753 (2023)

Talk No 14.

Novel charge trap mechanism in amorphous silicon nitride

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Polaron formation is a phenomenon where excess charge supplied from the outside becomes spatially localized, accompanied by lattice distortion [1]. In this talk, I report on a mechanism similar to polaron but fundamentally different. This phenomenon has been observed in amorphous silicon nitride and is accompanied by the breaking and formation of chemical bonds [2]. Excess charge becomes localized only on atoms undergoing these changes in chemical bonding. As a result, a shift in trap level occurs, stabilizing the stored charge. This discovery holds significant implications for Flash memory technology [3]. Charge trap flash (CTF) stores information by inserting a charge trap layer into the oxide layer of a standard MOSFET structure and injecting charge there to adjust the threshold voltage. So far, it has been believed that excess charge is stored in Si dangling bonds present in amorphous silicon nitride, guiding semiconductor processes and device modeling such as TCAD. However, this discovery suggests that stable charge traps can be explained better even without relying on Si dangling bonds. As miniaturization of memory devices continues, understanding phenomena occurring at the atomic level becomes increasingly important. Therefore, this discovery is highly significant at this point of time.

[1] C. Franchini, M. Reticcioli, M. Setvin, and U. Diebold, *Polarons in Materials*, Nat. Rev. Mater. **6**, 560 (2021).

[2] W. I. Choi, W.-J. Son, R. Dronskowski, Y. Oh, S.-Y. Yang, U. Kwon, and D. S. Kim, *Switchable Chemical-Bond Reorganization for the Stable Charge Trapping in Amorphous Silicon Nitride*, Adv. Mater. **36**, 2308054 (2024).

[3] D. Kahng and S. M. Sze, *A Floating Gate and Its Application to Memory Devices*, Bell Syst. Tech. J. **46**, 1288 (1967).

Talk No 15.

Development of a Virtual Quantum Computer based on Multi-scale Simulations of Si Quantum Dot Structures

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Needs for large-scale simulations of semiconducting systems have been obvious since they not only present a practical method for understanding electrical properties in a systematic level that would be hard to be captured with pure *ab-initio* simulations but can accelerate potential device designs including realistic aspects of controls. In this talk, we introduce our ongoing project whose focus is to develop a virtual quantum computer based on electrically created quantum dots in Silicon. Including details of multi-scale modeling based on the bulk physics augmented with empirical simulations of electrical structures [1], we present a short review on how to mitigate spin-qubit errors with bias controls [2], how to couple the Bayesian Optimization technique to improve the performance of a two-qubit entangling gate device [3], and designs of a five-qubit programmable quantum circuits with a Si structure that includes up to five quantum dots [4]. If time allows, we will discuss the parallelization scheme of our multi-scale modeling approach, including its parallel efficiency measured in high-performance computing resource.

Acknowledgement
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References
[1] J. Kang, J. Ryu and H. Ryu, *Nanoscale* **13**, 322
[2] H. Ryu and J. Kang, *Scientific Reports* **12**, 15200
[3] J. Kang, T. Yoon, C. Lee, S. Lim, and H. Ryu, Accepted to *Scientific Reports*.
[4] J. Ryu and H. Ryu, *arXiv:*2403.19551 [quant-ph].

ABSTRACTS OF POSTERS

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Poster No.1

Significant Anomalous Hall Conductivity in Fe_3GaTe_2 Due to Flat Nodal Line Topology

Yoon-Gu Kang[1], Woohyun Cho[1], Jaehun Cha[1], Dong Hyun David Lee[1], Do Hoon Kiem[1], Jaewhan Oh[1], Jongho Park[2], Changyoung Kim[2], Yongsoo Yang[1], Yeong Kwan Kim[1], Heejun Yang[1], and Myung Joon Han[1]

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The confluence of magnetism and band topology in materials results in unique quantum phenomena, among which the anomalous Hall effect (AHE) is prominent. This effect, arising from the breaking of time-reversal symmetry, is observed in various magnetic systems, including ferromagnets, non-collinear antiferromagnets, and altermagnets. Recent studies on the van der Waals ferromagnetic semimetal Fe_3GeTe_2 have identified a significant AHE owing to the Berry curvature associated with a dispersive nodal line [1]. In our research, we investigated Fe_3GaTe_2, another van der Waals ferromagnetic semimetal, which is notable for its substantial AHE and high Curie temperature [2]. Our first-principles calculations reveal that Fe_3GaTe_2 features a flat nodal line at the Fermi level, which induces a significant Berry curvature and thereby enhances the AHE. The flatness of the nodal line ensures distinct energy separation at the Fermi level, with the lower energy states predominantly contributing to the AHE. This contribution was considerably greater than that of the dispersive nodal lines. Owing to its robust room-temperature ferromagnetic properties and intricate band topology, Fe_3GaTe_2 is a promising material for advanced quantum devices. Our findings highlight the potential of Fe_3GaTe_2 in quantum technology driven by its unique electronic and magnetic properties.

[1] K. Kim, J. Seo, *et al*., *Nat. Mater.* **17**(9), 794-799 (2018).
[2] W. Cho, Y.-G. Kang, J. Cha, *et al*., *Adv. Mater.* 2402040 (2024).

Poster No.2

Surface Reaction Analysis Using Pretrained Machine Learning Potentials for NAND Flash Processes

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As semiconductor processes become increasingly miniaturized, new processes and techniques are being introduced. Although processes such as atomic layer deposition (ALD) and area selective deposition (ASD) are widely used, there are still some uncertainties due to the limitations of experimental equipment and the difficulty of mechanism analysis. Consequently, the importance of atomistic simulation in these processes is growing.

In studies conducted to date, reaction mechanism analysis based on density functional theory (DFT) has been commonly performed due to its high accuracy. However, DFT calculations for surface reactions are computationally expensive, making it challenging to analyze all complex surfaces and reactions.

Recently, research utilizing pretrained machine learning potentials (MLPs) has garnered significant interest, enabling atomistic simulations with DFT-level accuracy at much higher speeds without the need for exhaustive detail in constructing the training set. However, validation of these models for complex scenarios such as surface reactions has not been widely conducted.

Therefore, in this study, we aim to focus on the NAND Flash process and apply pretrained MLPs to analyze surface reactions occurring on silicon oxide and silicon nitride surfaces, particularly those involving ALD and ASD reactions. We intend to verify if these results exhibit sufficient consistency and accuracy compared to existing DFT results and to analyze the causes of any discrepancies.

Poster No.3

Layered Transition Metal Dichalcogenides as Ca/Mg Intercalation electrode: A Systematic First-Principles Study

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Multivalent-ion batteries have attracted attention as promising alternatives to conventional Li-ion atteries. However, few electrode materials can reversibly intercalate multivalent ions like Ca and Mg ecause strong interaction between the host framework and the guest ions impedes the facile intercalation reaction. Herein,Here, we focus on layered transition metal dichalcogenide polymorphs with a range of transition metal substitutions. Transition metal dichalcogenide can be classified into three polymorphs such 1T, 2H, and 3R, where the guest ions can occupy either octahedral sites or trigonal prismatic sites. Our investigation includes Ti, Zr, V, Nb, Ta, Cr, Mo, and W as substituted transition metals across six structure types. Considering two intercalating ions and two chalcogenide elements, 192 electrode candidates are generated. (Ion : Ca and Mg, Chalcogenide : S and Se) Using first-principles calculations based on density function theory, we assess four key properties - thermodynamic properties, electrochemical properties, ion mobility, and redox activity of transition metals - to pinpoint the optimal intercalation electrode materials for Ca and Mg batteries.

Poster No.4

Polytypic Variants of the Adaptive Ta_2O_5 Structures

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Tantalum oxide (Ta_2O_5) has a variety of suggested crystalline phases. Among them, the phases with an adaptive structure have similar related structures within the same composition, resulting in numerous configurations [1]. The effective search for an infinite number of possible ionic configurations in the adaptive structure can be initiated from the construction of the structural variants of the well-known phases. This work suggests a unified procedure for constructing the structural variants of the λ, γ, and Pmma phases of the Ta_2O_5 and calculates their energetic and dynamic stabilities. This procedure applies the polytype idea, a stacked structure of identical unit layers [2]. The polytypes composed of the same unit layer can have different structures depending on the stacking sequences. The unit layer is defined by the glide and screw symmetry elements of the λ, γ, and Pmma phases, forming distinct groups of polytypes. The resulting groups of polytypes share a common configuration of the Cmmm phase. The stacking sequence and the interaction between adjacent unit layers affect the energetic and dynamic stabilities of the polytypes.

[1] J. S. Anderson, J. Chem. Soc., Dalton Trans., 1107-1115 (1973)
[2] A. Guinier et al., Acta Cryst. A40, 399-404 (1984)

Poster No.5

First-principles-based relativistic magnon excitations

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Magnetism is a key issue in condensed matter physics. The magnetism in materials is often achieved by finding magnetic interactions. However, their evaluation is quite challenging due to its small energy scale and complex origins. Magnetic force theorem provides a powerful approach to obtaining these interactions [1-4]. In this work, we present an expansion of our code 'Jx' [5-7] using the magnetic force theorem for non-collinear spins (NC-MFT), which includes spin-orbit couplings. Based on these, we also provide a computational code development for describing magnon excitations [8].

[1] A. I. Liechtenstein et al. J. Phys. F: Met. Phys. 14, L125 (1984)
[2] A. I. Liechtenstein et al. J. Magn. Magn. Mater. 67, 65-74 (1987)
[3] V. P. Antropov et al. Phys. B: Condens. Matter. 237-238, 336-340 (1997)
[4] M. J. Han et al. Phys. Rev. B 70, 184422 (2004)
[5] H. Yoon et al. Phys. Rev. B 97, 125132 (2018)
[6] H. Yoon et al. Comput. Phys. Commun. 247, 106927 (2020)
[7] https://kaist-elst.github.io/Jx.jl/
[8] https://dhkiem.github.io/SpinMax.jl/

Poster No.6

Ab initio study of the effect of stacking order on the flat band size in rhombohedral graphene

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Rhombohedral graphene (RG) has attracted widespread attention for its extraordinary properties, the occurrence of the flat band near the Fermi level, which could lead to superconductivity. In addition, advances in experimental fabrication methods have made it easier to measure RG properties experimentally. This has led to an active research effort on RG structures, but there are still more challenges to be solved and a comprehensive understanding of the exotic properties that depend on the stacking composition is needed.

Our study aims to clarify the correlation between the stacking configuration and the low energy band structure. First, we use Density Functional Theory (DFT) and choose proper van der Waals option. On this basis, we study the tendency of the flat band size in multiple layers of RG up to 33 layers and determine the limits of the flat band size by analyzing the bulk properties. And we try to calculate different configurations introducing ABA structure configuration and sort out the changes in band structure along the configuration. We also calculate project band onto each layer to know the effects of layers on low energy band and calculate the density of states of each structure to characterize the electronic structure of graphene according to the configuration. Based on these results, we aim to identify if there are other structures, apart from the RG structure, that demonstrate unique behavior, and to explore ways to further enhance the properties of the RG structure.

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Poster No.7

Property-networking deep learning model for materials

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There is a growing need to develop artificial intelligence technologies capable of accurately predicting material properties. This requires expanding material databases beyond density functional theory (DFT) and developing deep learning (DL) models effective with limited high-fidelity data. We developed a DL model using a crystal structure representation based on the orbital field matrix (OFM), modified to include information on elemental properties and valence electron configurations. This model, capturing interrelations among elemental properties in crystals, is called PRoperty-networking Orbital Field maTrix-convolutional Neural Network (PROFiT-Net). Remarkably, PROFiT-Net demonstrates high accuracy in predicting dielectric constants, experimental band gaps, and formation enthalpies compared to other leading DL models. Moreover, our model accurately identifies physical patterns, such as avoiding unphysical negative band gap predictions and exhibiting a Penn-model-like trend while maintaining scalability. We envision PROFiT-Net accelerating the development of functional materials.

Poster No.8

Theoretical *ab-initio* investigation on polaronic dielectrics: dynamics of self-trapped polarons in perovskite $SrTiO_3$

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As well known, the technological progresses of the electric vehicles, airplanes, motorcycles, bicycles, robots and various other electric machinery devices have been very remarkable in recent days. The electronic capacitors, which are very important electronic components installed in large quantities into these devices and our representative core competence, have strongly supported these progresses. With further progresses of these devices, the requirements for the electronic components from the markets are expected to be higher and higher. Thus, it is inevitable to explore new dielectric materials and to develop new capacitors with much higher performances for the next generation.

At the beginning of this century, very sensational findings were reported, that is, $(Ca,Cu_3)Ti_4O_{12}$ oxides show huge dielectric constants (HDC) [1,2] much larger than those of usual ferroelectric materials. Although understanding of fundamental mechanism to express HDC has been quite important, theoretical elucidation has hardly been made clearly yet.

In the present study, we theoretically investigated the electronic states of one of the representative HDC materials, Nb doped $SrTiO_3$ perovskite, in detail by *ab-initio* calculations. Then, it was found that electron/hole carriers generated by dopants stably form polaron states in $SrTiO_3$. Moreover, the F color center, where polarons are self-trapped at the oxygen vacancy site, was formed as metastable states in hopping processes. Furthermore, we also examined detailed local hopping behaviors of self-trapped polarons by *ab-initio* molecular dynamics calculations and successfully observed their hoppings. Based on these results, we propose a new mechanism for the HDC materials, by which HDC are expressed. That is, in short, the polaron oscillations by local hoppings give rise to huge dielectrics. Our results show qualitatively good agreements with experiments [3].

In this presentation, we show our results and make discussion on them.

References

[1] M. A. Subramanian *et al*., J. Solid State Chem., 151, 323-325 (2000).
[2] C. C. Homes *et al*., Science, 293, 673-676 (2001).
[3] I. Kim *et al*., preparing for publication.

Poster No.9

Hybrid functional investigation of native crystallographic defects in Weyl semimetal LaAlGe

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Among the Weyl semimetal (WSM) *Ln*AlX (*Ln* = lanthanide, X = Ge, Si) family, the Fermi arc electron states on the surface were observed in the $I4_1md$ phase of LaAlGe [1]. However, no anomalous Hall effect or chiral anomaly, which are fingerprints of the WSM, was observed [2,3]. In addition, although the observed normal state transport property in LaAlGe is consistent with conventional metal, the large residual resistivity is comparable with that of a magnetic counterpart WSM CeAlGe [2]. The $I4_1md$ phase of LaAlGe single crystals is typically grown out of Al self-flux [2,3], the volatile nature of Al may result in crystallographic defects that can be sources of electric charges [4]. In this study, we investigate the native crystallographic defects including vacancy and antisite in LaAlGe using hybrid density-functional theory calculations [5]. The Ge-on-Al antisite (Ge_{Al}) and the Al-on-Ge antisite (Al_{Ge}) are the most abundant defects in LaAlGe, and the energetic preference depends on the growth conditions in experiment. Since the Ge_{Al} and Al_{Ge} antisites are donor-like and acceptor-like, respectively, they can be scattering centers in the electronic transport process and/or can induce the substantial vertical shift of the electronic chemical potential in LaAlGe .

[1] S.-Y. Xu *et al*., Sci. Adv. **3**, e1603266 (2017).
[2] H. Hodovanets *et al*., Phys. Rev. B **98**, 245132 (2018).
[3] Z. Hu *et al*., Appl. Phys. Lett. **117**, 222410 (2020).
[4] Y. G. Yu, X. Zhang, and A. Zunger, Phys. Rev. B **95**, 085201 (2017).
[5] I. Kim *et al*., Phys. Rev. Mater. **8.5**, 054203 (2024).

Poster No.10

Data-efficient construction of high-fidelity machine learning force field by multi-fidelity training

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One major advantage of machine learning force fields (MLFFs) is that the machine learning model can be fitted to any *ab initio* database, regardless of the choice of theory. For example, meta-generalized gradient approximation (meta-GGA) exchange-correlation functional has high-fidelity but more computationally expensive than conventional GGA methods. However, MLFF trained with meta-GGA data requires the same computational cost as one trained with GGA data, given the same machine learning architecture. Despite this, constructing high-fidelity MLFFs is still challenging due to the substantial computational costs of creating high-fidelity databases.

A promising solution to this problem is using both low- and high-fidelity data in MLFF construction. By training on the rough trends of the potential energy surface (PES) using abundant low-fidelity data and refining with the differences captured by the high-fidelity data, the model can accurately determine the ground truth with minimal high-fidelity data.

We have developed a new MLFF architecture capable of training on both low- and high-fidelity databases concurrently. Specifically, we use the SevenNet (Scalable EquiVariance-Enabled Neural NETwork), an equivariant graph neural network. By incorporating one-hot encoding of data fidelity into the node features, our modified SevenNet includes both common parameters used for every training data, and fidelity-dependent weights used for each fidelity database. This allows the MLFF to learn the general trends of the PES with common parameters while capturing detailed PES differences with fidelity-dependent parameters.

To validate our approach, we tested it on wurtzite $In_xGa_{1-x}N$, used in light-emitting diodes, and argyrodite Li_6PS_5Cl, used as a Li-ion conductor. For the low-fidelity database, we used GGA functionals to calculate various configurations, including strained crystal structures and molecular dynamics (MD) simulations. A small portion of this low-fidelity database was then recalculated using single-point calculation with meta-GGA functionals to create a high-fidelity database. Our results show that knowledge from the low-fidelity database can be effectively transferred, significantly improving the accuracy and MD stability of high-fidelity MLFFs in unsampled chemical environments.

Based on these findings, we extended our approach to construct a general-purpose MLFF with meta-GGA fidelity. We found that our approach substantially enhances the capability of high-fidelity general-purpose MLFFs, successfully predicting energy ordering, equilibrium volume and bulk modulus of oxide polymorphs by applying our multi-fidelity training to the GGA and meta-GGA databases from the Materials Project. However, this MLFF tends to underestimate forces since the meta-GGA database primarily contains near-equilibrium structures. We anticipate that our method marks a significant step toward creating the ultimate high-fidelity general-purpose MLFF by augmenting the database.

Poster No.11

Magnetic and Electronic Properties of Cr_2Se_3

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Recently, two-dimensional transition metal dichalcogenides (TMDC) have attracted much attention, and subsequently, materials with transition metals intercalated between TMDC layers have also received considerable attention. We performed charge density functional theory (cDFT)+U calculations for several spin configurations of one of these materials, bulk Cr_2Se_3. To obtain the appropriate values of U and J, the interaction parameters used in the cDFT+U calculation, the constrained random phase approximation (cRPA) calculation was performed. As a result, we obtained an antiferromagnetic ground state with a collinear order approximating the spin configuration proposed in previous neutron diffraction studies.

Poster No.12

First-Principles Study of the Dzyaloshinskii-Moriya interaction of self-intercalated CrTe2

Hyeong-Ryul Kim

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

Non-collinear spin-textures such as skyrmion have attracted much interest because of its potential for applying novel nano-spintronic devices. Recently, self-intercalated chromium telluride (Cr(1+δ)Te2) has been chosen as one of the interesting materials that represent the non-collinear spin-textures. In this research, we select several compounds of Cr(1+δ)Te2 and calculate Dzyaloshinskii-Moriya interaction (DMI) to simulate the non-collinear spin-textures. Since it is hard to get exact DMI due to the material being bulk material, we use the Clockwise/Anticlockwise (CW/ACW) fitting method to get bulk DMI. Using the calculated DMI parameters, we estimate the spin-textures of each structure.

Poster No.13

Density Functional Theory study of CDW structure in $TiSe_2$

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1T-$TiSe_2$ is a well-studied TMDC (Transition Metal Dichalcogenide) material known for exhibiting a CDW (Charge Density Wave) at 165K. Despite extensive research, it is not clear whether this material is a semimetal or a semiconductor. Additionally, a second CDW transition at 165K has been identified. Here, we perform first-principles electronic structure calculations to investigate potential CDW patterns in 1T-$TiSe_2$ and their impact on electronic structures. When considering a 2x2x1 supercell, only a single type of CDW pattern is observed, as reported in previous theoretical studies. However, in the case of a 2x2x2 supercell, we found four different types of CDW orders, which are almost degenerate in energy. Furthermore, we utilized the band unfolding technique to compare the band structures of the four CDW phases with angle-resolved photoemission data and discussed the effects of spin-orbit coupling on the band structures. Additionally, we computed lattice-induced free energies to determine the presence of potential thermal phase transitions.

Poster No.14

Quantifying thermoelectric-driven triboelectric charge

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The fundamental understanding of tribocharging has not been fully accomplished, despite its ubiquity in daily life and industry. Recently, our group revealed that thermoelectric effect plays a pivotal role in charge transfer induced by frictional heat [1]. However, this work primarily indicated the direction of tribocharging, leaving the quantification of the transferred charge unresolved. In this study, we quantify the charge transfer driven by thermoelectricity at material interfaces. Using the steady-state condition of total current density, we evaluated the transferred charge between two semi-infinite materials and examined the charging behavior for finite-sized interfaces. As a result, the transferred charge is determined by the averaged electronic reservoir of each material and increases as the contact area diminishes. The calculated triboelectric force explains the adhesion phenomena observed in daily life. Our findings provide essential theoretical insights into identical or granular charging and propose potential advancements for applications such as nanogenerators and nanoadhesion technologies.

[1] E.-C. Shin, J.-H. Ko, H.-K. Lyeo, and Y.-H. Kim, *Derivation of a governing rule in triboelectric charging and series from thermoelectricity*, Phys. Rev. Research **4**, 023131 (2022).

Poster No.15

First-Principles Study on the Defect-Induced Phenomena in Hexagonal Boron Nitride/Tungsten Diselenide Heterostructure

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Recent studies have demonstrated that defects can lead to exotic phenomena such as photoluminescence in different spin states or wavelength ranges. Two-dimensional materials are particularly suitable for hosting these phenomena, as their natural surfaces allow for easy manipulation of defects. Hexagonal boron nitride (hBN) and tungsten diselenide (WSe_2) have garnered significant interest due to their direct bandgap, which facilitates photoemissions. Although these phenomena have been experimentally observed, their underlying mechanisms remain unclear, necessitating comprehensive investigation and evaluation. In this study, various atomic defects in these materials were examined, with their energetic, electronic, and magnetic properties calculated using first-principles density functional theory. We analyzed their formation energy, defect state energy levels, and spin states. Additionally, we scrutinized how these defects play roles in the hBN/WSe_2 heterostructure, commonly fabricated for encapsulation, focusing on how interlayer complex defects influence their spin and valley characters.

Poster No.16

Temperature-dependent phase diagram of charge density wave in monolayer H-$TaSe_2$ calculated from accurate interatomic potential

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Charge density wave (CDW) is a spontaneous modulation of electron density and lattice at low temperature. Due to its ubiquity in numerous transition metal dichalcogenides, its origin and interplay with a superconductivity, metal-insulator transitions, and other correlated phases are of fundamental importance in modern condensed matter physics. Among various CDW materials, 2H-$TaSe_2$ is the one of the most studied ones and its successive phase transitions (commensurate, two or three incommensurate, and normal phases) on temperature are well established from X-ray scattering and resistance measurements. Though these phase transitions have been phenomenologically understood by a McMillan's Landau free energy model [PRB **12**, 1187 (1975)] with a handful of parameters, the absence of first-principles calculations on the phase transitions makes it difficult to understand the microscopic origin of the parameters. In this work, using accurate (<1 meV/atom) interatomic potential learned from first-principles calculations, we have calculated the temperature-dependent phase diagram reproducing essential phase transitions between commensurate, incommensurate and normal phase in monolayer H-$TaSe_2$. From the eigenmode decomposition analysis of total energy [J. Phys.: Condens. Matter **34**, 315401 (2022)], we have found that the anharmonic interaction is the origin of commensuration locking and the experimentally observed satellite Fourier peak in incommensurate CDW, clarifying the microscopic meaning of the parameters in Landau free energy model.

Poster No.17

SevenNet-0: A Pretrained Universal Machine Learning Potential.

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Machine learning potentials enable the development of interatomic potentials that achieve the accuracy of density functional (DFT) theory calculations with significantly enhanced computation speeds and scalability. However, these methods have been restricted to specific chemical species or applications, necessitating extra human efforts and DFT computations for generating the training set. To address this limitation, recent studies have concentrated on developing pretrained universal machine learning potentials. In this study, we present SevenNet-0, a foundational model trained on 180,000 crystal structures from the Materials Project. We investigated the generalizability of SevenNet-0 through several tests and observed the extrapolative ability of the model. For example, SevenNet-0 reasonably predicts the energies of crystal compounds which consist of the element combination absent in the training set. This indicates that fine-tuning the model with additional data is not mandatory. We found that the trained elemental embeddings of SevenNet-0 exhibit a continuous, spiral-like pattern along with atomic numbers. The pattern is analogous to periodic table and rationalize generalizability of SevenNet-0.

Poster No.18

Large scale molecular dynamics of phase-change material Ge-Sb-Te using machine learning potentials

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Ge-Sb-Te (GST) has garnered significant attention as a phase-change memory material due to its rapid switching between disordered and ordered states that exhibit substantial thermal and electrical contrasts. Understanding its atomic-level physical characteristics demands extreme computational power of simulating large-scale disordered structures and still remains a challenging task. We studied the mechanical and thermal properties of GST during the crystallization using large-scale molecular dynamics simulations with machine learning potentials. Initial amorphous structures were generated by melting-quenching process followed by annealing at 600 K for 10 ns that leads a phase change to cubic-GST. During crystallization, the bulk modulus and the shear modulus showed different behaviors, and the low-frequency vibrational anomaly known as the boson peak becomes weaker. We found that lattice vibrations associated with Te atoms are most responsible for the change in the shear modulus and the boson peak.

Poster No.19

Lindblad dephasing dynamics in strongly correlated electron systems

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Dephasing dynamics plays a critical role in describing light-matter interactions, particularly in the context of electron-electron scattering. In this study, we adopt the Lindblad master equation to investigate the dephasing process of high-harmonic generation (HHG) in the one-dimensional Hubbard model. The present approach could serve as a pertinent platform for understanding the dephasing processes in strongly correlated electron systems.

Poster No.20

Exploiting switching behavior of ferroelectric metal by joining metal contact

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Contact grants emergent properties that are beyond the innate characteristics of individual materials. The advent of two-dimensional ferroelectric metals has opened up a new avenues for contact engineering. We observed significant conductance hysteresis in contact composed of Pt and ferroelectric semimetal WTe_2 depending on the polarization direction. Considering that the conductance response of contact surpasses that of the ferroelectric channel, it is evident that contact plays the predominant role. Nevertheless, the absence of a band gap prevents direct elucidation of contact properties. Here, using first-principles calculations, we illustrate the origin of polarity-dependent conductance response in Pt/WTe_2 contacts. Initially, we demonstrate that the difference in charge transfer due to polarization direction, which agrees with the work function model. Our analysis further reveals that different doping levels of WTe_2 result in a distinctive gating response of conductance, leading to a butterfly-shaped hysteresis. These findings suggest an effective approach to harnessing the switching characteristics of ferroelectric metals.

Poster No.21

Disassembling gapless edge states; Insight from local Hamiltonians

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A topological insulator (TI) is a category of an insulator that hosts conduction channels on its surface, protected by the topology. While the origin of the edge states is apparent, it is hard to predict the shape of gapless edge states since it depends on the structure of the boundary. In the case of the gapped bilayer graphene, which is a well-known topological insulator, the AB stacking order smoothly transits into a BA stacking pattern across a wide domain boundary. Here, we propose a novel modeling method accounting for large domain wall structure that reduces large Hamiltonian into small local Hamiltonians. By using the local Hamiltonian picture, we found that effective potential energy landscape depends on the pseudospin character, which spatially separates two edge states across the bilayer graphene domain wall. This separation of pseudospin leads to a double-line feature in charge density, well agrees with the literature. Our work provides a new way of both predicting and understanding the properties of gapless edge states, unveiling the devil lies in the details.

Poster No.22

Phonon Renormalization by Electron-Phonon Coupling in Monolayer 1T-$IrTe_2$

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Layered transition metal dichalcogenides (TMDs) serve as a unique flatform to study intriguing electronic properties of two-dimensional materials [1]. Monolayer 1T-$IrTe_2$ exhibits diverse structural transitions from Ir dimerization as temperature or substrates are changed [2,3]. Yet, their physical origin is not comprehensively understood. In this study, we showed that the conventional model of the Fermi surface nesting does not account for the phonon-softening in $IrTe_2$. We investigated the phonon renormalization to find that the phonon-softening is indeed properly explained by considering the electron-phonon coupling. We demonstrated that the biaxial strains in $IrTe_2$ effectively modulate *pd* orbital hybridization and thus affect the electron-phonon coupling matrix elements. Our finding suggests that the structural transition of $IrTe_2$ upon changes in substrates or temperature may be associated with the strains induced by these changes.

References

[1] M. Chhowalla et al., Nature Chem 5, 263 (2013).
[2] J. Hwang et al., Nat Commun 13, 906 (2022).
[3] H. K. Kim et al., Phys. Rev. B 107, 045112 (2023).

Poster No.23

DFT analysis of influence of Oxygen Vacancies and Diffusion on Magnetic Properties at Co/HfO_2 Interfaces

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Multiferroic materials, composed of ferroelectrics and ferromagnets, exhibit significant magnetoelectric coupling, which allows magnetic properties to be controlled by electric fields. This property is highly valuable for engineering applications in memory and logic devices, and has led to extensive research in this area. Previous studies using Density Functional Theory (DFT) have analysed the magnetic moment and electronic structure at the Ni/HfO_2 interface. These studies have investigated changes in the magnetic moment of the ferromagnetic material as a function of polarization direction, and explored the effect of oxygen vacancies and diffusion on the multiferroic properties. In addition, experimental results have shown that the magnetic anisotropy energy changes when an electric field is applied to a Co/HfO_2 sample. In this study, we used DFT calculations to determine the interface geometry of Co/HfO_2 under different polarization directions, taking into account the effects of oxygen vacancies and diffusion. We then calculated the magnetic moment and electronic structure to explain the changes in magnetic anisotropy energy.

Poster No.24

Advancing Cesium Removal and Ammonia Recovery on Prussian Blue Analogs Using DFT Calculations

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Cesium, a radioactive material, and ammonia, which causes environmental issues such as eutrophication and soil acidification, require effective removal methods. Adsorption removal using adsorbents is advantageous due to its low energy consumption and resource recovery potential. Among various adsorbent materials, Prussian blue (PB) is known for its high selectivity towards monovalent cations. This study aims to evaluate the adsorption capabilities of cesium and ammonia using Prussian blue and its analogs (PBAs) through density functional theory (DFT) calculations. By calculating the adsorption energies, the adsorption strength of different adsorbents is compared, while desorption energies are calculated to assess durability. The density of states (DOS) is analyzed to identify the most effective adsorbents, and the total DOS (TDOS) and partial DOS (PDOS) are used to analyze the contribution of each atomic orbital.

Poster No.25

Electronic structures of marginally twisted trilayer graphene: a large scale tight-binding study

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The energetically favored stacking configuration for bilayer graphene is the Bernal type (AB stacking). In twisted bilayer graphene (TBG), each layer is distorted to maximize the Bernal-stacked area. For trilayer graphene, the Bernal stacking of three layers (ABA) is slightly more stable than the rhombohedral stacking (ABC). Their energy difference is negligible for moderately small twist angles while this difference can play a crucial role in marginally twisted trilayer graphene (mTTG), where the twist angle is smaller than ~0.1˚ [1]. A recent study [1] showed that the energy difference induces novel spontaneous symmetry breakings in mTTG, resulting in kagome and hexagram patterns for disparate stacking domains. In this work, we studied low-energy electronic structures of the mTTG using tight-binding theory calculations. To deal with at least three million orbitals in a single mTTG system, we developed an accurate tight-binding method for large twisted systems, employing a Lanczos algorithm-based eigenproblem solver. We find that several distinct electronic states appear at vertex sites of the grain boundaries between different stacking domains in mTTGs and provide a possible way of their controls.

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[1] D. Park, C. Park, KY, et al., *arXiv*:2402.15760.

Poster No.26

Atomistic simulation of dry etching using machine learning potential

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With the growing demand for high-performance semiconductor devices in the industries, etching has become an important process for size reduction. Dry etching is widely used to build the high-aspect ratio profile on the device for its anisotropy.

However, the underlying reactions are cumbersome, and atomistic interactions are not easily observable with experimental methods. Instead of experiments with large effort and budget, Molecular dynamics (MD) can be a way to observe these interactions on the atomic scale

Etching simulation requires a long, large-scale MD to extract various properties such as yield, byproduct, and surface morphology which demands huge computational costs. Machine learning potential (MLP) uses machine learning methods to learn interactions from accurate density functional theory calculations. MLP can accelerate large-scale MD simulations over DFT methods while maintaining sufficient accuracy to perform etching simulations.

In this work, we build a potential model for etching simulation with neural network, van der Walls, and ZBL universal potential that covers a wide range of interactions. We also propose the protocol to generate the training sets for Si_3N_4 and HF, CH_xF_y etching system. After validating and refining the trained potential with DFT calculations, etching MDs are then performed to obtain properties under process conditions in terms of incident ion type, energy, and angle.

We introduce the possibility of simulating etching MD using a ‘foundation model’, a graph-based machine learning potential trained with databases of DFT calculations. This foundation model is promising in that it requires less effort to generate a training set and is not dependent on a specific element system, so it can be used to explore diverse etching systems.

Poster No.27

Understanding Structural and Electronic Changes in the Surfaces of MA3Sb2I9 during Annealing and Cooling Processes

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Perovskites are highly promising materials for solar cells, especially lead-free perovskites, which offer the potential for non-toxic and environmentally friendly applications. Also, the stability of these materials is crucial, so research into 2D perovskites is essential, as their layered structures provide enhanced protection against environmental factors, contributing to improved durability. Our collaborative research team shared significant findings on MA3Sb2I9. Ultraviolet Photoelectron Spectroscopy (UPS) experiments revealed distinct changes in the electronic structure of MA3Sb2I9 during annealing and cooling. However, reannealing did not restore the original electronic structure. To understand these observations, we employed Density Functional Theory (DFT) calculations. To address this limitation, we conducted Molecular Dynamics (MD) simulations to capture dynamic properties at finite temperatures, considering the rotational behavior of MA at room temperature. Our analysis indicates that MA3Sb2I9 undergoes structural changes, caused by MA evaporation and Sb atom migration, affecting its electronic structure during annealing and cooling. These findings explain why the original electronic structure cannot be restored after reannealing due to these structural changes. This study enhances our understanding of the surface structure of perovskites at room temperature.

Poster No.28

Predicting Physical and Structural Properties of Liquid Electrolytes via Pretrained Machine Learning Potential

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Understanding the physical, structural, and transport properties of liquid electrolytes (LEs) is crucial to develop high-performance lithium-based batteries. To achieve higher lithium-ion conductivity and a stable inorganic solid-electrolyte interphase for enhanced cycle life, researchers are exploring new solvents and designing more complex electrolyte systems that incorporate high-concentrated electrolytes with diluents. These advancements often require engineering intermolecular interactions and ion solvation structures, where atomistic modeling becomes essential for development and optimization.

Analyzing the properties of LEs by molecular dynamics requires large cell sizes and long timescales, which restrict the use of *ab initio* approaches. Instead, machine learning potentials (MLPs) trained on data from density functional theory (DFT) calculations offer a promising alternative to accelerate simulations. Given the vast chemical diversity, compositional range, and varied local structures in LEs, defining a training domain is challenging. One promising way to overcome this is pretraining MLP on large databases, which can grant higher transferability to describe a wider range of chemistries outside the training data.

In this study, we utilize a pretrained MLP, SevenNet-0, to examine the physical and structural properties of LEs. SevenNet-0 is a graph neural network interatomic potential trained on a subset of the Materials Project database, which comprises over 180,000 crystal structures. Although molecular liquid configurations are not included in the training set, the model has shown proficiency in predicting key features of LEs. Our results show that the model predicts the order of liquid densities for seven commonly used carbonates consistently with experimental values. It is important since the diffusion constant of lithium ions can be largely affected by a small change in density. Additionally, it correctly captures the difference in solvation behavior of $LiPF_6$ salt between two representative solvents: ethylene carbonate (EC), which has higher permittivity, and dimethyl carbonate (DMC), which has lower. This demonstrates the generalizability of pretraining MLPs on a large dataset and highlights their possibility to model more complex LE systems for advanced battery technologies.

Poster No.29

Effect of solute elements on the performance of Mg_2Ni-based hydrogen storage alloys: A first-principles study

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Development of relevant hydrogen storage alloys, a kind of the solid-state hydrogen storage method, is a key issue in realizing the hydrogen economy. The Mg-based hydrogen storage alloys have attracted much attention due to their high hydrogen storage capacity, lightweightness, and economic feasibility. However, a difficulty of the dehydrogenation reaction due to their excessively high thermodynamic stability makes them difficult to use in practical applications. To resolve this issue, Mg alloys combined with elements which exhibits a low hydrogen affinity, such as alloys based on the Mg_2Ni intermetallic compound, have been studied, but the dehydrogenation process is still facing challenges. In this study, we conducted first-principles density functional theory calculations to examine the effect of ternary solute elements for improving the dehydrogenation performance of Mg_2Ni-based alloys. Especially, enthalpy and volume changes due to the hydrogenation reaction (i.e., from Mg_2Ni compound to Mg_2NiH_4 hydride) were analyzed considering various substitutional solute elements placed at different occupation sites of the Mg_2Ni compound. We also examined the physical origins of the effect of selected solute elements by analyzing the change in the bonding characteristics. We expect that the present results can provide a relevant guidance for deriving new alloying conditions to improve the performance of Mg_2Ni-based hydrogen storage alloys.

Keywords: Hydrogen storage alloys, Mg_2Ni alloy, Density Functional Theory, Metal hydrides

Poster No.30

Schottky Barrier Modulation via Oxygen Vacancy-Induced Gap States in $RuO_2(110)/TiO_2(110)$ for Interface-Type Resistive Switching

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The switching of interface-type resistive random access memory (RRAM) is governed by the modulation of the Schottky barrier height (SBH), which is induced by the oxygen vacancies (V_O) at the interface between electrode and oxide. Conventional explanations for this switching usually involve models based on the image force from uniform dopants or changes in band bending and depletion region widths due to the redistribution of V_O. However, these models are inadequate for interface-type RRAMs, which have thin interfaces where V_Os are spatially localized. In this study, the SBH was determined as a function of the interface V_O concentration by using the partial density of states, considering surface charge. Additionally, a model for SBH modulation was proposed. Rutile-structured RuO_2 and TiO_2 are selected as the electrode and oxide layer, and $RuO_2(110)/TiO_2(110)$ interface is used as a model system. As the interface V_O concentration increases, the SBH decreases monotonically. The V_Os act as donors, which result in the formation of defect-induced gap states near the conduction band minimum. Consequently, the Fermi level at the interface is pinned to the defect level. These findings emphasize the SBH modulation by the charge accumulation at the interface due to V_O, which is crucial for understanding the interface-type resistive switching mechanism.

Poster No.31

First-principles study on phonon transport properties of fluorographene for advanced thermal interface materials

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As electronic devices become increasingly integrated and miniaturized in the semiconductor industry, there is a growing demand for high-performance thermal interface materials. These materials need to exhibit both high thermal conductivity and low electrical conductivity. Additionally, strong anisotropy can enable more efficient heat control. Fluorographene, a derivative of graphene with fluorine atoms attached, possesses these desired characteristics and is being explored as a potential candidate for next-generation thermal interface materials. In our study, we investigated the heat transport properties of fluorographene compared to pristine graphene using density functional theory (DFT) and density functional perturbation theory (DFPT). We obtained the room-temperature in-plane lattice thermal conductivity of monolayer fluorographene: 112.2 W/mK and 145 W/mK using the single mode relaxation time approximation (RTA) and the full linearized Boltzmann transport equation (LBTE) solutions, respectively. Notably, the LBTE value for fluorographene is significantly lower than that of graphene, which can mainly be attributed to the heavy substituent fluorine atoms. We meticulously examined each phonon mode to understand their individual contributions to heat transport properties. Furthermore, we analyzed the thermal conductivity of multilayer fluorographene, observing variations with the number of layers. Overall, our research sheds light on the potential of two-dimensional thermal interface materials and provides valuable insights for the development of next-generation solutions in this field.

Poster No.32

Extended Hubbard corrected tight-binding model for rhombohedral few-layer graphene

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Rhombohedral multilayer graphene (RnG) featuring partially flat bands has emerged as an important platform to probe strong Coulomb correlation effects. Theoretical consideration of local electron-electron interactions are of particular importance for electronic eigenstates with a tendency to spatially localize. We present a method to incorporate mean-field electron-electron interaction corrections in the tight-binding hopping parameters of the band Hamiltonian within the extended Hubbard model that incorporates ab initio estimates of on-site (U) and inter-site (V) Hubbard interactions for the π bands of RnG. Our Coulomb-interaction renormalized band structures feature electron-hole asymmetry, band flatness, band gap, and anti-ferromagnetic ground states in excellent agreement with available experiments for $n \geq 4$. We reinterpret the putative gaps proposed in $n = 3$ systems in terms of shifting electron and hole density of states peaks depending on the range of the Coulomb interaction models.

[1] Lee, D., Yang, W., Son, Y.-W. & Jung, J. Extended Hubbard corrected tight-binding model for rhombohedral few-layer graphene. Preprint at https://doi.org/10.48550/arXiv.2403.00530 (2024).

Poster No.33

Thickness-evolution of the electronic structure and magnetic transition in multilayer Fe_3GeTe_2

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Van der Waals (vdW) two-dimensional (2D) magnets have gained widespread attention due to their potential in fundamental physics as well as in spintronic applications. Among them, the ferromagnetic (FM) layered compound Fe_3GeTe_2 (FGT) has attracted considerable interest due to its itinerant magnetism, correlated phenomena, and tunable high Curie temperature T_C. Previous studies have shown that FGT's T_C can be adjusted by the number of quintuple layers (QL) and carrier concentrations (n). However, it remains challenging to understand the underlying mechanism. Here, we demonstrate the thickness evolution of band structure and the role of itinerant carrier density in the ferromagnetism of FGT. Angle-resolved photoemission spectroscopy (ARPES) observes substantial changes in the band structure from 1 QL to 2 QL of FGT films grown by molecular beam epitaxy (MBE). Our density functional theory (DFT) calculations unveil that the observed band evolution is primarily driven by interlayer coupling. As a result, the bands gradually split into two parts with reduced inter-QL distance, where the upper and lower parts exhibit node and antinode wavefunctions at the interface, respectively. In addition, the n normalized to QL numbers shows a unified critical value at the T_C, suggesting the pivotal role of itinerant carriers in the ferromagnetism of FGT films. Our calculated Stoner parameters for the itinerant Fe II site indeed reveal an interesting coincidence with experimental T_C. Our study provides unique and valuable insights into the evolution of electronic structure and ferromagnetism in FGT thin films, shedding light on similar phenomena in other itinerant vdW FM materials.

Poster No.34

Effect of Electrolyte Additive Coating on Electrode Interface in Aqueous Zinc-Ion Batteries: A First-Principles Study

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Aqueous zinc-ion batteries (AZIBs) are attracting significant attention as a potential post-lithium-ion battery technology due to their advantages in safety and cost. However, numerous challenges must be addressed to improve the energy density and cycle stability for the commercialization of AZIBs. For instance, Mn-based cathodes, which are widely used in aqueous ZIBs, face the significant issue of Mn^{2+} dissolution into the electrolyte. To address this concern, various strategies are under investigation, such as the addition of extra Mn^{2+} into the electrolyte and crystal structure modification. In this work, we utilized MnO_2 as the cathode material and introduced an organic additive into the electrolyte. The organic additive formed a protective coating on the cathode surface, effectively inhibiting Mn^{2+} dissolution and resulting in enhanced battery performance. To understand the effect of the organic coating and the atomistic mechanisms governing the formation of the coating film on the cathode and its role in surface protection, we employed density functional theory (DFT) calculations. These calculations theoretically investigated the interfacial reactions on the cathode surface and identified the origin of the inhibition of Mn^{2+} dissolution.

Poster No.35

First-principles theory of purely ionic thermoelectricity

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While thermoelectricity (TE) is ubiquitous in electrically conducting materials, the fundamental understanding of ionic TE lags behind its electronic counterpart, hindering the development of efficient ionic TE materials. Here, we develop a microscopic theory of ionic TE based on the Green-Kubo formalism, leveraging three key symmetries of ionic transport (energy gauge invariance, Onsager reciprocal relation, and topological invariance of adiabatic charge transport). These symmetries uniquely determine the coupling between heat and charge transport, allowing for the extraction of thermoelectric coefficients directly from molecular dynamics (MD) simulations at equilibrium conditions. As a proof-of-concept demonstration, we calculate the thermoelectric coefficients of KCl (molten salt), Cu_2S (solid-liquid hybrid phase), and Li_3N (solid-state electrolyte) using MD simulations with machine-learned potentials.

Poster No.36

Multiple band inversions and their Floquet topological engineering in two-dimensional systems

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In a two-dimensional (2D) system with four time-reversal invariant momenta (TRIM) points, the $\mathbb{Z}_2$ invariants of a system with one band inversion and a system with three band inversions are topologically indistinguishable, according to diagnostic techniques like the Fu-Kane formula. However, multiple band inversions unlock rich possibilities for topological band engineering in Floquet systems. We found that band inversion is present at three equivalent M points in the 2D van der Waals material In_2Te_3 monolayer, and by manipulating the characteristics of the incident light, we can transition between different topological states. First, we showed that adjusting the light's phase can alter the effective time-reversal symmetry (TRS) in the Floquet system, allowing transitions between quantum spin Hall insulators and Chern insulators. Additionally, by manipulating the light's geometric propagation, we could control the number of band inversions at M points, thus managing various topological numbers and their corresponding edge states. Finally, using the light's handedness, we demonstrated that we could change the sign of the Chern number and control the chirality of edge states. Our findings open a new platform for rich topological phases through Floquet engineering in 2D systems with multiple band inversions. These often-overlooked aspects in topological diagnostics hold great promise for future topological quantum devices.

Poster No.37

Superconductivity in magic-angle twisted bilayer graphene: Thermal decoupling in domain wall

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In magic-angle twisted bilayer graphene (MATBG), not only AA or AB stacking, but also domain wall (DW) stacking, also called saddle point stacking, exists. Recently, it has been reported that DW stacking is the origin of the pseudo landau level and C_3 symmetry breaking, as well as theoretical calculations showing that the hole band in the flat band of MATBG emerges from DW stacking. In particular, in the flat band, the transport of carriers such as electrons and holes are slowed down, leading to a breakdown of the Wiedemann-Franz law, where the thermal phenomenon is dominated by phonons. This decoupling of electron and phonon provides a similar environment to High-T_c Cuprate superconductors. We discovered thermal decoupling in YBCO, which solved several important superconducting mysteries at once. Using *ab initio* molecular dynamics simulation and temperature-dependent effective potential method, we show that this thermal decoupling is driven by DW stacking in MATBGs. Surprisingly, the linear-T resistivity observed in experiments are fully explained by the thermal decoupling. We also confirmed that the superconductivity is closely related to quantum geometry in MATBG that have recently been reported experimentally. In particular, we show that the thermal decoupling can explain the superconductivity at extremely low Fermi temperatures due to flat bands as well as the Uemura relation between Fermi temperature and T_c, which has been found in the existing unconventional high-T_c superconductors.

Poster No.38

Monte-Carlo simulation exploring the connectedness of thru-holes in multi-layer stacking

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A recent study by Jang et al. (Adv. Mater. Interfaces, 2023, 10(4), 2201406) highlighted the potential of thru-hole epitaxy to align the growth of detachable domains with the crystallographic orientation of the substrate, using a 2D mask material transferred onto the substrate. Notably, this technique has practical implications, demonstrating the capability to reuse thick h-BN stacks to grow pristine, detachable GaN domains. However, the persistence of thru-holes in h-BN stacks through multiple stacking still needs to be better understood. We employed Monte Carlo simulations to evaluate the likelihood of thru-hole connectedness across each layer of the 2D mask. Our analysis indicates that the survival of a hole within the stack largely depends on the hole's shape. Notably, holes displaying a significant anisotropic form maintain their thru-hole status by extending upwards and downwards. This finding demonstrates the practical survival of thru-hole epitaxy across multiple stackings and provides valuable insights into growth conditions for its effective implementation.

Poster No.39

Revisiting LaMnO3: A density functional theory

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We systematically investigate $LaMnO_3$ employing various functionals and DFT+U schemes. Our study reveals that the response of the electronic structures on Coulomb interaction parameters are similar across different functionals. However, the magnetic properties vary significantly with changes in Hund's coupling J_H. We compare the different DFT+U schemes, with a particular focus on the magnetic interactions in the system.

Poster No.40

First-principles Study of Surface-Originated Quantum Confinement in III-V Colloidal Quantum Dots

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The colloidal quantum dots (QDs), semiconductor nanocrystals synthesized through wet chemistry methods, exhibit unique optoelectronic properties due to quantum confinement (QC) dependent on QD size. Conventionally, the QC phenomenon was described using the particle-in-a-box (PIB) model. This model suggests that tetrahedral QDs exhibit stronger QC than spherical ones of the same size due to their higher surface-to-volume ratio. [1,2]. While the PIB model successfully explains the sizing curve trend of the InP QDs, it fails to account for the unconventional sizing curve trend of the InAs QDs. To address this discrepancy, we propose a novel theory that the QC arises from interactions between the QD surfaces and passivating ligands, which operate alongside the PIB model.

We conducted first-principles calculations to analyze the surface effects on the electronic structure of QDs. With ligand passivation, the (100) surface undergoes reconstruction, whereas the (111) surfaces do not. As a result, (111) surface displays strong hybridization between in-gap surface states and the bulk conduction band. Therefore, the band gap of the (111) surfaces is strongly influenced by the in-gap surface state, resulting in a substantial reduction compared to the (100) surfaces. Additionally, the surface-dependent band gap reduction is more pronounced in materials with narrower band gaps, such as InAs or InSb. Our findings suggest the surface-originated QC, which will provide an innovative approach to understanding and controlling nanoscale physical properties.

References

[1] Kim, K., Yoo, D., Choi, H., Tamang, S., Ko, J., Kim, S., Kim, Y., and Jeong, S., Angewandte Chemie International Edition, 55, 3714–3718 (2016).
[2] Kim, M., Lee, J., Jung, J., Shin, D., Kim, J., Cho, E., Xing, Y., Jeong, H., Park, S., Oh, S.H. and Kim, Y.H., Journal of the American Chemical Society, 146, 10251 (2024).

Poster No.41

Ab Initio Study on TCNQ-Activated Ag Nanoparticles for 1-Hexene/n-Hexane Separation Enhancement

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Linear alpha olefins (LAOs) such as 1-hexene and 1-octene are experiencing a continuous increase in demand as value-added petrochemical feedstocks. Due to the high energy consumption associated with separating LAOs from their mixtures using distillation and extraction methods, there is a pressing need for more efficient separation approaches, such as membrane technology. Here, we develop facilitated transport membranes containing Ag nanoparticles for the separation of 1-hexene from n-hexane. These membranes exhibit high selectivity at ambient temperature and high downstream pressure due to specific interactions with TCNQ-activated Ag nanoparticles. We use density functional theory (DFT) to investigate the activation of Ag surfaces by TCNQ. We examine changes in the surface charge density of Ag depend on TCNQ coverage and calculate atomic charge differences through Bader charge analysis. Furthermore, we compute the adsorption energies of n-hexane, 1-hexene, 2-hexene, and 3-hexene on the Ag surface with various TCNQ coverages, and confirm the impact of carbon bonding on adsorption. These results demonstrate that the facilitated transport membrane has enhanced separation performance.

Poster No.42

Ultrafast thermal and nonthermal disordering of semiconductor investigated through nonadiabatic quantum molecular dynamics study

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We investigate the phase transition of ultrashort and intense laser-induced semiconductor. To elucidate the origin of the ultrafast lattice disordering occurring in semiconductor, we quantify the thermal and nonthermal contributions to disorder in ultrashort laser-irradiated germanium through nonadiabatic quantum molecular dynamics. The nonadiabatic quantum molecular dynamics employed in this study describes the electronic excitation within the linear-response time-dependent density functional theory framework. The nonadiabatic electron–ion dynamics are described through fewest switches surface hopping method. This provides us a unique capability to separate the time-evolving lattice disorder into fundamental components, thereby identifying the main driver of the disordering at each time stage. Our results show that, although the bond softening effect dominates in the beginning irrespective of the excitation density, the eventual ultrashort laser-driven phase transition involves both the thermal and nonthermal elements in it with the level of their effects regulated by the electronic excitation density.

Poster No.43

Enhancing Spin Hall Conductivity in Bi_2Se_3 through Bi Layer Incorporation: A First-Principles Study

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Several new materials have been identified with high Spin Hall Angle (SHA) defined as the ratio of spin Hall conductivity to electrical charge conductivity, indicating the effectiveness of charge-to-spin and spin-to-charge conversion, though their theoretical explanations remain insufficient. For instance, Bi_2Se_3 has been experimentally found to have a large SHA of 2-3.5, while theoretical predictions estimate it to be around 0.26, nearly ten times lower. Our research has shown that this discrepancy can be alleviated by introducing a few layers of Bi between two Bi_2Se_3 quintuple layers. First-principles calculations revealed that the presence of these Bi layers can enhance spin-Hall conductivity nearly tenfold. Additionally, structures incorporating Bi layers exhibit large SHA values, supported by more precise electrical conductivity measurements that account for electron-phonon coupling and sample thickness. We propose that integrating Bi layers could improve spin transport properties, leading to more efficient nanoscale spin-based devices.

Poster No.44

Evolution of charge-ordered phase in $SrTiO_3$ surface

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Charge ordering (CO), characterized by a periodic modulation of electron density and lattice distortion, has been a fundamental topic in condensed matter physics, serving as a potential platform for inducing novel functional properties. The charge-ordered phase is known to occur in a doped system with high *d*-electron occupancy, rather than low occupancy. Using first-principles calculations, here we design the charge-ordered phase in (001) surface of the electron-doped (001) $SrTiO_3$ that have the lowest *d*-electron occupancy i.e., d^1-d^0. We predict the presence of a metastable CO state in the bulk state of electron-doped $SrTiO_3$ and we reveal that the atomic distortion of the $SrTiO_3$ (001) surface favors electron-lattice coupling, thus triggering the stabilization of the CO phase from a correlated metal[1]. This stabilization extends up to six unit cells from the top surface to the interior. Our approach offers an insight into the means of stabilizing a new phase of matter, extending CO phase to the lowest electron occupancy and encompassing a wide range of 3*d* transition metal oxides.

[1] Eom, K., Chung, B. et. al (2024). Surface triggered stabilization of metastable charge-ordered phase in $SrTiO_3$. *Nat. Commun.* **15**, 1180 (2024).

Poster No.45

First-principles investigation on Mitigating Interfacial Degradation in Semi-Transparent Perovskite Solar Cells

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Recently, perovskite materials have gained prominence in semi-transparent and flexible solar cell applications due to their thin-film characteristics. In semi-transparent perovskite solar cells with n-i-p structure buffer layers on the hole transporting layer (HTL) are sometimes essential to prevent damage from sputtering of transparent conductive oxides. Organic materials like LiTFSI-doped Spiro-MeOTAD are commonly used as HTLs for their effective carrier extraction. However, the mobile nature of Li ions in the HTLs allows interactions with adjacent layers , necessitating research on the HTL-buffer layer interface to address stability issues in semi-transparent perovskite solar cells. This study investigates Li-ion migration into MoO_x buffer layer from LiTFSI-doped Spiro-MeOTAD HTL, and explores lithium oxide passivation through a collaboration of experiments and first-principles calculations. The impact of Li-ion migration on MoO_x is assessed through determination of transition levels and Li diffusion barriers in MoO_3. The results successfully explain that the gradual diffusion of Li-ion into MoO_3 reduces the work function of the buffer layer, thereby accelerating the degradation of the solar cell efficiency. Considering our experimental observations that the degradation can be suppressed by partial oxidation of HTL surface, we also compared the defect formation energies of possible lithium oxides to investigate the possibility of Li-ion passivation. We suggest that a forming lithium oxide layers on the HTL can effectively suppress Li migration to the buffer layer, thereby enhancing stability of the solar cell.

Poster No.46

First-principles study on intrinsic defects inducing *n*-type property during InAs crystal growth

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InAs, a III-V semiconductor, exhibits a small direct band gap of 0.43 eV and high electron mobility, making it advantageous for applications such as infrared photodetectors and field-effect transistors [1]. Recent findings indicate that the InAs crystal displays intrinsic *n*-type properties not only under In-rich conditions but even in As-rich environments [2]. This phenomenon is attributed to native defects in InAs. And the density functional theory (DFT) is an effective tool for analyzing the defect physics. However, in DFT, due to severe band gap underestimation in InAs, it is challenging to analyze defect energy states and charges within the bandgap [3].

In this study, we opted for hybrid exchange-correlation functionals and finite-size correction at charged-defect supercell calculations, eventually, we obtained the accurate band gap and defect formation energy [4]. We employed these two schemes, increasing the supercell size from 64, 216 to 512 atoms to clarify defect states within the narrow 0.43 eV band gap. Consequently, we revealed that In-interstitial and As-antisite defects were the dominant intrinsic defects under In-rich and As-rich growing conditions, respectively, acting as donors within the entire band gap.

Our results explain the experimental result that the synthesized InAs crystals inherently show *n*-type properties under both In- and As-rich growing conditions [2]. Our findings will offer quantitative guidelines to calculate defect energy states and formation energies of defects within narrow-band-gap materials including InAs. Also, it will be the pivotal framework to advance the understanding of carrier dynamics and defect physics in crystals.

References

[1] Kuech Thomas F., Progress in crystal growth and characterization of materials, **62**, 352-370 (2016).
[2] Shen G. *et al.*, Materials Research Express, **4**, 036203 (2017).
[3] Höglund A. *et al.*, Physical Review B, **74**, 075332 (2006).
[4] Freysoldt C. *et al*, Physical Review Letters, **102**, 016402 (2009).

Poster No.47

Physical model of $Ag/HfO_2/RuO_2$ diffusive memristor for p-computing application

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The electrochemical metallization-based memristors showed stochastic delay time, the interval for the memristor to reach a SET state after applying a voltage pulse. The SET probability and voltage exhibit a sigmoid-like relationship, making the memristor a promising candidate for a next-generation probabilistic bit (p-bit) device. However, the factors affecting this stochastic behavior remain unclear, impeding the device optimization. This work proposes a physical model of an $Ag/HfO_2/RuO_2$ diffusive memristor-based p-bit device by combining statistical thermodynamics and the finite element method. The material parameters for Ag^+ ions in amorphous HfO_2 were calculated using *ab initio* calculations. It was found that transport parameters, such as the diffusion barrier, differ significantly between amorphous and crystalline phases and that only the amorphous parameters adequately describe the device's diffusive behavior. This model feasibly reproduces the behavior of the fabricated device. Finally, factors affecting stochasticity are explored, and guidelines for controlling the device performance are provided.

Poster No.48

Search for magnetic ground states using DFT calculation: Cr_2Se_3 case

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Our study systematically searches the magnetic ground state of Cr_2Se_3, a non-van der Waals but layered material and a potential half-metal candidate. In our collinear calculations, we discovered that Wycoff symmetry is effective, leading to numerous degenerate spin configurations that significantly reduce the computational load. Noncollinear calculations further provide valuable easy axis information. By combining both approaches, we comprehensively understand the material's magnetic properties. We firmly believe that this approach has significant and immediate practical implications for the design of new materials with specific magnetic properties, thereby advancing the field of materials science and condensed matter physics.

Poster No.49

First-principles study of dielectric properties of ferroelectric perovskite oxides with on-site and inter-site Hubbard interactions

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We study the electronic and dielectric properties of ferroelectric perovskite oxides $BaTiO_3$, $LiNbO_3$, and $PbTiO_3$ using fully ab initio extended Hubbard functional in which the on-site (U) and intersite (V) Hubbard interactions are determined self-consistently by adopting the Agapito–Curtarolo–Buongiorno Nardelli (ACBN0) pseudo hybrid functional. We compare the atomic structures, band gaps, polarizations, and Born effective charges calculated with extended Hubbard functional, standard LDA, GGA, and Hybrid (HSE06) functionals. We find that the properties of all three ferroelectric perovskite oxides calculated by extended Hubbard functionals are in good agreement with experimental data. Moreover, we find a substantial increase in band gap values from the intersite interaction, having values similar to those from HSE06 calculations, and that the inclusion of the intersite interaction is crucial for stabilizing the ferroelectric ground state of BaTiO3. Our work presents a way to efficiently calculate the ferroelectric properties of oxides in which the inclusion of both on-site and intersite Hubbard interaction is important in predicting structural, dielectric, and electronic properties.

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Poster No.50

New Two-dimensional Carbon Networks Derived from Biphenylene

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Beginning with prototype structures formed by introducing acetylenic linkages between hexagonal carbon rings within a biphenylene network (BPN), we have discovered ten unique two-dimensional (2D) carbon allotropes with rectangular symmetry, all of which exhibit both dynamic and mechanical stability. Furthermore, they offer a high likelihood of successful synthesis, as evidenced by larger cohesive energies than the experimentally synthesized ɣ-graphdiyne. Notably, two allotropes, BPN-02 and BPN-04, display metallic band structures characterized by highly tilted Dirac cones positioned above the Fermi level, which consist of both flat and linearly dispersive band branches. Under 5 % biaxial strains, their Dirac cones descend to the Fermi level, forming critically-tilted type-III Dirac points with their flat band branches placed at the Fermi level. Conversely, BPN-22 demonstrates semiconductor behavior with a band gap of 0.45 eV, accompanied by a van Hove singularity in its density of states at the valence band maximum. It is found to exhibit highly anisotropic carrier mobility, which, along with a pronounced discrepancy between electron and hole mobilities, holds promise for the advancement of novel electronic and optoelectronic devices. Our investigation sheds light on the expansion of the stable 2D carbon allotrope family, unveiling exotic electronic and optical properties diverging from the hexagonal symmetry of graphene.

Poster No.51

Accelerating Polar Phase Discovery in Ferroelectric Oxides Using Machine Learning

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Machine learning is revolutionizing first-principles calculations in materials discovery and property prediction. However, developing accurate models requires large datasets of relaxed structures, which are computationally expensive. Crystal structure prediction algorithms show promise but often fail to predict the ground state accurately. We propose an alternative and efficient method of finding ground states by utilizing the total energy of random unrelaxed structures utilizing a crystal graph convolutional neural network [1]. Trained on a small dataset of unrelaxed energies from first-principles calculations, our model predicts the total energy of random structures with near-first-principles accuracy. This approach constructs the energy landscape of perovskite oxide in a cost-effective way, enabling a polar phase stability map of strained $BaTiO_3$, a representative ferroelectric oxide. Our method bypasses the computationally intensive structure optimization process, accelerating the search for the ground state and efficiently mapping the phase stability of strained perovskite materials.

[1] Rahman, M. M., Janwari, S., Choi, M., Waghmare, U. V., Lee, J., (2023). Accelerating search for the polar phase stability of ferroelectric oxide by machine learning. *Mater. Des.* ***236***, 112518.

Poster No.52

Electronic band gap of kesterite materials predicted by machine learning

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Recently, a lot of research has been reported on machine learning using the band gap obtained through first-principles density functional theory (DFT) calculations. To develop a machine learning model, a sufficiently large number of learning data is required. In many previous studies, DFT calculations were performed by employing Generalized Gradient Approximation (GGA) exchange-correlation potential due to its relatively small computation cost. However, the electronic band gap is severely underestimated in GGA calculations, and therefore the machine learning model learned from GGA data is also inaccurate. To overcome this problem, in some previous studies, the electronic band gap was obtained by performing hybrid density functional theory calculations with the structures optimized by using GGA. In some cases, however, the band gap errors are significant due to the inaccurate structure.

In this study, we developed a cost-effective approach to optimize the atomic structure using hybrid DFT, and obtained the band gap of kesterite materials accrurately. Machine learning models were obtained for predicting the band gap values. Among several models, the brute force searching (BFS) model exhibited the smallest error with the root mean square error (RMSE) of 0.137 eV and the R-squared value of 0.921. Machine learning model also show that the distance between group-IV and group-VI atoms in kesterite material affect the band gap most.

[1] D. Lee, S. Kim, and J.-S. Park, Curr. Appl. Phys. 59, 214 (2024).

Poster No.53

Atomic structure and electronic structure of SiC polymorphs

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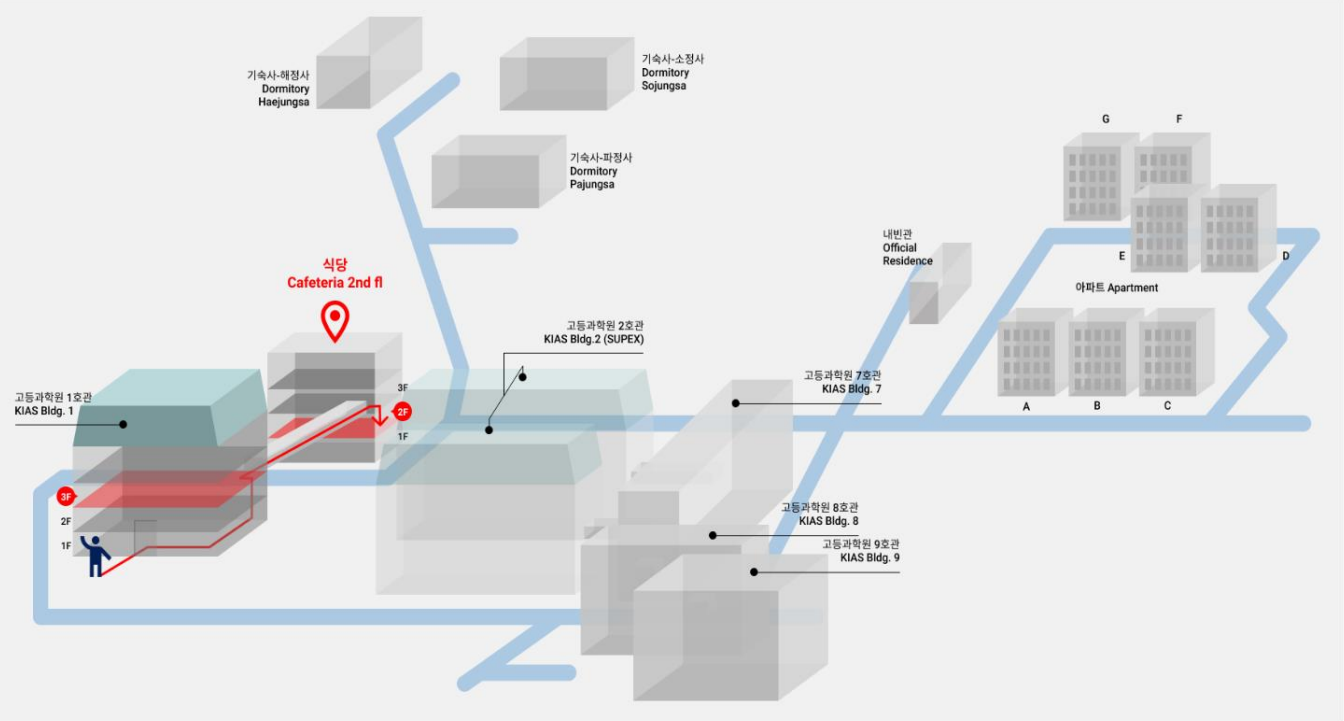
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SiC has been regarded as an important semiconductor material for power electronics applications. Among various polymorphs (or polytypes) of SiC, the 4H structure is widely used in power electronics. In this study, we performed the first-principles density functional theory (DFT) calculations to investigate the atomic structures and the electronic structure of SiC. We examined various exchange-correlation functionals and found that PBEsol predicts the lattice constants of 4H SiC in good agreement with experiments. The electronic structure of 2H, 3C, and 6H SiC were obtained by performing HSE06 calculations using the atomic structure optimized by using the PBEsol. 2H SiC and 4H SiC are calculated to have similar band gap values, and 3C SiC has a smaller band gap than the other structures. All polymorphs of SiC have indirect band gaps.

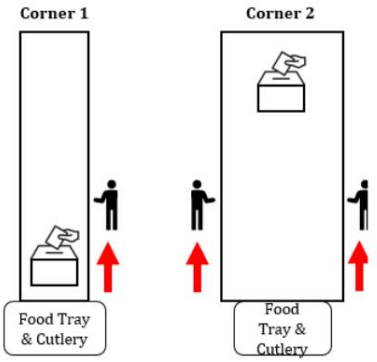
Bldg.1 to Cafeteria

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

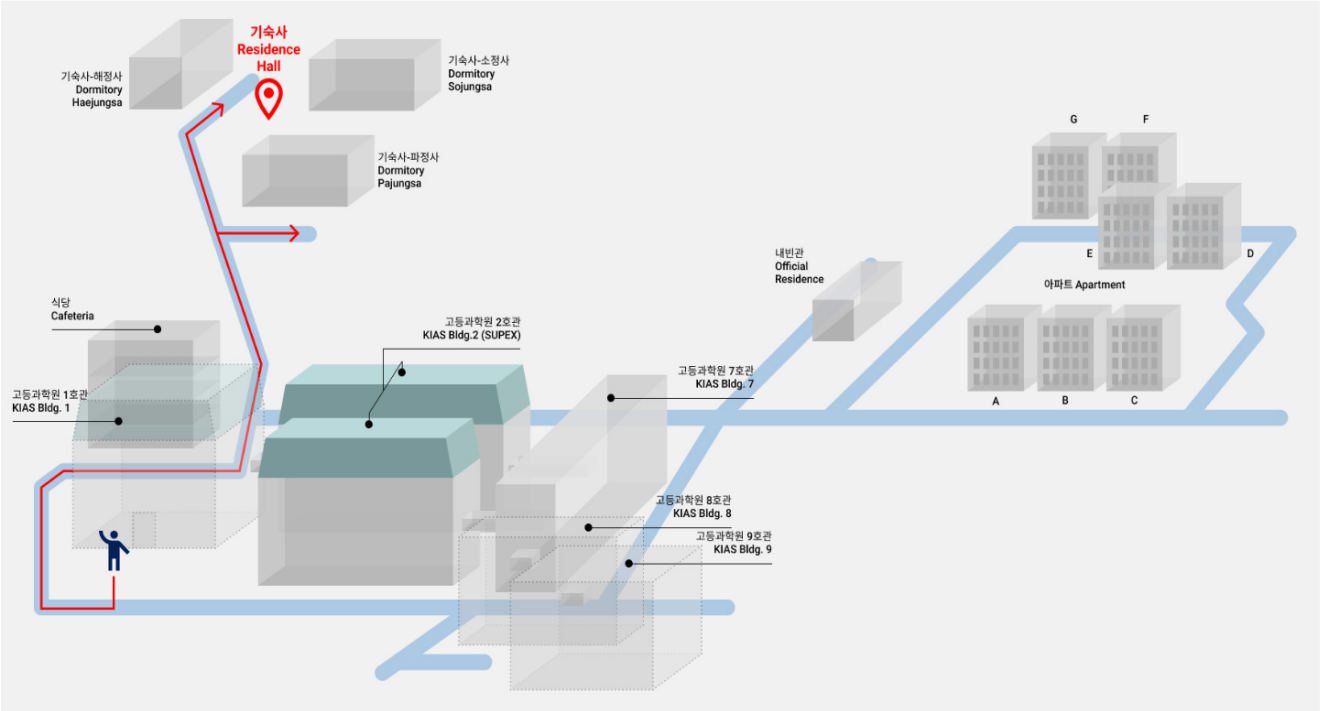


Lunch Coupon Usage

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



Bldg.1 to Residence Hall



Transportation

Bus – 201, 273

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

Metro – line no.1

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

From Hoegi Station

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

From Cheongnyangni Station

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