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최상국 (고등과학원)
한승우 (서울대학교 재료공학부)

자문위원회

권영균 (경희대학교), 김용현 (한국과학기술원),
김용훈 (한국과학기술원), 박철홍 (부산대학교),
심지훈 (포항공과대학교), 유재준 (서울대학교),
이승미 (한국표준과학연구원), 조준형 (한양대학교),
정유성 (한국과학기술원), 최형준 (연세대학교),
한명준 (한국과학기술원), 한상수 (한국과학기술연구원),
한승우 (서울대학교)

조직위원

김세중 (과학기술연합대학원대학교),
손영우 (고등과학원), 최상국 (고등과학원)

담 당 자 : 김혜미 (고등과학원)
전 화 : 02-958-2638
이 메 일 : hmkim@kias.re.kr
홈페이지 : http://events.kias.re.kr/h/ESCW2023

제19회 고등과학원

전자구조 계산학회

일시 : 2023년 7월 13일 (목) – 7월 14일 (금)
장소 : 고등과학원 1호관 대강당

KIAS 고등과학원 KOREA INSTITUTE FOR ADVANCED STUDY

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박지상 (성균관대학교 나노공학과)

박창원 (고등과학원)

박희철 (부경대학교 물리학과)

서동화 (한국과학기술원 신소재공학과)

신동빈 (광주과학기술원 물리광과학과)

이재광 (부산대학교 물리학과)

임진오 (한국화학연구원)

최상국 (고등과학원)

한승우 (서울대학교 재료공학부)

자문위원회

권영균 (경희대학교), 김용현 (한국과학기술원), 김용훈 (한국과학기술원), 박철홍 (부산대학교), 심지훈 (포항공과대학교), 유재준 (서울대학교), 이승미 (한국표준과학연구원), 조준형 (한양대학교), 정유성 (한국과학기술원), 최형준 (연세대학교), 한명준 (한국과학기술원), 한상수 (한국과학기술연구원), 한승우 (서울대학교)

조직위원

김세중 (과학기술연합대학원대학교), 손영우 (고등과학원), 최상국 (고등과학원)

연락처

김혜미 (고등과학원) 이메일: hmkim@kias.re.kr

제19회 고등과학원 전자구조계산학회 프로그램

7월 13일(목)		7월 14일(금)	
8:30 – 9:20 등록		8:30 – 9:20 등록	
9:20 – 9:30 개회 인사			
Session 1 **Artificial Intelligence 1** **좌장 이인호** **(한국표준과학연구원)**	**09:30~10:10** 한승우 (서울대학교 재료공학부) Machine learning potential: explained	**Session 5** **Applications of DFT 1** **좌장 이병주** **(한국과학기술연구원)**	**09:30~10:10** 서동화 (한국과학기술원 신소재공학과) First-principles calculations on the stability of oxidized oxygen in Li-excess cathode materials
	10:10~10:50 명창우 (성균관대학교 에너지과학과) Development of ab initio Machine Learning General Potential		**10:10~10:50** 박지상 (성균관대학교 나노공학과) Cost-effective screening of materials using hybrid density functional theory calculations
10:50 – 11:20 Coffee Break		10:50 – 11:20 Coffee Break	
Session 2 **Artificial Intelligence 2** **좌장 이예리** **(한국화학연구원)**	**11:20~12:00** 김우연 (한국과학기술원 화학과) Generative AI for accelerated materials discovery	**Session 6** **Applications of DFT 2** **좌장 최형준** **(연세대학교)**	**11:20~12:00** 김한슬 (충북대학교 신소재공학과) First-principle simulations toward practical semiconductor device applications of low-dimensional materials
	12:00~12:40 **임진오 (한국화학연구원)** Electronic structure-based descriptors for machine learning study of thermoelectric properties		**12:00~12:40** 신동빈 (광주과학기술원 물리광과학과) Exploring light-induced phenomena in condensed matter systems with ab initio approach
12:40 – 14:00 Lunch Break & Poster Session		12:40 – 14:00 Lunch Break & Poster Session	
Session 3 **Topological Physics** **좌장 박문집** **(한양대학교)**	**14:00~14:40** 김세권 (한국과학기술원 물리학과) Intrinsic Magnon Orbital Hall Effect in Honeycomb Antiferromagnets	**Session 7** **Many-Body Physics** **좌장 최철호** **(경북대학교)**	**14:00~14:40** 김아람 (대구경북과학기술원 화학물리학과) Misleading convergence of the bold-line diagrammatic technique: when the correct solution can be found
	14:40~15:20 박희철 (부경대학교 물리학과) Quantum chaos encounters Bloch theorem		**14:40~15:20** 김흥식 (강원대학교 물리학과) Emergence of flat bands via orbital-selective electron correlations in Mn-based kagome metal
15:20 – 16:00 Coffee Break			**15:20~16:00** **최상국 (고등과학원)** Ab initio DMFT methodologies for correlated quantum materials
Session 4 **Electron-Phonon Interactions** **좌장 김용현** **(한국과학기술원)**	**16:00~16:40** 이재광 (부산대학교 물리학과) Phonon Decoupling in Oxides	**Session 8** **시상 및 폐회** **좌장 손영우** **(고등과학원)**	**16:00~16:10** **포스터 시상식 및 폐회**
	16:40~17:20 민승규 (울산과학기술원 화학과) Correlated Electron-Nuclear Dynamics Toward Extended Systems		
	17:20~18:00 박창원 (고등과학원) Condensation of preformed charge density waves in kagome metals		
Poster Session **좌장 김세중** **(UST)**	**18:00~** **포스터 발표**		

Talk Abstracts

Talk No.1

Machine-learned potential: explained

Seungwu Han

Department of Materials Science and Engineering, Seoul National University, Seoul 08826, Korea

The machine-learned potential (MLP) infers total energies using machine learning models trained over reference DFT datasets. The accuracy and usefulness of MLP are evidenced by impressive examples of large-scale and long-term simulations. Unlike first-principles methods developed on the orthodox theory, the black-box nature of machine learning makes it difficult to understand how the MLP works. In addition, a variety of machine learning techniques can be applied to construct MLPs. As such, numerous packages are available in the public domain, sometimes confusing users. In this presentation, I will try to 'explain' the basic ideas underlying popular types of MLPs. In particular, the descriptors and regression methods will be compared among the descriptor-based MLPs. In addition, the equivariance-type graph-based models will be also discussed.

Talk No.2

Development of ab initio Machine Learning General Potential

Chang Woo Myung

Department of Energy Science, Sungkyunkwan University, Suwon, 16419, Korea

In recent years, machine learning has transformed numerous scientific disciplines by tackling key challenges. Machine learning potentials offer a promising avenue for surmounting the stringent limitations on size and speed, which are inherent to *ab initio* simulations [1]. We develop the sparse Gaussian process regression (SGPR) machine learning potential, which scales linearly and is transferable to any systems [2,3,4,5]. By taking advantage of the kernel structure, the SGPR machine learning potential can be expanded into a general potential for all known compounds. The SGPR machine learning potential has been developed for a variety of materials, including Li solid electrolytes [2], hydrocarbons [3], Li-battery cathodes [4], and aqueous solutions [5]. Presently, machine learning potentials only predict ab initio energy based on geometric information, which lacks crucial electronic details such as charge states, excited states, and spin interactions. To address this limitation, we incorporate the missing electronic structure information, including electron transfer [5] and spin-spin interactions [6], enhancing its predictive capabilities of the SGPR potential. The ultimate goal is to build and apply this general-purpose ab initio machine learning potential to investigate various complex reactions such as catalysis, electron transfer, protein folding, and adsorption phenomena on surfaces.

References

[1] C. W. Myung, B. Hirshberg, M. Parrinello, *Phys. Rev. Lett.* 128, 045301 (2022).
[2] A. Hajibabaei, C. W. Myung, K. S. Kim *Phys. Rev. B* 103, 214102 (2021).; C. W. Myung *et al. Adv. Energy Mater.* 12, 2202279 (2022).
[3] M. Ha *et al.*, *ACS Phys. Chem Au*, 2, 260–264 (2022).
[4] M. Ha *et al. Adv. Energy Mater.* 12, 2201497 (2022).
[5] C. W. Myung *et al*, Active multi-task sparse Gaussian process regression machine learning potential: Redox chemistry of aqueous solutions, to be submitted, (2023)
[6] T. H. Park, C. J. Kang, C. W. Myung, Spin-dependent sparse Gaussian regression potential using renormalized spin-exchange function, in preparation, (2023)

Talk No.3

Generative AI for accelerated materials discovery

Woo Youn Kim

Department of Chemistry and AI Institute, KAIST, Daejeon, Republic of Korea

HITS Incorporation

Deep learning is attracting great attention for various applications including materials discovery. In particular, generative AI is used to design materials with target properties directly unlike virtual screening that prioritizes pre-constructed candidates according to selection criteria. Here, we first overview representative AI models developed for organic molecule-based molecular design. Then, we propose a building block-based molecular generative AI which designs new molecules with target properties by sequentially adding molecular building blocks to any given starting molecule. A key feature of our model is a high generalization ability in terms of property control and building block types. The former becomes possible by learning the contribution of individual building blocks to the target properties in an auto-regressive manner. For the latter, we used a deep neural network that predicts the bonding probability of two molecules from the embedding vectors of the two molecules as input. The high synthetic accessibility of the generated molecules is implicitly considered while preparing the building block library with the BRICS decomposition method. We show that this model can generate molecules with the simultaneous control of multiple target properties at a high success rate. As a practical application, we demonstrate that the model can be applied to materials design with an example study on drug and OLED design.

Talk No.4

Electronic structure-based descriptors for machine learning study of thermoelectric properties

Jino Im

Korea Research Institute of Chemical Technology

Thermoelectric performance is typically determined by $ZT=\sigma S^2T/\kappa$, consisting of the electrical conductivity (σ), Seebeck coefficient (S), and thermal conductivity (κ) at a given temperature T. Although achieving a high ZT value has been the ultimate goal, it is challenging due to the interdependence of these factors. Doping and alloying are fundamental strategies to improve the thermoelectric performance of raw materials. However, identifying outstanding elements and compositions for high ZT thermoelectric materials is difficult due to the vast chemical space of doping and alloying. To overcome the problem, the machine learning (ML) approach has been widely utilized.

In this presentation, we will show an ML-guided approach to identifying optimal doping and alloying compositions for improved thermoelectric performance in SnSe compounds. We built highly accurate ML predictive models for thermoelectric properties using experimental and computational data. We then used these models to explore a vast chemical space of 59 different doping and alloying elements. This allowed us to identify several elements that result in high ZT SnSe compounds. To enhance the accuracy and generalization of our models, we used electronic structures as descriptors for the SnSe-based materials. By doing so, we were able to improve the predictive power of the models for unknown doping/alloying elements, which is critical for the practical applications of models. Additionally, we will discuss several strategies for enhancing the predictive power of the ML models by incorporating various electronic structure-based descriptors.

Talk No.5

Intrinsic Magnon Orbital Hall Effect in Honeycomb Antiferromagnets

Se Kwon Kim

Department of Physics, Korea Advanced Institute of Science and Technology, Daejeon 34141, Korea

We theoretically investigate the transport of magnon orbitals in a honeycomb antiferromagnet [1]. We find that the magnon orbital Berry curvature is finite even without spin-orbit coupling and thus the resultant magnon orbital Hall effect is an intrinsic property of the honeycomb antiferromagnet rooted only in the exchange interaction and the lattice structure. Due to the intrinsic nature of the magnon orbital Hall effect, the magnon orbital Nernst conductivity is estimated to be orders of magnitude larger than the predicted values of the magnon spin Nernst conductivity that requires finite spin-orbit coupling. For the experimental detection of the predicted magnon orbital Hall effect, we invoke the magnetoelectric effect that couples the magnon orbital and the electric polarization, which allows us to detect the magnon orbital accumulation through the local voltage measurement. Our results pave a way for a deeper understanding of the topological transport of the magnon orbitals and also its utilization for low-power magnon-based orbitronics, namely magnon orbitronics.

[1] G. Go, D. An, H.-W. Lee, and S. K. Kim, "Intrinsic Magnon Orbital Hall Effect in Honeycomb Antiferromagnets," arXiv:2303.11687

Talk No.6

Quantum chaos encounters Bloch theorem

Hee Chul Park

Department of Physics, Pukyong National University, Busan, Korea, Republic of

We have studied the mesoscopic features of wavefunctions on microcavities induced by Bloch momentum. Let us explore three interesting systems: moiré superlattice and scar lattice. First, the moiré superlattice of misaligned atomic bilayers paves the way for designing a new class of materials with wide tunability. In this work, we propose a photonic analog of the moiré superlattice based on dielectric resonator quasi-atoms. We find that these flat bands are characterized by non-trivial band topology, originating from the moiré pattern of the resonator arrangement. The physical manifestation of the flat band topology is a robust one-dimensional conducting channel on the edge, protected by the reflection symmetry of the moiré superlattice.

Second, chaotic microcavities have been the primary testing ground for studying quantum chaos. In this work, we generalize the wave chaos theory to cavity lattice systems. We discover the intrinsic coupling of the crystal momentum to the internal cavity dynamics, which substitutes the role of the deformed boundary shape in the ordinary microcavity problem. In addition to the normal cavity, the next project involving topological materials will be presented in this workshop.

Talk No.7

Phonon Decoupling in Oxides

Jaekwang Lee

Dept. of Physics, Pusan National University

In general, a slight displacement of an atom from its equilibrium position act the forces on the rest of atoms simultaneously. That's why the phonon has been considered as collective excitation in a periodic arrangement of atoms in solids. Here, using the first-principles density functional theory calculations, we first demonstrate that, contrary to typical collective phonons, oxygen- octahedral and oxygen-tetrahedral phonons can be fully decoupled over the whole range of phonon spectra in particular ternary oxides. This decoupled oxygen tetrahedral phonon would be strongly localized and can greatly induce the band flattening along a specific crystal orientation, which enables the unusual site-selective control of unit cell width domain wall.

Talk No.8

Correlated Electron-Nuclear Dynamics Toward Extended Systems

Seung Kyu Min

Department of Chemistry, Ulsan National Institute of Science and Technology (UNIST)

Correlated electron-nuclear dynamics is crucial in various phenomena, including photosynthesis, photovoltaics, photocatalysis, radiation chemistry, polaron chemistry, and quantum computing. Electron-nuclear correlations are handled using mixed quantum-classical approaches for small and intermediate molecular systems.[1] However, for extended molecular systems, real-time time-dependent density functional theory (RT-TDDFT) is used frequently. RT-TDDFT propagates electronic density with time-dependent Kohn-Sham orbitals and time-dependent external potentials while the classical nuclei move according to the Ehrenfest-type equation of motion. While the electronic equation of motion can describe nonadiabatic transitions, it cannot account for nuclear wave packet splitting and quantum decoherence, which are crucial for describing long-time behavior. To overcome this limitation, we propose a Hermitian form of an electron-nuclear correlation operator, which is equivalent to the original non-Hermitian operator.[2] This approach obtains a stable real-time and real-space electronic propagation with quantum decoherence in correlated electron-nuclear dynamics, which is essential for condensed phase simulations. Furthermore, we devise a modified version of the time-dependent Kohn-Sham equation by employing a Hermitian correlation operator within the RT-TDDFT framework. The approach is demonstrated to work well for molecular and condensed matter systems. The proposed method may pave the way for using the RT-TDDFT framework with the electron-nuclear correlation from the exact factorization approach for the simulation of extended systems for material science applications where a large number of electronic BO states are involved in the dynamics.

[1] Ha, J.-K.; Lee, I.S.; Min, S.K., Surface Hopping Dynamics beyond Nonadiabatic Couplings for Quantum Coherence, J. Phys. Chem. Lett. 2018, 9, 1097-1104.
[2] Han, D.; Ha, J.-K.; Min, S.K., Real-Space and Real-Time Propagation for Correlated Electron-Nuclear Dynamics based on Exact Factorization J. Chem. Theory Computat., 2023, 19, 2186-2197.

Talk No.9

Condensation of preformed charge density waves in kagome metals

Changwon Park

Korea Institute for Advanced Study, Seoul, 02455, Korea

Charge density wave (CDW) is a spontaneous spatial modulation of charges in solids whose general microscopic descriptions are yet to be completed. Layered kagome metals of AV_3Sb_5 (A = K, Rb, Cs) provide a unique chance to realize its emergence intertwined with dimensional effects as well as their special lattice. In this talk, based on state-of-the-art molecular dynamics simulations, I will show that the phase transition to CDW state in kagome metals is a condensation process of incoherently preformed CDWs. It will be demonstrated that charge modulation first forms on each kagome layer at a well-defined temperature but its phase still fluctuates with 10^5 times slower frequencies than typical phonon vibrations until reaching their freezing temperature. The size of spacer A layers controls the competition between the fluctuation and condensation of preformed orders, results in a maximized CDW transition temperature with Rb atom. Our results resolve controversial observations on CDW formations and highlight roles of weak interlayer interactions for CDWs in kagome metals.

Talk No.10

First-principles calculations on the stability of oxidized oxygen in Li-excess cathode materials

Dong-Hwa Seo

School of Energy and Chemical Engineering, UNIST

Center for Multidimensional Carbon Materials, Institute for Basic Science

Li-ion batteries are widely used for power sources in small electronic devices and increasingly in larger applications such as electric vehicles. Developing suitable electrode materials for these batteries is a key area of research, with a focus on materials that are stable, high-powered, high-energy, and cost-effective. Oxygen redox in Li-excess oxide cathodes has recently received great attention due to its potential to provide extra capacity in addition to the capacity from transition metal redox. However, the stability of oxidized oxygen is a critical issue for cathode performance, and the factors affecting its stabilization are not yet clear. In this talk, I will present the first-principles results of the effect of the spatial distribution of oxidized oxygen and the type of coordinated transition metal on the stability of oxidized oxygen in Li-excess cathode materials.

Talk No.11

Cost-effective screening of materials using hybrid density functional theory calculations

Ji-Sang Park[1]

[1]*SKKU Advanced Institute of Nanotechnology (SAINT) and Department of Nano Engineering, Sungkyunkwan University, Suwon 16419, Republic of Korea*

Several computational databases were constructed with the aim of screening and machine learning, however, most of them have been suffering from low accuracy in the electronic structure. Hybrid density functional theory (DFT) is currently being regarded as a remedy for improving accuracy in a wide discipline, however, it is not currently an ideal method for high-throughput calculations due to the high computational cost. In this presentation, we discuss how to reduce the computational cost of hybrid DFT without losing too much accuracy with respect to the conventional method [1,2]. Further analysis has revealed that the accuracy of the eigenvalues is determined by the downsampled reciprocal grid for the Hartree-Fock potential [3]. Studies on halide perovskite alloys and defects in Si will be also discussed [4,5].

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[2] J.-S. Park, J. Jung, and S. Lee, *Cost-Effective High-Throughput Calculation Based on Hybrid Density Functional Theory: Application to Cubic, Double, and Vacancy-Ordered Halide Perovskites*, J. Phys. Chem. Lett. **12**, 7885–7891 (2021).
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Talk No.12

First-principle simulations toward practical semiconductor device applications of low-dimensional materials

Han Seul Kim

Department of Advanced Material Engineering, Chungbuk National University, Chungdae-ro 1, Seowon-Gu, Cheongju 28644, Chungbuk, Republic of Korea

Low-dimensional materials such as two-dimensional and quantum dot materials, and crystal materials with internal polyhedral structures attract great attention due to their extraordinary controllability over electrical/optical properties. In this regard, they are expected to be the key materials for various next-generation semiconductor devices such as memory, display, and sensor. In this presentation, I would like to introduce several electronic structure calculation studies for the practical application of low-dimensional materials to semiconductor-type sensors and memory devices. In particular, it will be highlighted that the material engineering parameters revealed by electronic structure calculations can act as key components toward seamless collaborations with experiments.

References

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[3] *ACS Appl. Mater. Interfaces* 14, 20, 23617 (2022)

Talk No.13

Exploring light-induced phenomena in condensed matter systems with *ab initio* approach

Dongbin Shin

Department of Physics and Photon Science, Gwangju Institute of Science and Technology (GIST), Gwangju 61005, Republic of Korea

Condensed matter systems have greatly interested due to their potential applications and intriguing physical properties. Recent studies have focused on the effects of light on materials that have given rise to unprecedented light-induced phenomena. One example is the light-induced topological phase transitions observed in materials like WTe_2 and $ZrTe_5$ [1-2]. These transitions have been explained as resulting from changes in the lattice dynamics caused by excited electronic structures [3]. Another fascinating case is the light-induced ferroelectric transitions observed in quantum paraelectric $SrTiO_3$, which were induced by mid-infrared and terahertz lights [4-5]. Theoretical evidence suggests that the unique properties of the quantum paraelectric phase are responsible for this terahertz field-induced ferroelectricity [6]. This talk will explore the theoretical explanations behind recent light-induced dynamics in the condensed matter systems, such as light-induced magnetic momentum under time-reversal symmetric conditions in $NbAs_2$, light-induced topological phase transition in HgTe, and light-induced ferroelectricity in $SrTiO_3$. By exploring these diverse examples, we hope to understand better the complex interactions between light and condensed matter systems and the potential applications of these phenomena in the fields of physics and technology.

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Talk No.14

Misleading convergence of the bold-line diagrammatic technique: when the correct solution can be found

Aaram J. Kim

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

Convergence of the self-consistent skeleton diagrammatic technique (SDT)—in which the full Green's function is determined through summation of Feynman diagrams in terms of itself—to the wrong answer has been associated with the existence of non-perturbative branches of the Luttinger-Ward functional. Although it has been possible to detect misleading convergence without the knowledge of the exact result, the SDT has remained inapplicable in the regimes where this happens. We show that misleading convergence does not always preclude recovering the exact solution. In addition to the established mechanism, convergence of the SDT to the wrong answer can stem from divergence of the inherent diagrammatic series, which allows us to recover the exact solution by a modified SDT protocol based on controlled analytic continuation. We illustrate this approach by its application to the analytically solvable (0 + 0)D Hubbard model, the Hubbard atom, and the 2D Hubbard model in a challenging strong-coupling regime, for which the SDT is solved with controlled accuracy by the diagrammatic Monte Carlo method.

Talk No.15

Emergence of flat bands via orbital-selective electron correlations in Mn-based kagome metal

Subhasis Samanta[1], Hwiwoo Park[2], Chanhyeon Lee[3], Sungmin Jeon[2], Hengbo Cui[4], Jungseek Hwang[2], Kwang-Yong Choi[2], Heung-Sik Kim[1]

[1]Department of Physics and Institute of Quantum Convergence Technology, Kangwon National University, Chuncheon 24311, Republic of Korea

[2]Department of Physics, Sungkyunkwan University, Suwon 16419, Republic of Korea

[3]Department of Physics, Chung-Ang University, Seoul 06974, Republic of Korea

[4]Department of Physics and Astronomy and Institute of Applied Physics, Seoul National University, Seoul 151-747, Republic of Korea

Kagome lattice has been actively studied for the possible realization of frustration-induced two-dimensional flat bands and a number of correlation-induced phases. Currently, the search for kagome systems with a nearly dispersionless flat band close to the Fermi level is ongoing. Here, by combining theoretical and experimental tools, we present $Sc_3Mn_3Al_7Si_5$ as a novel realization of correlation-induced almost-flat bands in the kagome lattice in the vicinity of the Fermi level. Our magnetic susceptibility, ^{27}Al nuclear magnetic resonance, transport, and optical conductivity measurements provide signatures of a correlated metallic phase with tantalizing ferromagnetic instability. Our dynamical mean-field calculations suggest that such ferromagnetic instability observed originates from the formation of nearly flat dispersions close to the Fermi level, where electron correlations induce strong orbital-selective renormalization and manifestation of the kagome-frustrated bands. In addition, a significant negative magnetoresistance signal is observed, which can be attributed to the suppression of flat-band-induced ferromagnetic fluctuation, which further supports the formation of flat bands in this compound. These findings broaden a new prospect to harness correlated topological phases via multiorbital correlations in 3d-based kagome systems.[1]

[1] S. Samanta et al., arXiv:2304.04928

Talk No.16

Ab initio DMFT methodologies for correlated quantum materials

Sangkook Choi

School of Computational Sciences, Korea Institute for Advanced Study, Seoul, South Korea

*Email: sangkookchoi@kias.re.kr

In materials with a large number of electrons, the quantum mechanical interactions between these electrons often dictate the material's properties. These so-called correlated quantum materials display a range of exceptional emergent phenomena, including transitions from metal to insulator states, colossal magnetoresistance, and high-temperature superconductivity and even topological superconductivity.

The prediction of correlated quantum materials properties from first principles poses a grand challenge for condensed matter physics and materials science. Correlated quantum materials defy current band-picture-based ab initio methodologies, such as density functional theory. In these materials, there are fine details beyond band-picture descriptions due to their quantum many electron nature. To illustrate, quasiparticle peak comes with finite width and there can be a satellite peak next to the quasiparticle peak. In some cases, there is no one-to-one correspondence between mean-field band structure and measured one-electron spectra and band-picture description fails.

In this lecture, we present ab initio DMFT as one of the most successful methodologies to understand correlated quantum materials. This Green's function based method goes beyond the band-picture and has been successful in explaining many features of correlated quantum materials. We discuss the theoretical basis of this Green's function based approach and introduce multiple variations of ab initio DMFT. Additionally, we provide supportive data to validate ab initio DMFT.

Poster Abstracts

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김범섭	2	Optoelectronic manifestation of orbital angular momentum driven by chiral hopping in helical Se chains
김성환	3	Diffusion-based Generative AI for Exploring Transition States from 2D Molecular Graphs
김세준	4	Many-body perturbation theory for solvated low-dimensional systems
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Poster No.1

First-principles linear response theory for relativistic spin exchange interactions

Do Hoon Kiem, Hongkee Yoon, Myung Joon Han

Department of Physics, Korea Advanced Institute of Science and Technology, Daejeon 34141, Korea

Relativistic spin exchange interactions, such as Dzyaloshinskii-Moriya (DM) or Kitaev interactions, play a crucial role in creating magnetic textures or excitations. However, accurately calculating these relativistic spin interactions is challenging due to spin non-collinearity. The magnetic force theorem provides a powerful approach to obtaining these interactions [1-4]. In this work, we present an expansion of our code 'Jx' [5-6] using the magnetic force theorem for non-collinear spins (NC-MFT), which includes spin-orbit couplings. To verify the reliability and applicability of our method, we apply it to various bulk and two-dimensional systems in fully relativistic density functional theory calculations. Our method successfully provides quantitative DM interactions for both bulk and two-dimensional systems.

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Poster No.2

Optoelectronic manifestation of orbital angular momentum driven by chiral hopping in helical Se chains

Bumseop Kim[1,2†], Dongbin Shin[3,4†], Seon Namgung[2], Noejung Park[1,2], Kyoung-Whan Kim[5*], Jeongwoo Kim[6*]

[1]*Graduate School of Semiconductor Materials and Devices Engineering, Ulsan National Institute of Science and Technology, Ulsan 44919, Korea*

[2]*Department of Physics, Ulsan National Institute of Science and Technology, Ulsan 44919, Korea*

[3]*Department of Physics and Photon Science, Gwangju Institute of Science and Technology, Gwangju 61005, Korea*

[4]*Max Planck Institute for the Structure and Dynamics of Matter and Center for Free Electron Laser Science, Hamburg 22761, Germany*

[5]*Center for Spintronics, Korea Institute of Science and Technology, Seoul 02792, Korea*

[6]*Department of Physics, Incheon National University, Incheon 22012, Korea*

[†]These authors contributed equally: Bumseop Kim, Dongbin Shin

Chiral materials have garnered significant attention in the field of condensed matter physics. Nevertheless, the magnetic moment induced by the chiral spatial motion of electrons in helical materials, such as elemental Te and Se, remains inadequately understood. In this work, we investigate the development of quantum angular momentum enforced by chirality using static and time-dependent density functional theory calculations for an elemental Se chain. Our findings reveal the emergence of an unconventional orbital texture driven by the chiral geometry, giving rise to a non-vanishing current-induced orbital moment. By incorporating spin-orbit coupling, we demonstrate that a current-induced spin accumulation arises in the chiral chain, which fundamentally differs from the conventional Edelstein effect. Furthermore, we demonstrate the optoelectronic detection of the orbital angular momentum in the chiral Se chain, providing a conceptually novel alternative to the interband Berry curvature, which is ill-defined in low dimensions.

Poster No.3

Diffusion-based Generative AI for Exploring Transition States from 2D Molecular Graphs

Seonghwan Kim[1†], Jeheon Woo[1†] and Woo Youn Kim[1,2*]

[1]*Department of Chemistry, KAIST, 291 Daehak-ro, Yuseong-gu, 34141, Daejeon, Republic of Korea.*
[2]*AI Institute, KAIST, 291 Daehak-ro, Yuseong-gu, 34141, Daejeon, Republic of Korea.*

[†]These authors contributed equally to this work.

The exploration of transition state (TS) geometries is crucial for elucidating chemical reaction mechanisms and modeling their kinetics. Recently, machine learning (ML) models have shown remarkable performance for prediction of TS geometries. However, they require 3D conformations of reactants and products often with their appropriate orientations as input, which demands substantial efforts and computational cost. Here, we propose a generative approach based on the stochastic diffusion method, namely TSDiff, for prediction of TS geometries just from 2D molecular graphs. TSDiff outperformed the existing ML models with 3D geometries in terms of both accuracy and efficiency. Moreover, it enables to sample various TS conformations, because it learned the distribution of TS geometries for diverse reactions in training. Thus, TSDiff was able to find more favorable reaction pathways with lower barrier heights than those in the reference database. These results demonstrate that TSDiff shows promising potential for an efficient and reliable TS exploration.

Poster No.4

Many-body perturbation theory for solvated low-dimensional systems

Se-Jun Kim [1], Sébastien Lebègue[2*], Stefan Ringe[3*], and Hyungjun Kim[1*]

1 Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST), 291 Daehak-Ro, Yuseong-Gu, Daejeon 34141, Republic of Korea

2 Université de Lorraine and CNRS, LPCT, UMR 7019, Vandoeuvre-lès-Nancy 54506, France

3 Department of Chemistry, Korea University, Seoul 02841, Republic of Korea

The discovery of graphene in 2004 ignited the evolution of two-dimensional (2D) materials, such as transition metal chalcogenides (TMDCs) and hexagonal boron nitride (hBN). The exotic optoelectronic properties attributed to thickness reduction, even down to a single atomic thickness, have enticed scientists to decipher the underlying physics or, in some cases, replace conventional bulk materials to utilize abnormal light-matter interaction. Owing to tremendous efforts, their electronic and optical properties have been disclosed, providing a new direction in the research field.

However, when these materials are submerged in a solution where solute-solvent interactions play a critical role, electronic or quasiparticle phenomena are rarely discussed or reported due to the absence of appropriate methodology. Theoretically, a high-level theory beyond density functional theory (DFT) is needed to accurately describe electronic structures or optical spectra, such as many-body perturbation theory.

Here, we address this issue by developing a new methodology called GW-GPE, which combines the GW approximation and the generalized Poisson equation in a harmonious manner. In this method, the solvent effects on 2D materials are defined by decoupling them into two effects: the polarization-field effect (PFE) and the environmental screening effect (ESE). We particularly discovered a structure-property relation where percolation can be strongly correlated with solvent effects. Additionally, the band alignments in the solution matched well with experimental band positions.

Next, we extended GW-GPE by conjugating the Bethe-Salpeter equation to GW-GPE (GW/BSE-GPE) to unveil optical behaviors of low-dimensional systems. We successfully reproduced experimental observations and captured new dielectric-dependent exciton evolution. Collectively, this methodology can shed light on distinct behaviors of 2D materials in solutions, ultimately suggesting design guidelines for future optoelectronic energy devices.

Poster No.5

Exploring decomposition mechanism of Hydroxylamine on Cu(111) surface using Pynta – Workflow code for heterogeneous catalysis reaction

Shinae Kim, Matthew S. Johnson, Judit Zádor

Combustion Research Facility, Sandia National Laboratories, Livermore, CA, USA

Predicting chemical changes for the heterogeneous catalytic process is important in order to build a fundamental understanding of kinetic models and chemical reaction pathways. Recently, we developed Pynta (https://github.com/zadorlab/pynta), an automated workflow code for exploring reaction paths that can automatically set up and process a large number of quantum chemistry calculations to study reactions of adsorbates and gas-phase species on metal facets. Pynta characterizes elementary chemical reactions relevant to heterogeneous catalysis and can provide adsorption-site-specific kinetic information. Using the harmonically forced saddle point searching method, Pynta can generate chemically sensible and comprehensive initial guesses for saddle point geometries by defining harmonic potentials based on the optimized adsorbate geometries and bonds that are forming and breaking during the reaction.

As an application of Pynta, hydroxylamine (HA) decomposition pathways on the Cu(111) surface are explored. Hydroxylammonium nitrate (HAN) is a promising monopropellant thruster that can replace toxic and highly explosive hydrazine-based monopropellant thrusters. Mass spectroscopy results have shown that HAN decomposes to hydroxylamine (HA), and the catalytic decomposition reaction of HA creates critical ignition conditions in HAN-based propellants. While copper is widely used for propellant catalysts, the mechanisms for the catalytic decomposition reaction of HA on copper surfaces have not yet been examined. We demonstrate that Pynta is able to identify transition states and generate rate coefficients for possible HA decomposition pathways and discuss the predicted products.

Poster No.6

Theoretical Investigation of the Electronic and Magnetic Properties of Cr_2Se_3

Jaewon Kim[1*], Do Hoon Kiem[1], Myung Joon Han[1*]

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

Half-metallic fully compensated ferrimagnetic (HM-FCFiM) materials have gained attention due to their potential for future spintronic devices. In the previous study, Cr_2Se_3 was proposed as a potential candidate material for HM-FCFiM [1]. In this work, we theoretically studied Cr_2Se_3 based on first-principles calculations. Our DFT+U calculations investigated a variety of spin configurations and successfully provide a phase diagram as a function of the interaction parameters U and J. Our calculation results can improve the understanding of electronic structures for Cr_2Se_3.

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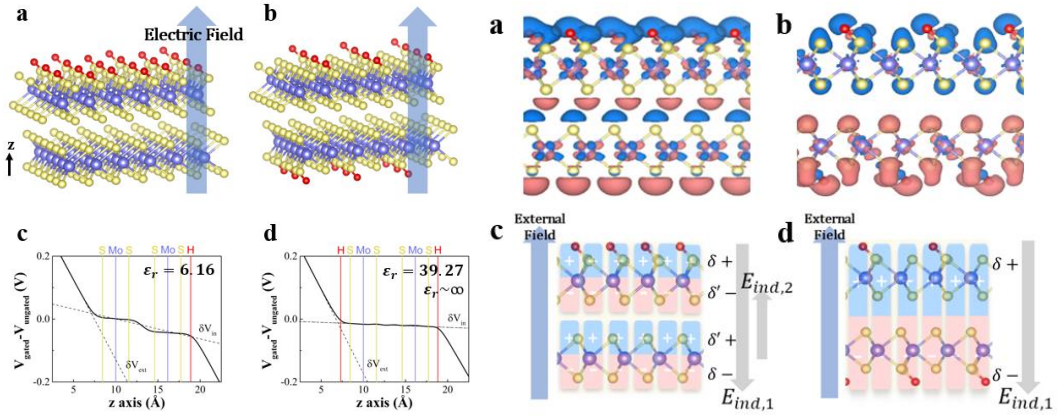
Poster No.7

Correlation of functionalization and screening length on vertical electric screening of few-layer MoS_2

Joohee Kim

Department of Physics, Konkuk University, Seoul 05029, Korea

We performed functionalization to few-layer MoS2 to study their vertical electric screening using first-principles calculations for dielectric constants based on linear response theory. We found that one side functionalized bilayer MoS2 shows semiconducting screening behavior, while both sides one show metallic screening behavior though all the MoS2 are semiconducting in terms of band theory. One side functionalized MoS2 has a shorter screening length than their thickness, while both sides one has close or longer screening lengths than their thickness. We also found that the screening of one side functionalized MoS2 remained unchanged as the functionalization concentration increased, while both sides functionalized MoS2 has increasing electric screening because the screening length for both sides functionalized MoS2 is only increased as the functionalization concentration increases. Our results indicate strong correlation among the functionalization side, its concentration, and screening length, which considerably influences the vertical electric screening of few-layer MoS2. We also show the dependence of the type of functionalization on the screening.



Poster No.8

AI-enabled active exploration of small molecules for n-charge generation layer in tandem organic light-emitting diode

Jisu Kim,[1] Jaesun Kim,[1] Jinmu You,[1] and Seungwu Han[1,2,*]

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

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

The rapid advancement of organic light-emitting diodes (OLEDs) has greatly influenced display technology, enabling the development of thin and flexible solid-state lighting devices. Tandem OLEDs, which consist of stacked electroluminescent units connected by a charge generation unit, offer a promising solution for achieving high efficiency and brightness. However, these devices face the issue of increased operational voltages due to additional layers. Therefore, it is crucial to develop an intermediate charge generation unit with efficient charge generation and transportation properties to mitigate voltage drop.

To address this, a two-step process involving unsupervised and supervised learning is proposed to investigate suitable organic semiconductors for the charge generation layer (CGL). Specifically, Li-doped phenanthroline derivatives are studied as potential CGL materials. Initially, unsupervised learning using k-means clustering is employed to generate a representative set of molecules from the vast chemical space of phenanthroline derivatives. This condensed set serves as a starting point for further exploration. Subsequently, a relational graph neural network, along with the Monte Carlo dropout method, is used for supervised learning to predict molecular properties relevant to CGL suitability. A scoring function is formulated based on these properties, and an active exploration algorithm is designed to enhance accuracy and generate new promising molecules.

This systematic approach resulted in the discovery of molecules that outperform known phenanthroline derivatives in terms of CGL suitability. The research also provides insights into common characteristics of promising molecules, such as the substituted carbon position in phenanthroline. Overall, this study presents an efficient strategy for exploring the challenging chemical space of CGL materials.

Poster No.9

Unveiling Wet Etching Mechanism of GaN Through Molecular Dynamics Simulations with Neural Network Potential

Purun-hanul Kim[1] , Youngho Kang[2], and Seungwu Han[1,*]

[1]*Department of Materials Science and Engineering and Research Institute of Advanced Materials, Seoul National University*

[2] *Department of Materials Science and Engineering, Incheon National University*

Micro-sized light emitting diodes (μLEDs) based on GaN hold great potential for augmented reality and virtual reality displays in our hyperconnected society. However, their performance is currently inferior to bulk LEDs due to the vulnerability of μLEDs to surface defects caused by their high surface-to-volume ratio. The wet-etching process in alkaline environments plays a critical role in shaping the structure of μLEDs during the fabrication of microscale GaN, necessitating a thorough understanding of the etching mechanism to establish reliable production processes. Traditional ab-initio molecular dynamics (AIMD) simulations based on density functional theory (DFT) have limitations in capturing the complex and diverse chemical reactions occurring at the solution-GaN interface during wet etching, primarily due to their restricted system size and time scale.

To overcome these limitations, Behler-Parrinello-type neural-network potential (NNP) based molecular dynamics (MD) simulations have emerged as an effective tool. In this study, we employ NNP-MD simulations, which are significantly faster than AIMD, to investigate the wet etching of GaN. To construct an accurate and reliable NNP model for simulating etching processes, we generate a comprehensive training set by sampling AIMD trajectories of KOH solution, GaN surface, and their interface models across various temperature and pressure ranges. The NNP constructed with SIMPLE-NN code accurately reproduces DFT energies, forces, and stress tensors. The NNP is validated extensively through comparisons with DFT results. Using the established NNP model, we conduct NNP-MD simulations to investigate the etching of the GaN($1\bar{1}00$) surface immersed in KOH solution. Our simulations reveal the crucial processes of OH^- (*aq*) attachment to the surface Ga and subsequent passivation of an N dangling bond by H^+ (*aq*) during the wet etching of GaN. These findings enable us to establish the etching mechanism and provide valuable insights into surface defects that can degrade LED performance. Moreover, we explicitly demonstrate the dependence of the etch rate on the surface orientation of GaN, which aligns with experimental observations.

Poster No.10

Understanding the Dielectric Relaxation of Liquid Water Using Neural Network Potential and Classical Pairwise Potential

Jae Hyun Ryu[1], Ji Woong Yu[2], Tae Jun Yoon[3,*], Won Bo Lee[1,*]

[1]*School of Chemical and Biological Engineering, Seoul National University, Seoul, 08826, Republic of Korea*

[2]*Center for AI and Natural Sciences, Korea Institute for Advanced Study, Seoul, 02455, Republic of Korea*

[3]*Department of Chemical Engineering and Applied Chemistry, Chungnam National University, Daejeon, 34134, Republic of Korea*

Understanding the role of hydrogen bond networks in determining the relaxation dynamics is essential for understanding natural phenomena in liquid water. Classical pairwise additive models have been widely utilized for elaborating the underlying mechanism behind the relaxation phenomena. However, they have shown their limits due to either the absence or inaccurate descriptions of many-body and medium-to-long-range interactions. This work demonstrates that the Deep Potential Molecular Dynamics (DPMD) model help calculate the dielectric relaxation at the accuracy of the first-principles simulations. The DPMD model outperforms the classical force field (SPC/Fw) in predicting dielectric spectra. Analyzing the simulation results, we discover that the improvement does not stem from accurately representing the tetrahedral order. Instead, including inherent many-body interactions and intramolecular dynamics makes water molecules adapt to their local environments, lowering the potential energy barrier of reorientation.

Poster No.11

Description of medium-range order in amorphous GeSe by machine learning potentials : descriptor versus graph

Minseok Moon[1], Seungwoo Hwang[1], Jaesun Kim[1], and Seungwu Han[1,2,*]

Department of Materials Science and Engineering, Seoul National University
Korea Institute for Advanced Study

Atomistic simulations based on density functional theory (DFT) play a crucial role in understanding the behavior of materials at the atomic level and gaining insights into complex phenomena within the field of materials science. However, these simulations are limited in terms of time and size scale due to their high computational costs. Recently, there has been a growing interest in machine-learned potentials (MLPs) as an alternative to the DFT method. MLPs can calculate energy and atomic forces much faster than DFT while achieving similar accuracy. However, MLP often fails to reproduce DFT properties in complex system. For instance, amorphous chalcogenide systems are difficult for MLPs to learn due to their complex medium-range order, which includes n-membered rings and Peierls distorted structures. Matching the medium-range order in amorphous chalcogenide system is crucial because it significantly impacts the electronic structure. Various types of machine learning models have been developed, including the descriptor-based Behler-Parinello neural network (BPNN), moment tensor potential (MTP), Gaussian approximate potential (GAP), and graph neural network (GNN). However, there is a lack of understanding regarding the differences between each model, as well as unresolved questions such as the difficulty of learning systems with medium-range order and determining which model can be more effective for this type of system.

In this study, we tested various MLP models in the amorphous GeSe system to determine which models can accurately reproduce this system. Three different MLP models were tested: BPNN with atom-centered symmetry function, MTP, and a message-passing graph neural network called NequIP. The amorphous structures generated by the MLP models exhibited subtle differences in local structure, such as radial distribution function (RDF) and angular distribution function (ADF). However, when it came to medium-range features like ring distribution and angular-limited three-

body correlation indicating the degree of Peierls distortion, only the NequIP model accurately reproduced the features of DFT and even matches the electronic structure. On the other side, the amorphous structures generated by the BPNN and MTP models failed to accurately describe structural distortions in chalcogenide amorphous materials and showed a preference for structures with resonant bonds. However, the MTP models showed better performance than BPNN by considering many-body terms. We confirmed that message-passing MLPs can overcome the limitations that atom-centered descriptor models have in learning medium-range interactions and can accurately reproduce electronic structure of DFT amorphous. Additionally, the atom-centered descriptor model can learn medium-range order to some extent by considering many-body terms. This work is expected to contribute to a better understanding of the differences between MLP models and provide insights for selecting appropriate models.

Poster No.12

Production of machine learning potentials including vdW interaction

Karam Park[1], Kangmo Yeo[2], Sukmin Jeong[1]

[1]Department of Physics and Research Institute of Physics and Chemistry, Chonbuk National University, Jeonju 54896, Korea
[2] Department of Artificial Intelligence Convergence, Chonnam National University, Gwangju 61186, Korea

The PAW potential and PBE exchange-correlation functional are widely practiced in computational science research for materials properties using density functional theory (DFT). However, these methods often do not adequately represent van der Waals (vdW) interactions, requiring additional approximation methods to include them. While some approximations can produce results comparable to experimental observations, they typically come with high computational costs and calculation time. In recent times, machine learning has made significant advancements in various fields, including computational science. We utilize machine learning to develop potentials that effectively describe vdW interactions. This study aims to construct atomic potentials that include vdW interactions using the VASP, DeepMD, and LAMMPS packages. And we test the effectiveness of these machine learning potentials by comparing them to DFT+vdW correction calculations. We create multiple generations of machine learning potentials (MLPs) and evaluate their effectiveness in accurately describing interactions among aromatic molecules. The convergence of different potentials by generations will be analyzed by assessing lattice distances, potential curvature, binding energy, and mean absolute error (MAE). Additionally, we will compare the computational efficiency of first-principles calculations with those using machine learning potentials. The results show that as the generations progress, various parameters exhibit convergence. MLP-based calculations offer a significantly faster and more efficient alternative while maintaining accuracy comparable to DFT calculations, albeit within a limited range.

Poster No.13

First-principles study on the defect states in the monolayer tungsten diselenide

Sunho Park[1)], Mina Yoon[3)], Young-Kyun Kwon[1) 2)]

1) Department of Physics, Kyung Hee University, Seoul, South Korea

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

3) Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN, USA

Monolayer tungsten diselenide has attracted significant interest among researchers due to its optical activity. Its intriguing aspects come from atomic defects, which generate electron transitions within the bandgap. Particular luminescence observed In this material has been regarded as a single photon emitter, having potential for applications in quantum information technology, specifically for flying qubits. However, comprehending each type of defect poses challenges as experiments can only capture collective signals from samples. To overcome such challenges, we employed density functional theory (DFT) calculations with a hybrid functional approach to explore how defect structures would affect the electronic structures of monolayer tungsten diselenide. Our investigation involves evaluating the formation energy to determine their energetic stability and examining defect states to estimate the transition energy associated with photon emission. Additionally, we analyzed the effects of hBN encapsulation on this system. Lastly, we present the features and properties of defect states in the band structures, which strongly depend on the symmetries of each defective system.

Poster No.14

Composition and Strain-Induced Effects on Magnetic Anisotropy in Co-Pt Alloy

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

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

E-mail: ykkwon@khu.ac.kr

Various Co-Pt alloys, Co_nP_{tm}, have attracted great attention due to their promising potential applications in spintronics and magnetic storage devices. However, the precise control of the magnetic anisotropy energy (MAE) in Co-Pt alloys is still poorly understood. We used density functional theory calculations to explore how the MAE is affected by the strain and composition ratio of Co and Pt. We systematically analyzed the strain effect on MAE by applying strain along the [001] and [111] crystal directions. Our results show an inverted parabolic variation of MAE when strain is applied along the [001] direction, while a direct parabolic trend is observed when strain is applied along the [111] direction. By varying the ratio of Co to Pt, we further observed that the perpendicular magnetic anisotropy (PMA) exhibits the highest stability at a 1:1 ratio of Co to Pt. To provide insight into these observed trends, we performed a comprehensive analysis of the magnetic properties by considering various orbital-resolved physical quantities, such as the orbital-resolved MAE.

Poster No.15

Machine learning ensemble for predicting the formation energy of oxygen vacancy in a latent chemical space

Seulyoung Park[1], Jun Oh Park[1], Jin Park[1], Yu Seong Heo[1], and Jaichan Lee[1,2]*

*Corresponding author: jclee@skku.edu

[1]*School of Advanced Materials Science and Engineering, Sungkyunkwan University, Suwon 16419, Korea*

[2]*CompAID Research, Suwon 16419, Korea*

Oxygen vacancy is an intrinsic defect in metal oxides and its concentration is susceptible to growth conditions and annealing processes. It also significantly affects the physical properties of metal oxides and the performance of devices in various fields. Consequently, the formation energy of an oxygen vacancy (E_V) is one of the primary factors in fabricating and investigating metal oxides. Traditional methods such as theoretical calculations and experiments have been used to obtain E_V, while they are expensive and have a limitation in exploring a large number of metal oxides. In this study, machine learning (ML) models are built up to rapidly predict the formation energy of oxygen vacancies in the latent chemical space. We show that an ensemble of multiple ML models enables accurate predictions of the formation energy of oxygen vacancies across a wide range of unexplored latent chemical space, from binary to quinary oxides.

Poster No.16

Scalable Parallel Algorithm for Graph Neural Network Potentials in Molecular Dynamics Simulations

Yutack Park,[1] Jaesun Kim,[1] and Seungwu Han[1,2,*]

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

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

Machine-learned potentials have emerged as a preferred method for addressing the scale limitations inherent in *ab initio* molecular dynamics (MD) simulations. Early-stage machine-learned potentials utilized invariant, atom-centered descriptors to encode the atomic environment. Recently, however, attention has been drawn to graph-based neural network interatomic potentials (GNNs), especially those of the equivariant type. These GNNs generally surpass descriptor-based models in accuracy and can efficiently manage multi-component systems. However, the message propagation in GNNs inherently makes them challenging to integrate with spatial decomposition, a conventional parallel algorithm used in MD. To the best of our knowledge, no GNN package currently supports distributed-memory parallelism in MD. Consequently, the length scale that GNNs can study is restricted by the memory size of a single processor.

To address the issue, we present SEVENNet (Scalable EquiVariance-Enabled Neural Network), an implementation of a parallel algorithm that integrates GNNs with spatial decomposition. The baseline GNN model is the same as NequIP, and we employed the LAMMPS package for spatial decomposition. To optimize the parallel implementation, we have included a communication routine for GNNs with multiple GPUs, leveraging NVIDIA GPUDirect® technology for fast inter-GPU communication. To assess the parallelization efficiency of our algorithm, we conducted MD simulations for SiO_2 on A100 GPU clusters. We tested up to 5 message passing layers and 32 GPUs, where intensive communication of atomic features and gradient information between processors occurs in each message passing layer. SEVENNet demonstrated over 80%-90% parallel efficiency when scaling the number of atoms proportionally with the number of GPUs. This result indicates that the simulation using SEVENNet can be linearly scaled up to accommodate a large number of atoms. We believe that this study paves the way for the application of GNNs in large-scale simulations.

Poster No.17

Comparative analysis of machine learning potential.

Pyung Jin Park, Young-Jae Choi and Seung-Hoon Jhi

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

Molecular dynamics (MD) simulations have proved to be a valuable tool for investigating the dynamical behavior of materials across various scientific disciplines. Yet, the MD study of phenomena involving extensive time and size scales demands computationally efficient methods without sacrificing accuracy. Machine-learning methods, such as neural networks and kernel methods, promise a great potential in achieving high accuracy while significantly reducing computational costs. In this study, we present a comprehensive summary of the applications of machine learning potentials in MD simulations, focusing on chalcogenide phase change materials (GeTe, GST) and silicon. Specifically, we compare the effectiveness of neural networks and kernel methods in terms of construction efficiency and accuracy for lattice dynamics. We vary the number of training sets generated by a randomized atomic-system generate [1] to perform this analysis and compare the results (radial distribution function, phonon dispersion, etc) of three representative machine learning potentials (DPMD [2], NequIP [3], GAP[4]).

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Poster No.18

Calculate the ground state for a fully connected tight-binding model using gradient descent with quantum(simulated) annealing

Hayun Park

Kangwon National University

Gradient descent (GD) is a widely used method in machine learning. However, due to the non-convexity of the loss function, GD may become trapped in local minima. On the other hand, quantum(simulated) annealing can globally find the ground state. In this study, we calculate the ground state for a fully connected tight-binding model using only GD, and then by combining GD and annealing. We demonstrate that this hybrid method finds the ground state faster as compared to conventional GD method . .

Poster No.19

Decoherence of MoS_2 in high harmonic generation

Gimin Bae and J. D. Lee*

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

Decoherence time T_2 describes electron-electron or electron-phonon scattering, which changes the dynamics of electrons, e.g., the intensity and phase of the high-harmonic generation (HHG) spectra. While the HHG has been extensively investigated in real space and time-domain, research into its decoherence processes has been lacking. In this study, we use the quantum master equation to investigate the electron dynamics in MoS_2, with a specific focus on T_2 values below 20 fs. In a linearly polarized pulse, which is rotated by a specific angle between 0 and 30 degrees with respect to the crystal mirror plane, we find that a rotation along the $\hat{\mathbf{x}}$ (zigzag) direction of the polarization direction of the even-order HHG varies with T_2. This rotation is because MoS_2 has a honeycomb structure designed in different structures along parallel and perpendicular directions with broken inversion symmetry. These findings present a possible application to measure the decoherence time T_2 and an understanding of the underlying physical process of decoherence time in two-dimensional materials.

Poster No.20

Origin of spatial variations in atomic-scale thermopower profiles

Seungil Baek[1], Eui-Cheol Shin[1], Yong-Hyun Kim[1,2]*

[1]*Department of Physics, Korea Advanced Institute of Science and Technology (KAIST), Daejeon 34141, Republic of Korea.*

[2]*Graduate School of Nanoscience and Technology, KAIST, Daejeon 34141, Republic of Korea.*

**Correspondence to: yong.hyun.kim@kaist.ac.kr*

To realize the full potential of thermoelectricity, a comprehensive understanding of an atomic-scale thermopower is imperative [1,2]. Recently, a thermoelectric study on defective systems revealed that the decaying wave function of localized states exerts far-reaching constant influence up to nanometers [3]. However, the question of what causes the spatial variations in the local thermopower profile still remains open. Here, we show that energetical distance is the leading factor that causes spatial fluctuations in the mesoscopic thermopower. *Ab initio* scanning Seebeck microscopy revealed that a single wave function at a specific K-point generates a flat profile regardless of its magnitude. Only after states with different energetical distance comes into account, does the outcome image starts to possess spatial variations. Moreover, when the wave function population becomes exactly zero, especially for antibonding nodes, energetical distance undergoes drastic alteration and its presence is expressed as a local peak nearby. Therefore, nodal points/lines can be captured via a sharp signal in the thermopower profile. Our results not only provide exquisite node sensing technique, but also suggest fundamental understanding of atomic thermoelectricity.

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Poster No.21

Strain-Induced Stabilization of monolayer $IrTe_2$ Phases: Insights from Thermal Expansion

Sungmin Song and Seung-Hoon Jhi

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

Layered transition metal dichalcogenides (TMDs) offer a valuable platform for investigating intricate electronic phases in two dimensional materials [1]. In the case of monolayer $IrTe_2$, the origin of the dimerized phase observed at low temperatures and the 1T phase at room temperature has remained elusive [2]. In this study, we present the evidence that the phase of $IrTe_2$ can be modulated by external strains. We also demonstrate that this strain is induced thermally. Our findings shed light on the underlying mechanisms governing the phase transitions in $IrTe_2$, and highlight the significant role of strain in modulating its phase properties.

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Poster No.22

Atomistic kinetic Monte Carlo simulation for atomic layer deposition of TiN thin film

Hyungmin An[1*], Sangtae Kim[1], Sangmin Oh[1], and Seungwu Han[1]

1 Department of Materials Science and Engineering and Research Institute of Advanced Materials, Seoul National University, Seoul 08826, South Korea

E-mail address: andynn@snu.ac.kr

In the semiconductor industry, titanium nitride (TiN) plays a crucial role in metal gates and diffusion barriers, due to its low electrical conductivity and high thermal stability. For depositing TiN thin films, atomic layer deposition (ALD) is a preferred method which employs a $TiCl_4$ precursor and NH_3 reductant. By surface reactions from alternating precursors, TiN ALD enables production of highly conformal crystalline films with low resistivity.

Nevertheless, alongside technical problems such as Cl contamination impacting the film's resistivity, the kinetics of surface reactions and even the overall thermodynamics in TiN ALD remain obscure. Hence, a thorough comprehension of the surface reaction mechanism is crucial to address problems in TiN ALD and to optimize the process conditions.

The use of *ab initio* molecular dynamics to study surface reactions has limits on both time and length scales. In this study, we propose an on-lattice type kinetic Monte Carlo (kMC) model to model the TiN ALD process. We calculated reaction energies and activation barriers of elementary surface reaction mechanisms with DFT. We pay particular attention to comparing our data on growth per cycle (GPC) and Cl contamination ratios with experimental results, while examining the atomic-level origin.

Poster No.23

Ab initio-based understanding of charge density wave phases in TaS_2

Jinseok Oh[1], Dongbin Shin[2*], Noejung Park[1]

[1]*Department of Physics, Ulsan National Institute of Science and Technology, Ulsan 689-798, Republic of Korea*

[2]*Department of Physics and Photon Science, Gwangju Institute of Science and Technology, Gwangju 61005, Republic of Korea*

jsoh23@unist.ac.kr, dshin@gist.ac.kr, noejung@unist.ac.kr

TaS2 is a fascinating material that exhibits a range of unusual properties associated with its charge density wave phases, which were initially thought to be due to in-plane lattice distortions. However, recent research has shown that the CDW phases in TaS2 are more complex than originally thought, and that the behavior of TaS2 monolayers cannot fully explain all of the phases observed in bulk TaS2. In this study, we investigate the effects of stacking order on the electronic properties of TaS2, using first-principles calculations to explore the effect of different stacking orders.

Poster No.24

Development of an Efficient Preconditioned Eigenvalue Solver for Real-Space Density Functional Theory Calculations and Multi-GPU Acceleration

Jeheon Woo, Woo Youn Kim

Department of Chemistry, KAIST, Daejeon 34141, Republic of Korea

Various real-space methods optimized on massive parallel computers have been developed for efficient large-scale density functional theory (DFT) calculations of materials and biomolecules. The iterative diagonalization of the Hamiltonian matrix is a computational bottleneck in real-space DFT calculations. Despite the development of various iterative eigensolvers, the absence of efficient real-space preconditioners has hindered their overall efficiency. An efficient preconditioner must satisfy two conditions: appropriate acceleration of the convergence of the iterative process and inexpensive computation. This study proposed a Gaussian-approximated Poisson preconditioner (GAPP) that satisfied both conditions and was suitable for real-space methods. A low computational cost was realized through the Gaussian approximation of a Poisson Green's function. Fast convergence was achieved through the proper determination of Gaussian coefficients to fit the Coulomb energies. The performance of GAPP was evaluated for several molecular and extended systems, and it showed the highest efficiency among the existing preconditioners adopted in real-space codes. We also combine GAPP with a shift-and-inverse preconditioning scheme. The new preconditioning method enables efficient multi-GPU parallelization with minimal communication overhead. As a result, we have successfully harnessed the computational power of multiple GPUs to achieve high multi-GPU acceleration.

Poster No.25

Investigating the Athermal Charge Effect on Electro-Plasticity of Metals through First-Principles Calculations

Seungwoo Yoo, Young-Kyun Kwon

1.Physics, Departments of Science, Kyung Hee University

The phenomenon of enhanced plasticity in metals under the influence of electric current has long been recognized and has been exploited for industrial purposes such as structural manipulation. To understand the effect of charge on plasticity, we have performed first-principles density functional theory calculations on various charged systems undergoing structural deformation. Our work demonstrates that the introduction of charge doping, regardless of the excess or deficiency of electrons, can induce notable changes in the energy barriers associated with structural deformations such as layer sliding and shear deformation. We have also explored the dynamic changes in the local charge distribution during deformation, revealing that excess charge migrates to the deformed region. Such migration effectively mitigates the charge instability caused by structural changes and ultimately reduces the deformation barrier. It is noted that slab calculations of charged systems inevitably lead to significant discrepancies between calculated and desired potentials due to the periodicity inherent in the calculation method. To address this issue, a charge compensation scheme was applied to successfully compensate for the desired localized potentials, allowing for more precise calculations.

Poster No.26

Resonant and non-resonant high harmonic generation from twisted bilayer graphene.

Gwanjin Lee[1] and J.D. Lee[1]*

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

Twisted bilayer graphene (TBG) has gained renewed attention as an important van der Waals material with atomic thinness, especially following the discovery of its superconducting state. Despite several experimental and theoretical studies focusing on the nonlinear optical properties of TBG, the research has been limited to linear or circular polarized pump pulses. Moreover, after the experimental observation of resonant second harmonic generation and third harmonic generation, theoretical investigations of resonant high harmonic generation (HHG) of TBG have not been reported.

In this study, we examine the minimal commensurate TBG structure using a tight-binding Hamiltonian and theoretically calculate the harmonic response induced by an ultrafast pulse via the quantum master equation. We present selection rules for both linear and circular-polarization pump pulses within the sublattice exchange even parity structure. Particularly, we investigate the 5^{th} harmonic response to an elliptically polarized pulse using a mid-infrared pump pulse. In addition, we calculate the dependence of dephasing time (T_2) on harmonic ellipticity, phase difference, and harmonic rotation using elliptically polarized pump pulses. Our study further reveals resonant 5th harmonic generation in TBG near the 3 eV transition energy. This study could contribute to the understanding and application of TBG in the field of nonlinear optics.

Poster No.27

Molecular Dipole Layers for Improving Exciton Dissociation in Self-powered Photodetectors

Noki Lee, Sehoon Oh, and Jaichan Lee*

School of Advanced Materials Science and Engineering, Sungkyunkwan University (SKKU), Suwon 16419, Republic of Korea

This research discusses the design of self-powered photodetectors, devices that do not need an external power source, making them perfect for low-energy applications like the Internet of Things. We explore the potential of two-dimensional (2D) materials by introducing a strategy to enhance exciton dissociation in a specific 2D material, bilayer tungsten diselenide (bi-WSe_2). This approach uses molecular dipole layers (MDLs) to induce an internal electric field within the bi-WSe_2, promoting exciton dissociation and increasing photocurrent generation. Our research indicates that the surface potential from the MDLs and charge redistribution at the bi-WSe_2/MDL interface contribute to this internal field. By avoiding a phenomenon known as degenerate doping, a common issue in low-dimensional materials, we further optimize the energy band offset, resulting in the enhancement of the photodetector's sensitivity to light and the reduction of dark current currents. These insights provide insights for developing more efficient self-powered photodetectors for low-power applications.

Poster No.28

Van der Waals metal 1T-$CrTe_2$: Self-Doped double-Exchange ferromagnet

Dong Hyun David Lee[1*], Taek Jung Kim[1], Min Yong Jeong[1] and Myung Joon Han[1†]

[1]*Department of Physics, KAIST, Daejeon 34141, Republic of Korea*

1T-$CrTe_2$ is a van der Waals ferromagnetic metal that has been gaining significant attention as a potential spintronics device due to its interesting properties including high Curie temperature even in the atomically thin-film form, intriguing transport phenomena, and wafer-size fabrication via molecular beam epitaxy. Nevertheless, the orbital-dependent electron correlation and its relation with ferromagnetism is still not well understood. Here, we argue the ferromagnetism of 1T-$CrTe_2$ is best understood within `self-doped' double-exchange mechanism. By using density functional theory plus dynamical mean-field theory (DFT+DMFT), we show that self-doping together with the aid of Hund's interaction imposes dual nature of Cr-*d* orbitals: Albeit they are all metallic, e_g and t_{2g} electrons exhibit itinerant and localized nature, respectively. These electrons are coupled through the Hund's interaction, which in turn facilitates double-exchange mechanism. Our study provides deeper understanding of basic electronic properties and their connection with the ferromagnetism in 1T-$CrTe_2$.

Poster No.29

Investigation of Al-ion intercalation in vanadium-based 2D materials via First-principles calculation

Moonwon Lee[1,2], and Kanghoon Yim[1*]

[1]*Computational Science & Engineering Lab., Korea Institute of Energy Research, Daejeon, 34129, South Korea*

[2]*Graduate School of Energy Science and Technology, Chungnam National University, Daejeon, 34134, South Korea*

[*]Corresponding Author E-mail Address: khyim@kier.re.kr

Recently, the aluminum-ion battery (AIB) has attracted great attention as a promising alternative to conventional lithium-ion batteries (LIBs) due to its high theoretical capacity and abundance. In particular, aqueous AIBs (AAIBs) are being actively researched since the Al-metal anode can be utilized in aqueous electrolytes without safety issues, unlike LIB. To enhance the energy density and stability of AAIBs, researchers are exploring cathode materials that can facilitate the intercalation of Al^{3+} ions. Among these materials, V_2CO_2 MXene and α-V_2O_5 have shown potential for intercalating Al^{3+} ions. However, little research has been done on the structural change in host materials as Al^{3+} ions are intercalated. In addition, the exact intercalation mechanism of Al-ion is still not clear. In this study, we investigated the differences in the intercalation behavior of Al^{-}ions in V_2CO_2 MXene and α-V_2O_5 through density functional theory (DFT) calculations. Based on the result, we compare the differences in capacity and stability depending on the cathode material types.

Poster No.30

Polymorphic and dual topological insulating phases of van der Waals layered InTe

Sangmin Lee[1], Miyoung Kim[1], and Young-Kyun Kwon[2,*]

[1]*Department of Materials Science & Engineering and Research Institute of Advanced Materials, Seoul National University*

[2]*Department of Physics, Department of Information Display, and Research Institute for Basic Sciences, Kyung Hee University*

We present a study on the unique properties of InTe, exhibiting characteristics of both a topological insulator (TI) and a topological crystalline insulator (TCI). This remarkable behavior gives rise to a dual topological insulator (DTI) in InTe, revealing nontrivial $\mathbb{Z}_2$ invariants and a mirror Chern number $C_M = \pm 1$. By investigating the stacking order of InTe as a van der Waals layered material, we discovered the formation of an additional mirror symmetry that enhances the robustness of the surface state against perturbations. These polymorphic variations give rise to a triply protected surface state, combining the newly formed mirror symmetry with the existing mirror symmetry and time-reversal symmetry. Furthermore, we demonstrate that the gapless Dirac state in InTe not only withstands time-reversal symmetry-breaking magnetic fields but also exhibits displacement away from the time-reversal invariant momentum (TRIM) points, with the direction of movement determined by the spin texture. The dual topological nature induced by vdW stacking offers exciting possibilities for controlling the stability and mobility of Dirac states, thereby opening avenues for the development of highly versatile and reliable DTI-based devices.

Poster No.31

Size-dependent electrical conductivity of PdCoO2 calculated using the momentum-dependent mean free path model

Youngjun Lee[1] , Seoung-Hun Kang[2] and Young-Kyun Kwon[1]

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

[2]*Materials Science and Technology Division,*

Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

With the continuous downsizing of modern CMOS devices, minimizing interconnect resistance has become crucial. Copper, a widely-used interconnect material due to its high conductivity in bulk, faces challenges at current technology scales due to the significant increase in resistance as the size decreases. This resistance upsurge stems from the excessively-increased scattering probability at the surface caused by copper's long mean free path. To overcome these limitations, delafossite materials, such as PdCoO2, have emerged as promising alternatives for electronic applications. PdCoO2 exhibits very anisotropic electronic properties originating from its 2D-like Fermi surface resulting in high planar conductivity. It is, however, to predict its size-dependent conductivity since currently-available models that predict the resistivity of thin-film metals rely on phenomenological fitting to experimental data, requiring real experimental measurements. Even with them, these models still cannot provide accurate predictions since they do not consider the anisotropic behaviors of charge carriers in samples. We present a new model method to evaluate the size-dependent resistivity through the modified relaxation time, which is a function of both energy and momentum. By employing our method, we present our understanding of the electrical properties of PdCoO2 at reduced thickness leading to the prediction that PdCoO2 maintains favorable electrical conductivity even at reduced thicknesses. These findings highlight the potential of PdCoO2 as a promising candidate for ultrathin electronic devices. In addition, our work provides valuable insights into the potential practical applications in the realm of electronic devices.

Poster No.32

Electronic and optical properties of monolayer hexagonal boron nitride on a graphite substrate

Woncheol Lee[1], Ping Wang[1], Mackillo Kira[1], Zetian Mi[1], and Emmanouil Kioupakis[2]

[1]*Department of Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, MI 48109, USA*

[2]*Department of Material Science and Engineering, University of Michigan, Ann Arbor, MI 48109, USA*

In this work, we investigate the electronic and optical properties of monolayer boron nitride (mBN) grown on Highly Ordered Pyrolytic Graphite (HOPG) substrate based on density functional theory and many-body perturbation theory. Our results indicate that the screening of the semi-metallic graphite substrate results in a giant bandgap renormalization of mBN. Also, we find a huge reduction of exciton binding energy in the presence of HOPG substrate and a blue-shifting of the 1s-exciton energy to above 6 eV. Furthermore, we demonstrate that strong electron-phonon interactions also play an important role in the optical process of mBN and give rise to the multiple phonon sidebands as observed from photoluminescence measurements. As a result, we propose that both the strong dielectric screening from the substrate and the strong electron-phonon interaction must be explicitly included to the analysis of luminescence measurements.

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Poster No.33

Origin of high quantum efficiency of bulk hexagonal boron nitride

Woncheol Lee[1], David Arto Laleyan[1], Yuanpeng Wu[1], Zetian Mi[1], and Emmanouil Kioupakis[2]

[1]Department of Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, MI 48109, USA

[2]Department of Material Science and Engineering, University of Michigan, Ann Arbor, MI 48109, USA

In this work, we theoretically investigate the electronic, phononic, optical, and excitonic properties of bulk h-BN using first-principles calculations. We demonstrate that the quasi-2D nature of h-BN leads to the enhanced confinement effect and the strong exciton binding energy. Additionally, we report that the efficient exciton-phonon coupling and the exceptionally flat exciton dispersion in h-BN both contribute to the effective phonon-assisted illumination in h-BN. Furthermore, we directly calculate the absorption spectrum of bulk h-BN using special displacement method and confirm that even though h-BN is an indirect-gap material, it shows much stronger absorption intensity than direct-gap AlN.

The work is supported by the University of Michigan College of Engineering Blue Sky Research Program. W.L. was partially supported by the Kwanjeong Educational Foundation Scholarship. Computational resources were provided by the DOE NERSC facility.

Poster No.34

Ab Initio Investigation of MoS_2-Graphene Composite for Li-ion Battery Anode

Suim Lim[1,2], Wonzee Jung[1,3], Kyu Yeon Jang[4,5], Hana Yoon[4], and Kanghoon Yim[1*]

[1] *Computational Science & Engineering Laboratory, Korea Institute of Energy Research, Daejeon, 34129, South Korea*

[2] *Department of Mechanical Engineering, Chungnam National University, Daejeon, 34134, South Korea*

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

[4] *Energy Storage Laboratory, Korea Institute of Energy Research, Daejeon, 34129, South Korea*

[5] *Advanced Energy and System Engineering, University of Science and Technology, Daejeon, 34129, South Korea*

In commercial Li-ion batteries (LIBs), graphite is still widely used as anode materials despite the limitations in capacity and diffusivity. To overcome the limitations and improve the performance of LIB anode, development of new materials with high capacity and high rate performance is required. The 1T phase of MoS_2, known for its superior electrical conductivity compared to the 2H phase, offers improved efficiency in charge/discharge processes and overall battery performance, making it a suitable material for use in LIBs. Recently, the 2D heterostructures composed of 1T/2H mixed phase MoS_2 nanosheets assembled on multi-layer graphene sheets are synthesized and exhibit enhancement in energy density and rate performance. To characterize the 2D heterostructure of MoS_2-graphene composite as LIB anode, we conducted first-principles calculations using the slab structure consist of 1T/2H mixed MoS_2 monolayer and graphene bilayer. First, we investigated the intercalation energies at various sites at the MoS_2/graphene interface, considering MoS_2 phases; 1T, 2H and 1T/2H phase boundary. In addition, we calculated the migration barriers of Li-ion in each region. The results show that interfaces on 1T MoS_2 and 1T/2H phase boundary can provide faster Li intercalation channel in the MoS_2-graphene composite.

Poster No.35

Atomic and electronic structures at Al_2O_3/ZnO heterostructure interfaces

JunOh Jeon, Deok-Yong Cho, Sukmin Jeong

Department of Physics and Research Institute of Physics and Chemistry, Jeonbuk National University, Jeonju 54896, Korea

A two-dimensional electron gas (2DEG), which is frequently found in semiconductor heterostructure, has been studied intensively in view of applications and academic reasons. This research focuses on investigating the 2DEG formed at the interface of insulating materials, specifically Al_2O_3/ZnO. To model the Al_2O_3/ZnO heterostructure, we utilize Al_2O_3, which has the α-alumina structure at room temperature, and ZnO, characterized by the wurtzite structure. By comparing the formation energy while controlling the number of oxygen atoms at the interface, we determine the stable structures. However, in structures with oxygen vacancies, defect states appear below the Fermi level resulting in gap states. The defect states primarily localize at the interface between Al_2O_3 and ZnO. These states can be verified by analyzing the plane-average local density of states (PLDOS) as well as the layer density of states. We propose that vacancy states contribute to the formation of the 2DEG.

Poster No.36

Manipulating Spin-Dependent Surface Band Gap in $MnBi_2Te_4$ via Antisite Defects: A First Principles Study

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

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

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

[3] *Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN*

MnBi2Te4 (MBT) is a promising material for spintronics due to its unique magnetic and topological properties. Despite the lack of time-reversal symmetry, MBT exhibits unique topological surface states due to their invariance under nonsymmorphic time reversal, or time reversal combined with a half-translation. While theoretical studies have suggested that the surface state should have a band gap, experimental measurements have observed a gapless surface state. This observation has been theoretically suggested to be possible when the spins of the system are aligned along the in-plane direction. We used density functional theory to investigate under which conditions, the system would prefer the in-plane spin direction and whether such conditions would exhibit the gapless surface state. We found that MBT with antisite defects has a negative magnetic anisotropy energy favoring the in-plane spin orientation. It was also observed that even in the presence of antisite defects, mirror symmetry protects the Dirac state on its surface. We present that the defect concentration can tune the Fermi level of the system enabling us to estimate a possible concentration of antisite defects in MBT samples observed in ARPES experiments.

Poster No.37

Study of the Effect of Light on In_2Se_3 Ferroelectric Field Effect Transistor(FeFET) for Synaptic Device using First-principles Calculations

Wonzee Jung[1,2], Seokju Kang[2], Young-Jun Yu[2*], Kanghoon Yim[1*]

[1]*Computational Science & Engineering Laboratory, Korea Institute of Energy Research*

[2]*Department of Physics, Chungnam National University*

In recent years, there have been significant advancements in neuromorphic systems employing nonvolatile memory as a next-generation computing system. As a promising potential material for neuromorphic systems, two-dimsional (2D) In_2Se_3 simultaneously exhibits stable ferroelectric, semiconducting, and photoelectric properties. In this study, we fabricated a synaptic device using α-In_2Se_3/h-BN/SiO_2 structure on a p^{++} Si wafer and observed a higher recognition rate when the device was exposed to LED illumination. In order to understand the origin of the light effect on the α-In_2Se_3 channel, we investigate the increase in Fermi-level based on the asymmetric density of states(DOS) that contributes to the built-in electric field. For further investigation to the built-in electric field, we also examine the hypothetical system of an illuminated α-In_2Se_3/h-BN interface. We suggest that both contributions to the built-electric fields enhance the electric field in a specific direction, resulting in an improvement of the imbalance of potentiation/depression curve.

Poster No.38

Impact of native point defects on intrinsic *n*-type conductivity of bulk InAs

Authors: Jae-Gwan Jung[1], Minwoo Jeong[1], Ho-Hyun Nahm[1], Manmhin Choi[2], Hyoin Kim[2], Sohee Jeong[2], Yong-Hyun Kim[1,3*]

Affiliations:

[1]*Department of Physics, Korea Advanced Institute of Science and Technology (KAIST), Daejeon 34141, Republic of Korea.*

[2]*Department of Energy Science, Sungkyunkwan University, Gyeonggi-do 16419, Republic of Korea.*

[3]*Graduate School of Nanoscience and Technology, KAIST, Daejeon 34141, Republic of Korea.*

**Correspondence to: yong.hyun.kim@kaist.ac.kr*

InAs, possessing a small direct band gap of 0.4 eV, exhibits high electron mobility which is ten times greater than Si. Therefore, electronic applications such as field effect transistors and infrared photodetectors are anticipated, but in order to optimize carrier dynamics it is essential to understand native point defects in InAs. However, the tiny band gap poses challenges in identifying defect bands in the electronic band structure because they easily disperse due to hybridization with neighboring host band edges, which hinders the precise analysis of the defect charge states. Here, by using the supercell and Hartree Fock method with first-principles calculations, we clarified defect energy levels and their relation with bulk band edges and demonstrated the intrinsic *n*-type nature of bulk InAs. Considering vacancy, interstitial, and antisite defects, we revealed that In-interstitial and As-antisite consistently act as stable donors across all Fermi levels within the band gap. Our results serve quantitative guiding principle for investigating the carrier dynamics of small-band-gap materials, including their surfaces.

Poster No.39

Efficiency Enhancement of Saddle Point Search Algorithms with SHERPA and machine-learned potentials

Jisu Jung[1], Hyungmin An[1], Deokgi Hong[1], and Seungwu Han[1,2,*]

[1]*Department of Materials Science and Engineering, Seoul National University, Seoul 08826, Korea.*

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

**E-mail address: wjdwltn928@snu.ac.kr*

Advanced atomistic modeling techniques offer a detailed understanding of chemical processes at the atomic level, but their application to long-term processes is often limited. Kinetic Monte Carlo (KMC) simulations can investigate such processes. They do this through the use of an event table, built using saddle point searching algorithms like ARTn. However, the efficiency of these algorithms, particularly when dealing with surface-level reactions such as oxidation and catalysis, has not been sufficiently studied.

In this study, we focus on reaction pathways of Pt (111) 2 nm × 2 nm surface with adsorbed oxygen atoms, a configuration often encountered during platinum surface oxidation. We found that the presence of low barrier reactions on the surface compromises the efficiency of conventional algorithms like ARTn. To improve efficiency, we introduce SHERPA (Saddle points Hunting based on Energy surface for Reaction Pathways) package, which integrates two key features: constrained-orthogonal relaxation within ARTn and dynamic-active volume. SHERPA demonstrated a 30% higher success ratio and reduced computational time compared to ARTn, successfully identifying all expected reactions even with constraints. Additionally, to accelerate the computation of the potential energy surface, we used Behler-Parinello type machine-learned potentials (MLPs) as surrogate models of DFT. Trained MLP displayed energy and force root-mean-square errors of 7 meV/atom and 0.22 eV/Å, respectively, on the DFT validation set consisting of various platinum oxide phases and randomly distributed oxygen atoms on platinum surface. We believe that this study enhances the efficiency of the saddle points searching algorithm. Furthermore, it paves the way for on-the-fly kMC simulations, pushing the frontier of atomistic modeling in capturing long-term chemical processes.

Poster No.40

Exploring Li-Ion Diffusion in Argyrodite Solid-State Electrolytes Using Machine-Learned Potentials

Suyeon Ju,[1] Jiho Lee,[1] Jinmu You,[1] Jisu Jung,[1] and Seungwu Han[1,2,*]

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

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

Solid-state batteries with solid Li-ion conductors have gained attention for their safety and higher energy density compared to liquid electrolyte batteries. However, these conductors exhibit low ionic conductivities at room temperatures. Argyrodite systems, such as Li_6PS_5Cl, have shown promising results with ionic conductivity exceeding 10 mS/cm at room temperature. The high conductivities in argyrodites are attributed to anion disorder, although the precise mechanisms of Li-ion diffusion remain unclear. Theoretical investigations based on density functional theory (DFT) have been informative but encounter challenges in accurately quantifying diffusivities and ionic conductivities across different disorders. Discrepancies with experimental results arise from the selection of exchange-correlation functionals and small simulation cells that do not adequately account for anion disorder. Additionally, the simulation of rare Li-ion jumps at room temperature requires timescales that extend beyond the capabilities of current DFT calculations.

In this study, we employ Behler-Parrinello type neural network potentials (NNPs) to estimate Li-ion conductivities in argyrodite Li_6PS_5Cl with varying Cl disorder at 4c sites. Leveraging the speed and accuracy of NNPs, we directly predict Li-ion conductivity at room temperature, considering S/Cl disorder and ergodicity of Li distributions. The NNPs are trained using strained bulk crystals and *ab initio* molecular dynamics (MD) data at elevated temperatures. By conducting NNP MD simulations with large supercells containing over 3,000 atoms and extended simulation times of up to 15 ns at 300 K, we minimize statistical fluctuations in conductivity. Our predicted activation energies and ionic conductivities align well with experimental data. Notably, the Li-ion conductivity peaks at 25% Cl disorder at 4c sites, and free energy analysis confirms the thermodynamic accessibility of these structures. Furthermore, we analyze diffusion mechanisms in both ordered and disordered structures, focusing on Li-ion jumps between cages. Our work demonstrates the capability of accurate and cost-effective NNPs in predicting and analyzing the properties of disordered complex solid-state electrolyte materials.

Poster No.41

First-principles study on A-site dependent metastable polar states in perovskite $AZrO_3$

Min Chul Choi[1, 2], Se Young Park [1, 2]

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

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

We investigate the structural, electronic, and ferroelectric properties of ABO_3 centrosymmetric perovskites with different atomic radii of the A-site using first-principles density functional theory. We create initial structures with octahedral rotation patterns commonly observed in bulk perovskite oxides, and systematically investigate phonon dispersion and unstable modes in each rotation pattern to search for the ferroelectric metastable structures. $CaZrO_3$, which has a relatively large rotation angle, has numerous ferroelectric metastable structures, unlike $SrZrO_3$, which has a small rotation angle and does not exhibit any ferroelectric metastable structure. The octahedron rotation is known to suppress ferroelectricity in ABO_3 perovskite oxides, but if the specific rotation patterns are maintained, the larger rotation angle is more advantageous for obtaining ferroelectricity. The ferroelectric metastable structure can be stabilized by growing perovskite in the form of a thin film on a substrate with a specific rotation pattern as a ground state. The most promising phase is R3c of $CaZrO_3$ at $P=53\mu C/cm^2$, which exhibits nonlinear polarization slopes for tensile and compressive strain.

Poster No.42

Divergence of the phonon Edelstein effect

Young-Jae Choi[1,2] and Seung-Hoon Jhi[2]

[1]*Center for Artificial Low Dimensional Electronic Systems, Institute for Basic Science (IBS), Pohang 37673, Republic of Korea*

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

The phonon heat current naturally generates phonon angular momentum (PAM), namely the phonon Edelstein effect. This effect is analogous to the spin Rashba-Edelstein effect and yet displays unique phenomena owing to the bosonic nature of phonons. Specifically, phonons exhibit a large deviation in their lifetimes in terms of eigenfrequency and temperature. In this study, we calculated the phonon Edelstein effect in wurtzite ferroelectrics (AlN and GaN) and graphene-like boron nitride (g-BN) using precise calculations of mode-specific phonon lifetimes. We identified intriguing critical behaviors in which the phonon Edelstein effect diverges under certain temperature and strain conditions. Chiral phonons with large coherence time result in asymmetric accumulation of phonon angular momentum. The keys to understanding these divergent phenomena lie in the phonon dispersion and their anharmonicity.

Keywords: chiral phonon, phonon angular momentum, thermal transport, anharmonicity

Poster No.43

Time-resolved photoemission spectroscopy simulation of black phosphorus with pseudospin

Youngchan Choi, Jiwon Jeon and J.D. Lee*

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

Black phosphorus is the material that has the optical selection rule because of pseudospin from its high anisotropic structure with two sublattices. The optical selection rule of pseudospin is crucial because it determines allowed transitions between different pseudospin states in two-dimensional materials. Here, we study the monolayer and bilayer black phosphorus with Time- and angle-resolved photoemission spectroscopy (TRPES) simulation to show its optically selective dynamics related to the pseudospin. Through comparison of the final-state based on the existing free electron approximation and the final-state obtained by analytically describing the Lippmann-Schwinger equation, the selection rule by the probe pulse in black phosphorus TRPES is confirmed. The matrix element effects by the probe pulse polarization in the monolayer and bilayer black phosphorus to observe the pseudospin of the excited electron by the pump pulse is discussed. By analyzing the pseudospin of the excited electron through our TRPES simulations, we gain a deeper understanding of the unique optical properties of black phosphorus and the implications of its pseudospin for future technological applications.

Poster No.44

Atomistic study of TaN_x-Cu Interfaces using Neural Network Interatomic Potentials

Jeong Min Choi[1], Jaehoon Kim[1], Seungwu Han[1]

[1] *Department of Materials Science and Engineering, Seoul National University, Seoul 08826, Korea*

In the field of semiconductor devices, the role of interconnect systems is of crucial importance, with Cu often serving as a key component within metal lines. When Cu comes into direct contact with dielectric materials, issues such as electromigration arise, leading to the formation of defect structures. To address this, TaN_x is introduced as a barrier material, acting as a protective layer between Cu and dielectric elements. With the pursuit of higher integration through device scaling, the stability of the interface becomes a significant concern, impacting adhesion properties and potentially compromising device reliability. These challenges become critical at the nanometer scale, where investigating interface properties with varying compositions of TaN_x experimentally becomes a formidable task. Therefore, efforts have been made to calculate the interface stability between TaN_x and Cu using density functional theory (DFT). However, due to the computational cost and the complexities associated with non-epitaxial interfaces, the atomistic simulation has been very limited.

Recently, the neural network interatomic potential (NNP) has emerged as a promising surrogate for DFT calculations. NNP enables fast calculation with accuracy comparable to the DFT for the targeted simulation when trained with suitable DFT training sets. In this work, we apply the NNP to describe the interface of the amorphous TaN_x-Cu system. Thanks to the capability of NNP to assign atomic energies to each atom, the interface energy can be conveniently calculated even for complicated interfacial structures. Based on this approach, we evaluate the stability of interfaces that are modelled in various ways such as bulk adjoining or simulated deposition. We also investigate the effects of varying TaN_x compositions on interface stability, considering that Cu exhibits a stronger bond with Ta than with N. Our analysis paves the way for systematically quantifying the stability of complicated interfaces that are commonly found in scaled-down semiconductor devices.

Poster No.45

Insights into the Durability of Platinum-Based Alloy Nanoparticle Catalysts for Fuel Cells via Kinetic Monte Carlo Simulation with Machine-Learned Potentials

Deokgi Hong[1], Jisu Jung[1], and Seungwu Han[1*]

[1] *Seoul National University*

Energy conversion through fuel cells has emerged as a promising avenue for achieving a carbon-neutral society. To facilitate wider utilization, it is imperative to reduce the cost and enhance the durability of fuel cells. The cost issue can be addressed by alloying platinum (Pt) catalyst with other metal elements. However, Pt-based alloy catalysts are susceptible to dissolution. Therefore, a comprehensive understanding of the structural factors influencing dissolution reactions at the atomistic level is crucial for designing durable Pt-based ternary alloy catalysts. Nevertheless, employing atomistic-level simulations, such as density functional theory (DFT) calculations, becomes impractical due to the spatial and temporal scales associated with catalyst dissolution reactions. Simulating nanometer-sized nanoparticles requires including thousands of atoms, and capturing dissolution reactions, which occur on a long timescale, demands substantial computational resources.

In this study, we utilize kinetic Monte Carlo (KMC) simulations with machine-learned potentials (MLPs) to investigate the dissolution of Pt-Co and Pt-Ni-Co nanoparticles. MLPs trained with DFT data offer DFT-level accuracy while reducing simulation time. KMC simulations are efficient tools for studying the kinetics of rare processes such as dissolution reactions. Firstly, an MLP is trained using DFT calculations to acquire data on the local atomic environment of alloy nanoparticles. The training process is carried out using SIMPLE-NN [1]. Subsequently, the trained MLP is employed in KMC simulations to calculate the barrier energy of dissolution and diffusion reactions of metal atoms. The dissolution rate of the nanoparticles is evaluated by analyzing the temporal evolution of the dissolution reaction. The Pt-Ni-Co nanoparticle exhibits a lower dissolution rate compared to the Pt-Co nanoparticle, thus providing evidence for the higher durability of the Pt-Ni-Co nanoparticle. Furthermore, the durability of Pt-Ni-Co nanoparticles with varying Ni and Co compositions is assessed, revealing the influence of alloying element composition on nanoparticle durability.

This study offers valuable insights into the requisite conditions for achieving durable Pt-based alloy catalysts suitable for fuel cell applications.

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Poster No.46

Understanding HF Etching of amorphous Si_3N_4 by Molecular Dynamics with Neural Network Potential

Changho Hong[1], Sangmin Oh[1], Seungwu Han[1]

[1] *Department of Materials Science and Engineering, Seoul National University, Republic of Korea.*

Dry etching is a critical process in semiconductor device fabrication, with recent advancements in high-aspect-ratio structures and 3D integrated circuits emphasizing the need for precise etching control. As these devices increase in complexity, optimizing process parameters to minimize sidewall deformations becomes crucial. Predicting the outcomes of these optimizations has been aided by macroscale modeling approaches, but these can lead to inaccuracies due to the omission of detailed chemical processes.

Molecular dynamics (MD) simulations have been used to investigate atomic processes in ion etching, providing a more detailed understanding than traditional macroscopic models. This approach has enabled the exploration of physical and chemical sputtering using classical potentials and the reactive force-field (ReaxFF). However, the range of these potentials is limited and their parametrization requires a deep understanding of chemical bonds and reactions. While density functional theory (DFT) is accurate, it is not feasible for etching simulations due to the extended time and length scales involved. Machine-learned potentials (MLPs) have shown promise in surface catalysis and physical sputtering simulations, but their application to etching reactions is still in its infancy, largely due to the complexity of predicting chemical reaction pathways.

In this study, we introduce two innovative strategies, guided MD and high-temperature MD, to sample the pathways of chemical reactions and capture the abrupt changes occurring during the etching process. We investigate the mechanism of Si_3N_4 etching by HF ions using MD simulations with a neural network potential (NNP), starting with an assessment of accuracy of the NNP. Our simulations reveal that at low angles of incidence, the surface layer is modified and the etched products result from chemical sputtering. At high angles of incidence, the surface remains unaltered, with the product originating from physical sputtering. We believe these new methods will enable MD simulations with DFT accuracy, shedding light on the mechanisms of chemical sputtering prior to laborious experiments and improving the prediction of feature profiles.

Poster No.47

Stability and equilibrium structures of unknown ternary metal oxides explored using machine-learned potentials

Seungwoo Hwang[1], Jisu Jung[1], Changho Hong[1], Wonseok Jeong[1], Sungwoo Kang[1], and *Seungwu Han[1]

[1]*Department of Materials Science and Engineering, Seoul National University, Seoul 08826, Korea*

Ternary metal oxides are extensively employed in diverse applications and have been extensively documented in experimental material databases like the Inorganic Crystal Structure Database (ICSD). However, there remains a considerable number of unexplored cation combinations in oxide forms in terms of their stability and structures. The conventional approach of discovering new ternary metal oxides through experimental methods alone is time-consuming and resource-intensive. Alternatively, theoretical databases provide hypothetical structures based on known prototypes, but they cannot identify ground states that are not represented by prototype structures. Overcoming this challenge requires the use of crystal structure prediction (CSP), which involves heuristic methods to find the lowest-energy structure for a given composition without prior knowledge. However, the effectiveness of this approach is limited due to the computational expense of density functional theory (DFT) calculations and the exhaustive search of the structure space, which is often impractical for complex equilibrium phases of ternary metal oxides.

Recently, there has been a growing interest in machine-learned potentials (MLPs) as an alternative to the DFT method. MLPs can compute energy and atomic forces much faster than DFT while achieving similar results. Our previous research has shown that MLPs trained with disordered phases have been successful as surrogate models for DFT in CSP. Building on this concept, we developed a systematic CSP program called SPINNER (Structure Prediction of Inorganic crystals using Neural Network potentials with Evolutionary and Random searches), which employs MLPs within an evolutionary algorithm. In benchmark tests using the experimental structure database, SPINNER accurately identified approximately 80% of the structures of 60 different ternary compounds with diverse crystal symmetries, and it did so 10^2 to 10^3 times faster than heuristic methods based on DFT.

In this study, we extensively utilize SPINNER to explore uncharted chemical spaces. We investigate 181 ternary metal oxide systems, encompassing most cations except

those with partially filled 3d or f shells, and determine their lowest-energy crystal structures using representative compositions derived from common oxidation states and a machine-learned recommender system. We discover 45 stable ternary oxides that do not decompose into binary or elemental phases, with the majority of them containing noble metals. Comparisons with other theoretical databases highlight the strengths and limitations of heuristic- and informatics-based material discovery. With relatively moderate computational costs, we firmly believe that heuristic-based structure searches, as exemplified in this study, present a promising approach for future material discovery endeavors.

Poster No.48

Real-space calculations on layered materials: from lattice reconstruction to electronic structure

Nicolas Leconte, Jiaqi An, Youngju Park, Srivani Javvaji, Appalakondaiah Samudrala and Jeil Jung

Department of Physics, University of Seoul, Seoul 02504, Korea.

In this poster, I illustrate our methodology to obtain the electronic properties of materials based on lattice calculations, both at the level of the lattice realxations and the tight-binding electronic structure calculations. I illustrate this approach on a variety of materials, including twisted bilayer graphene (tBG), alternated twisted multilayer graphene (tNG), t2G on hBN (t2G/hBN), graphene on hBN (GBN) and hBN-encapsulated bilayer graphene (hBN/BG/hBN), while focusing on relevant physics for each of these systems, from magic angle flat band signatures (tBG and tNG), primary and secondary gap behavior in presence of a substrate (GBN), commensuration torques (t3G and t2G/hbN) and substrate induced layer polarization of BG (hBN/BG/hBN).

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