초청연사

김건우 (중앙대학교)

김성곤 (미시시피 주립대학교)

김영국 (성균관대학교)

김용현 (한국과학기술원)

김형준 (한국과학기술원)

권용경 (건국대학교)

박노정 (울산과학기술원)

박문집 (기초과학연구원)

이병주 (한국과학기술연구원)

이승섭 (서울대학교)

이승원 (삼성전자 종합기술원)

임준원 (아주대학교)

최철호 (경북대학교)

최형준 (연세대학교)

홍순철 (울산대학교)

자문위원회

김용현 (한국과학기술원), 김용훈 (한국과학기술원),
권영균 (경희대학교), 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)

담 당 자 : 김혜미 (고등과학원)
전 화 : 02-958-2638
이 메 일 : hmkim@kias.re.kr
홈페이지 : http://events.kias.re.kr/h/ESCW2022

제18회 고등과학원

전자구조 계산학회

일시 : 2022년 7월 7일 (목) – 7월 8일 (금)

장소 : 고등과학원 1호관 대강당 및 온라인

KIAS 고등과학원 KOREA INSTITUTE FOR ADVANCED STUDY

초청연사

김건우 (중앙대학교)

김성곤 (미시시피 주립대학교)

김영국 (성균관대학교)

김용현 (한국과학기술원)

김형준 (한국과학기술원)

권용경 (건국대학교)

박노정 (울산과학기술원)

박문집 (기초과학연구원)

이병주 (한국과학기술연구원)

이승섭 (서울대학교)

이승원 (삼성전자 종합기술원)

임준원 (아주대학교)

최철호 (경북대학교)

최형준 (연세대학교)

홍순철 (울산대학교)

자문위원회

김용현 (한국과학기술원), 김용훈 (한국과학기술원), 권영균 (경희대학교), 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)

Contact

김혜미 (KIAS) 전화: 02-958-2638 이메일: hmkim@kias.re.kr

제18회 고등과학원 전자구조계산학회 프로그램

7월 7일(목)

8:30 – 9:20 등록

9:20 – 9:30 개회 인사

Session 1
Novel Properties of Solids

좌장
권영균 (경희대학교)

09:30~10:10
홍순철 (울산대 물리학과)
Design of Future Permanent Magnets

10:10~10:50
김용현 (한국과학기술원 물리학과)
Triboelectricity (마찰전기): Do we know it?

10:50 – 11:10 Coffee Break

Session 2
Surfaces and Interfaces

좌장
강준구 (대구경북과학기술원)

11:10~11:50
김성곤 (미시시피 주립대 물리학과)
Flat-surface-assisted and self-regulated oxidation resistance of Cu(111)

11:50~12:30
김형준 (한국과학기술원 화학과)
Electronic and Liquid Structures of the Electrified Interfaces: Seeing Both Sides at Once

12:30 – 14:00 Lunch Break & Poster Session

Session 3
Time-Dependent Phenomena

좌장
이재동 (대구경북과학기술원)

14:00~14:40
박노정 (울산과학기술원 물리학과)
Orbital angular momentum dynamics in the context of circular photogalvanics and current-induced magnetization: first-principles calculations of real-time time-dependent density functionals.

14:40~15:20
김건우 (중앙대 물리학과)
Floquet simulators for topological surface states in isolation

15:20 – 16:00 Coffee Break

Session 4
Layered Materials

좌장
지승훈 (포항공과대학교)

16:00~16:40
권용경 (건국대 물리학과)
Nature of interlayer binding in a blue phosphorene bilayer and graphene-supported Pt layers: Quantum Monte Carlo study

16:40~17:20
김영국 (성균관대 물리학과)
Monolayer vanadium-based kagome metals AV3Sb5 (A=K, Rb, and Cs)

Poster Session

좌장 김세중 (UST)

17:20~19:00 포스터 발표

7월 8일(금)

8:30 – 9:20 등록

Session 5
Correlated Phenomena and Methods Developments

좌장
이현용 (고려대학교)

09:30~10:10
이승섭 (서울대 물리천문학부)
Multipoint Correlation Functions: Spectral Representation and Numerical Evaluation

10:10~10:50
최철호 (경북대 화학과)
MRSF-TDDFT: Balancing Dynamic and Nondynamic Electron Correlations

10:50~11:30
임준원 (아주대 물리학과)
Bulk-interface correspondence of flat band systems

11:30~13:00 Lunch Break & Poster Session

Session 6
Twisted Layered Systems

좌장
방준혁 (충북대학교)

13:00~13:40
최형준 (연세대 물리학과)
Electronic and phononic structures of twisted layers of two-dimensional materials

13:40~14:20
박문집 (기초과학연구원)
Twisted Bilayer Magnetism

14:20~14:40 Coffee Break

Session 7
Machine Learning Applications

좌장
박지상 (경북대학교)

14:40~15:20
이병주 (한국과학기술연구원)
Machine-learning guided reactivity prediction in energy storage devices

15:20~16:00
이승원 (삼성전자 종합기술원)
Single Large Job @ 기술원 슈퍼컴

Session 8
시상 및 폐회

좌장 손영우 (고등과학원)

우수 포스터 시상식 및 폐회

Talk Abstracts

Talk No.1

Design of Future Permanent Magnets

D. Odkhuu[1], T. Ochirkhuyag[1], D. Tuvshin[1], T. Thuy Hoang[2], T. Tsevelmaa[2] and S. C. Hong[2]

[1]*Department of Physics, Incheon National University, Incheon 22012, South Korea*
[2]*Department of Physics and EHSRC, University of Ulsan, Ulsan 44610, South Korea*

Keywords: Permanent magnet, first-principles calculation, $ThMn_{12}$, $Fe_{16}N_2$, FeNi, MnBi, Heusler compounds

Permanent magnets are important components in electric motors, wind turbines, actuators, and data storage memory devices. High-performance permanent magnets are mainly characterized by their large saturation magnetization M_S, high uniaxial magnetocrystalline anisotropy (MCA) K_u, and high Curie temperature T_C in terms of intrinsic magnetic properties. Moreover, the structural and thermodynamic stabilities are also decisive factors to make permanent magnets practical. Although permanent magnets have been researched intensively for longer than one hundred years, practically only two magnets of Nd-magnet and ferrite magnet dominate the market for different reasons.

$Nd_2Fe_{14}B$ provides highest-performing permanent magnetic properties at present. This magnet exhibits a high $(BH)_{max}$ of about 45 MGOe, K_u of 4.5 MJ m^{-3}, and $\mu_0 M_S$ of 1.57 T at room temperature. However, practical usage of $Nd_2Fe_{14}B$ magnet is quite limited due to extremely fast degradation of $(BH)_{max}$ above room temperature and high price. On other hand, ferrites have the advantage of being very cheap despite the low performance of about 5 MGOe.

Nerveless, industry including automobile requires variety of permanent magnets to apply to diverse functionalities. Some alloys such as $Fe_{16}N_2$, FeNi, MnBi, $SmFe_{12}$ are supposed to be the best candidate materials for new permanent magnets. But permanent magnets based on them have not been realized mainly due to structure instability as well as not enough coercivity. In this talk, we propose two kinds of new materials for permanent magnets. The first one may show higher performance than the champion Nd-Fe-B magnet. The other one is rare-earth or heavy metal free materials including Fe-based, Mn-based, and Heusler compounds which may show medium performance and price competitiveness simultaneously. We will discuss the way to improve physical properties of the alloys, focusing on simultaneous optimization of structure stability, magnetic hardness, Curie temperature, and saturation magnetization by first principles calculation, atomic simulation, and Monte Carlo simulation, .

Supported by Future Materials Discovery Program (2016M3D1A1027831) and Development of Magnetic Materials for IE4 Class Motor (Grant No. 20192010106850).

Talk No.2

Triboelectricity (마찰전기): Do we know it?

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*

Electricity has a history of more than 2600 years to the ages of Thales and Plato in ancient Greece, and triboelectricity is the first notion that human recognized about electricity. Indeed, the origin of the word "electricity" comes from an amber that easily causes triboelectricity after being rubbed. The friction-driven static electrification is familiar and fundamental in daily life, industry, and technology, but its basics have long been unknown. The only way to characterize triboelectricity is to display triboelectric materials in a series called the triboelectric series. Surprisingly, no triboelectric series is 100% consented because it seriously lacks reproducibility. The triboelectric series is no longer taught in the second grade of middle schools since 2015 in Korea. It is very mysterious, in spite of the state-of-the-art quantum mechanics and condensed matter physics, why we do not know which material will be charged positively or negatively when two materials are rubbed. We jumped into this problem in 2014 when we realized that the thermoelectricity at the interface play an important role in scanning thermoelectric microscopy [1,2]. After seven years of struggle, we finally arrived at a satisfactory explanation [3] about triboelectricity and triboelectric series using heat transfer solutions and first-principle density-functional theory calculations. Here, I will introduce how we formulate a theory of triboelectricity based on thermoelectric physics between two rubbing materials, which leads us to profound understandings and new discoveries on the fundamental phenomenon.

[1] E.-S. Lee, S. Cho, H.-K. Lyeo, and Y.-H. Kim, Seebeck effect at the atomic scale, Phys. Rev. Lett. **112**, 136601 (2014).
[2] S. Cho, S. D. Kang, W. Kim, E.-S. Lee, S.-J. Woo, K.-J. Kong, I. Kim, H.-D. Kim, T. Zhang, J. A. Stroscio, Y.-H. Kim, and H.-K. Lyeo, Thermoelectric imaging of structural disorder in epitaxial graphene, Nat. Mater. **12**, 913 (2013).
[3] E.-C. Shin, J.-H. Ko, H.-K. Lyeo, and Y.-H. Kim, Derivation of a governing rule in triboelectric charging and series from thermoelectricity, https://arxiv.org/abs/2101.12485, Phys. Rev. Research, *accepted* (2022).

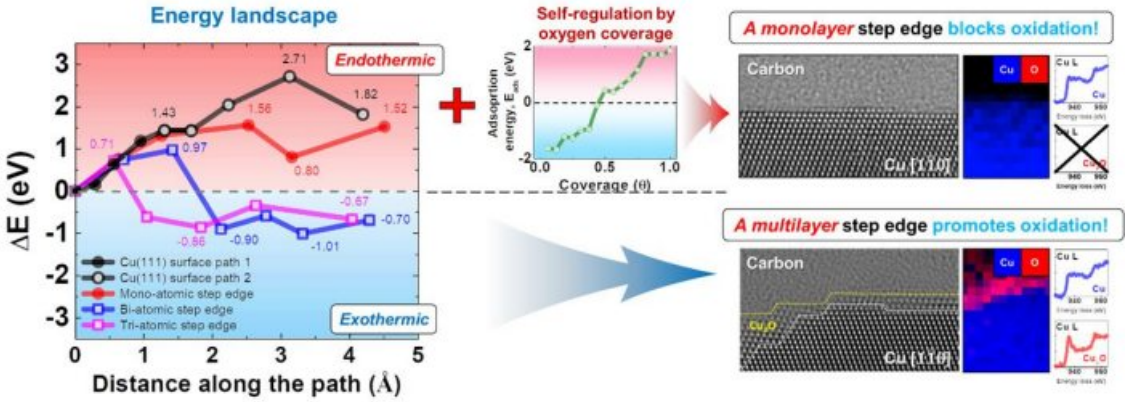
Talk No. 3

Flat-surface-assisted and self-regulated oxidation resistance of Cu(111)

Seong-Gon Kim

Mississippi State University

Oxidation can deteriorate the properties of copper that are critical for its use, particularly in the semiconductor industry and electro-optics applications. This has prompted numerous studies exploring copper oxidation and possible passivation strategies. In situ observations have, for example, shown that oxidation involves stepped surfaces: Cu_2O growth occurs on flat surfaces because of Cu adatoms detaching from steps and diffusing across terraces. But even though this mechanism explains why single-crystalline copper is more resistant to oxidation than polycrystalline copper, the fact that a flat copper surfaces can be free of oxidation has not been explored further. Here, we report the fabrication of copper thin films that are semi-permanently oxidation resistant because they consist of flat surfaces with only occasional mono-atomic steps. Our first principles calculations show that mono-atomic step edges are as impervious to oxygen as flat surfaces, and that surface adsorption of O atoms is suppressed once an oxygen fcc surface site coverage of 50% has been reached. These combined effects explain the exceptional oxidation resistance of ultraflat Cu surfaces.



We also introduce colossal oxidation resistance (COR), which not only provides permanent protection against room-temperature oxidation of oxidizable metals but also is robust even against high-temperature oxidation. Our first-principles calculations show that the COR originates from complete blocking of the oxygen entry path into the metal by oxygen atoms themselves and the reconstitution of the metal surface forms an atomically thin barrier impenetrable to oxygen at high temperature. This reliable approach to creating COR will open new directions for research fields and industries hesitating to use oxidizable metals.

Talk No.4

Electronic and Liquid Structures of the Electrified Interfaces: Seeing Both Sides at Once

Hyungjun Kim[1]

[1]*Department of Chemistry, KAIST, Daejeon*

The solid-liquid interface is ubiquitous in a variety of scientifically and technologically important systems such as heterogeneous photo/electro-catalysts, corrosion, fluid transport, etc. Despite recent research efforts to develop atom- and electron-level understanding of the solid-liquid interface, a reliable computational methodology is yet to be at hand. The difficulty stems from the intrinsic heterogeneity of the interface. On one hand, quantum-mechanics (QM)-based theory like a density functional theory (DFT) can provide a wealth of understanding about the electronic structure and material properties of the solid but limited information about the liquid structure. On the other hand, classical-mechanics-based molecular dynamics (MD) simulation can provide a full statistical picture of the liquid structure as well as its transport properties, but no electronic information. Hence, we develop a first-principles-based multiscale simulation method to properly see both sides of the interface at an atom resolution. Using our new simulation method, named a DFT in classical explicit solvents (DFT-CES), we recently elucidate the full atomic details of the electric double layer (EDL) structure formed at the single crystalline electrode in the dilute electrolytes, which will be introduced in the talk. We directly compare the computational results with the Poisson-Boltzmann analytic results (i.e., Gouy-Chapman model) and experiments. Of prime interest here is the finding of a microscopic origin in the well-known prototypical behavior of the EDL capacitance, which suggests a possible involvement of a phase transition. I further introduce the development direction of the DFT-CES for handling quasi-particle energies and exciton binding behavior of the materials immersed in the water, which will provide a useful computational tool for investigating photo/electro-catalytic systems.

Talk No.5

Intrinsic responses of materials in the context of circular photogalvanics and second harmonics: full first-principles calculations of statics and dynamics of angular momentum and Berry curvature family

Noejung Park

Department of Physics, Ulsan National Institute of Science and Technology, Ulsan, 689-798 Korea

We have developed the full ***ab initio*** density functional, static and time-dependent computation method and simulation package for orbital angular momentum (OAM) and Berry curvature family of Bloch band states wavepackets $\psi(\vec{r},t) = \sum_{m,\vec{k}} W_m(\vec{k},t) u_{m,\vec{k}}(\vec{r}) e^{i\vec{k}\cdot\vec{r}}$. We analyze the intrinsic response character, which is in some cases delicately associated with the topological natures of the band structures, in terms of circular photogalvanic effect (CPGE) and second harmonic responses. We propose that nonlinear optical responses can be utilized as a probe for diverse phase profiles that comes out on breaking the (time-reversal and/or inversion) symmetries, or on the formation of magnetic order or charge density waves.

Talk No.6

Title Floquet simulators for topological surface states in isolation

Kun Woo Kim[1]

[1]*Chung-Ang University, 84 Heukseok-ro, Dongjak-gu, Seoul, 06974, Korea*

We propose dynamical protocols allowing for the engineered realization of topological surface states in isolation. Our approach builds on the concept of synthetic dimensions generated by driving systems with incommensurate frequencies. As a concrete example, we consider 3d topological surface states of a 4d quantum Hall insulator via a (1+2)-dimensional protocol. We present first principle analytical calculations demonstrating that no supporting 4d bulk phase is required for a 3d topological surface phase. We back the analytical approach by numerical simulations and present a detailed blueprint for the realization of the synthetic surface phase with existing quantum linear optical network device technology. We then discuss generalizations, including a proposal for a quantum simulator of the (1+1)-dimensional surface of the common 3d topological insulator.

Talk No. 7

Nature of interlayer binding in a blue phosphorene bilayer and graphene-supported Pt layers: Quantum Monte Carlo study

Yongkyung Kwon

Dept. of Physics, Konkuk University, Seoul 05029, Korea

In this talk, I will present the results of our recent quantum Monte Carlo (QMC) calculations for some 2D materials, focusing on their interlayer binding. Our study reveals that an A_1B_{-1}-stacked bilayer blue phosphorene undergoes a semiconductor−metal transition as the interlayer distance decreases [1]. While the most stable bilayer structure is a semiconducting one with two monolayers coupled through a weak van der Waals interaction, the metallic bilayer at a shorter interlayer distance is found to be only metastable. Analysis of charge density distributions shows that the metastable metallic phase is induced by interlayer chemical bonding and intralayer charge redistributions. Our QMC calculations also confirm the formation of energetically stable Pt layers on graphene, among which a vertically buckled (111) packing structure adhered to graphene through van der Waals interactions is the most stable one. Especially, this buckled (111) structure is found to be more stable than a (100) packing structure registered at the bridge sites of graphene, which can be understood by a significant lattice mismatch ($>$ 10 %) between a pristine graphene and a free-standing (100) Pt layer. We find another buckled-(111) structure for a Pt bilayer whose formation energy is higher only by $\sim$ 0.1 eV per Pt atom than the lowest-energy (111) structure. This buckled-(111) Pt bilayer is found to be chemisorbed on graphene and is projected onto the graphene surface to form a rectangular structure, which is consistent with recently reported TEM images of Pt layers grown epitaxially on graphene [2].

[1] J. Ahn. I. Hong, G. Lee, H. Shin, A. Benali, and Y. Kwon, J. Phys. Chem. Lett. **12**, 10981 (2021).

[2] J. I. Choi *et al*., Adv. Funct. Mater. **29**, 1902274 (2019); A. W. Robertson *et al*., ACS Nano **13**, 12162 (2019).

Talk No.8

Monolayer vanadium-based kagome metals AV_3Sb_5 (*A*=K, Rb, and Cs)

Youngkuk Kim[1]

[1]*Department of Physics, Sungkyunkwan University, Suwon, Korea*

We present our first-principles and mean-field study of monolayer vanadium-based kagome metals AV_3Sb_5 (A = K, Rb, and Cs). Recently, layered kagome AV_3Sb_5 has attracted much attention as a fertile platform for strong correlation and topology. We show that AV_3Sb_5 can exist in a monolayer form in two dimensions, exhibiting intrinsically different electronic properties than the original layered systems. Notably, dimensionality significantly affects the van Hove singularities in their numbers and types. Various correlated states consequently occur when including the Hubbard-type electron-electron interactions. We compute electronic phase diagrams, which comprise diverse orders, including doublets of charge density waves and s- and d-wave superconductivity. Our finding suggests the advent of a novel platform for exploring exotic correlated phases in two dimensions.

Talk No.9

Multipoint Correlation Functions: Spectral Representation and Numerical Evaluation

Seung-Sup Lee[1]

[1]*Department of Physics and Astronomy, Seoul National University, Seoul 08826, Korea*

Many observables in the experiments of condensed matter and ultracold atoms, such as the conductivity and inelastic scattering spectra, are theoretically described as multipoint correlation functions. However, the analytic structure of multipoint functions has been elusive, and their non-perturbative, accurate computations have been intractable. Here I will talk about our recent two papers that provide a breakthrough in solving these problems. We derived the spectral representations of general multipoint functions, which reveal their structure with great clarity [1]. And we developed a numerical renormalization group (NRG) method for evaluating the spectral representations for local multipoint functions, which can treat temperatures and frequencies—imaginary or real—of all magnitudes, from large to arbitrarily small ones [2]. I will present the numerical results of four-point vertex functions and resonant inelastic x-ray scattering (RIXS) spectra of quantum impurity systems.

[1] F. B. Kugler*, S.-S. B. Lee*, and J. von Delft, Phys. Rev. X **11**, 041006 (2021).
*: These authors contributed equally to this work.
[2] S.-S. B. Lee, F. B. Kugler, and J. von Delft, Phys. Rev. X **11**, 041007 (2021).

Talk No.10

MRSF-TDDFT: Balancing Dynamic and Nondynamic Electron Correlations

Cheol Ho Choi

Department of Chemistry, Kyungpook National University, Daegu, South Korea, E-mail: cchoi@knu.ac.kr

A new quantum theory, MRSF-TDDFT (Mixed-Reference Spin-Flip Time-Dependent Density Functional Theory) has been developed[*] for both ground and excited electronic states within the context of the conceptual and practical simplicity of the linear response theory. After exhaustive investigations, it is found that the MRSF-TDDFT not only overcomes the limitations of current DFT, TDDFT, SF-TDDFT and CASSCF, but also exhibits quantitative accuracy as good as high level quantum theories in some cases, providing perhaps a breakthrough in the study of various difficult strongly correlated situations including NAMD (Nonadiabatic Molecular Dynamics).

Here, we present some of our recent results on excited state nonadiabatic dynamics, conical intersection, open shell singlet system, band structure by quasi-particle, nonadiabatic coupling, spin-orbit coupling, X-ray absorption/ionization applications. Finally, we show that our multi-Fock or mixed-reference approach is a new route of introducing various types of electron correlations effectively and economically.

[*] (a) Lee, S., Filatov, M., Lee, S., & Choi, C. H. (**2018**). Eliminating spin-contamination of spin-flip time dependent density functional theory within linear response formalism by the use of zeroth-order mixed-reference (MR) reduced density matrix. *The Journal of Chemical Physics*, 149(10), 104101. (b) Lee, S., Kim, E., Nakata, H., Lee, S. & Choi, C. H. (**2019**). Efficient implementations of analytic energy gradient for mixed-reference spin-flip time-dependent density functional theory (MRSF-TDDFT), *The Journal of Chemical Physics*, 150(18), 184111.

Talk No.11

Bulk-interface correspondence of flat band systems

Jun Won Rhim

Department of Physics, Ajou University, Suwon 16499, Republic of Korea

Triggered by the discovery of flat bands in twisted bilayer graphene systems, novel many-body and geometric physics of flat band systems have attracted great attention. Notably, it was recently found that quantum geometric quantities, such as quantum distance and cross-gap Berry connection, play a crucial role in determining the Landau level structures of flat bands. In the present work, we show that the maximum value of the quantum distance between Bloch wavefunctions near a singular point of a flat band is reflected in the band structure of the interface modes formed at an interface between two regions with different potentials or the maximum quantum distances. This new kind of bulk-interface correspondence offers us a way of measuring the quantum distance of the bulk by detecting the interface band dispersion.

Talk No.12

Electronic and phononic structures of twisted layers of two-dimensional materials

Hyoung Joon Choi

Department of Physics, Yonsei University, Seoul, Korea

Twisted layers of two-dimensional materials such as graphene, black phosphorus, and transition-metal dichalcogenides have emerged as a new platform of novel electronic structures. Since they have large moiré supercells typically, it becomes a challenge to perform density functional theory (DFT) calculations of their electronic structures. Here, we present an efficient method for electronic structure calculations of twisted graphene layers based on DFT [1], and discuss the doping dependence of electronic structures and spin-valley polarization [1]. We also present applications of a simplified atomistic approach to atomic and phononic structures of twisted graphene layers [2-4] and twisted transition-metal dichalcogenide layers [5], and discuss their atomic and phononic structures [2-5]. In addition, we discuss peculiar electronic structures of twisted black phosphorus layers [6]. This work was supported by NRF of Korea (Grant No. 2020R1A2C3013673) and KISTI supercomputing center (Project No. KSC-2021-CRE-0384).

[1] Yosep Cho, Young Woo Choi, and Hyoung Joon Choi, in preparation.
[2] Young Woo Choi and Hyoung Joon Choi, Phys. Rev. B 98, 241412 (2018).
[3] Young Woo Choi and Hyoung Joon Choi, Phys. Rev. B 100, 201402 (2019).
[4] Young Woo Choi and Hyoung Joon Choi, Phys. Rev. Lett. 127, 167001 (2021).
[5] Han-gyu Kim, Young Woo Choi, and Hyoung Joon Choi, in preparation
[6] Taesik Nam, Han-gyu Kim, and Hyoung Joon Choi, in preparation

Talk No.13

Twisted Bilayer Magnetism

Moon Jip Park[1]

[1]*Center of Theoretical Physics of Complex Systems, Institute for Basic Science (IBS) Daejeon 34126, Republic of Korea*

We develop a concrete theory of twisted bilayer magnetism. Starting from the first-principles calculations of two-dimensional honeycomb magnet CrI_3, we construct the generic spin models that represent a broad class of twisted bilayer magnetic systems. Using the Monte-Carlo method, we discover a variety of non-collinear magnetic order that has been overlooked in the previous theoretical and experimental studies. As a function of the twist angle, the collinear magnetic order undergoes the phase transitions to the non-collinear order and the magnetic domain wall phase. Within the domain wall phase, the magnetic skyrmion phase, caused by the non-trivial spatially varying interlayer exchange coupling, is additionally identified even in the absence of the Dzyaloshinskii–Moriya interaction. In addition, we describe the critical phenomena of the phase transitions of the magnetic phases by constructing the field theoretical model of the moire magnet. Our continuum model explains the nature of the phase transitions observed from the numerical simulations. Finally, we classify the topological properties of the magnon excitations, characterized by different mass gaps with the distinct physical origins of the mass terms. In the collinear magnetic order, the higher-order topological magnonic insulator phase occurs, and it serves as a unique example of the higher-order topological phase in magnonic system, since it does not require any non-collinear order or asymmetric interactions. In the noncollinear phases, the magnons of the noncollinear domain wall harbor one-dimensional topological edge mode, which is confined to the domain walls. As the domain walls form a network, the confined edge mode extends to form a network model of the topological magnons.

Talk No.14

Machine-learning guided reactivity prediction in energy storage devices

Byungju Lee[1]

[1]*KIST 5, Hwarang-ro 14-gil Seongbuk-gu Seoul, 02792, Korea*

Stability and compatibility between components are essential parameters which should be screened in the selection of materials in most applications. In configuring energy/environmental devices, e.g. batteries or solar cells, not only the functionality in the application, but also a proper combination of materials which do not lead to side reactions is critical in guaranteeing their reliable performance. While the universal theory that can generally predict the reactivity between materials is long awaited and has been the subject of studies with a long history, traditional ways proposed to date have been mostly rely on simple electronic properties of materials, e.g. electronegativity, ionization energy, electron affinity and hardness/softness, and the prediction were applicable to only a small group of materials. Moreover, prediction has often been far from accurate and has failed to offer general implications; thus it was practically inadequate as a selection criterion in high-throughput materials screening, i.e. data-driven material discovery. In this talk, we propose a new model for predicting the general reactivity and chemical compatibility among a large number of organic materials, realized by a machine-learning approach. We believe that the machine-learning model introduced in this talk will not only help accelerate the screening of materials for electrochemical systems that contain various chemical interfaces but also provide general insights into the relationship between materials properties and the reactivity between them.

Talk No.15

Single Large Job @ 기술원 슈퍼컴

이승원[1]

[1]*SAIT,130 Samsung-ro, Yeongtong-gu, Suwon-si, Gyeonggi-do, 16678 Korea*

기술원이 보유한 슈퍼컴 현황과 이를 통해 이룩한 21 년 주요 성과들과 Single Large Job 을 활용하는 과제들을 살펴본다. 또한, Single Large Job 을 가속할 수 있는 PIM(Processing-in-Memory)기법들에 대해 알아본다.

Poster Abstracts

제18회 고등과학원 전자구조계산 학회

Poster Session

Name	Poster	Board
권정안	1-POS	Board 1
김도훈	2-POS	Board 2
김민재-KIAS	3-POS	Board 3
김민재-POSTECH	4-POS	Board 4
김범섭	5-POS	Board 5
김성환	6-POS	Board 6
김영철	7-POS	Board 7
김인서	8-POS	Board 8
김지수	9-POS	Board 9
김태형	10-POS	Board 10
Li, Fengping	11-POS	Board 11
문창연	12-POS	Board 12
박민희	13-POS	Board 13
박선호	14-POS	Board 14
박성진	15-POS	Board 15
박소희	16-POS	Board 16
박슬용	17-POS	Board 17
박효섭	18-POS	Board 18
배기민	19-POS	Board 19
백승일	20-POS	Board 20
송유빈1	21-POS	Board 21
송유빈2	22-POS	Board 22
신동윤	23-POS	Board 23
신승재	24-POS	Board 24
신용진	25-POS	Board 25
신의철	26-POS	Board 26

Name	Poster	Board
심도은	27-POS	Board 27
An, Jiaqi	28-POS	Board 28
Yananose, Kunihiro	29-POS	Board 29
여강모	30-POS	Board 30
여현우	31-POS	Board 31
오상민	32-POS	Board 32
우재헌	33-POS	Board 33
유승우	34-POS	Board 34
이동현	35-POS	Board 35
이룡규	36-POS	Board 36
이벽송	37-POS	Board 37
이세호	38-POS	Board 38
이영준	39-POS	Board 39
이원규	40-POS	Board 40
이진수	41-POS	Board 41
이철완	42-POS	Board 42
이형우	43-POS	Board 43
Jharapla, Prathap Kumar	44-POS	Board 44
전지원	45-POS	Board 45
정다믈	46-POS	Board 46
정준	47-POS	Board 47
조운형	48-POS	Board 48
주예린	49-POS	Board 49
최민철	50-POS	Board 50
최영재	51-POS	Board 51
Tran, Van Quang	52-POS	Board 52
홍덕기	53-POS	Board 53
황재영	54-POS	Board 54

Poster No.1

밀도범함수이론과 클러스터 전개법 기반의 기계학습을 이용한 연료전지 환원전극 촉매 개발

권정안, 임동희*

충북대학교 환경공학과 환경계산과학연구실

합금 촉매 연구에서 합금의 벌크(bulk) 구조 안정성은 매우 중요하지만, 다전자 시스템에서 다양한 합금 조성비에 대한 원자 수준의 촉매 벌크 구조를 광범위하게 스크리닝 하기에는 컴퓨터 자원과 계산 소요시간의 한계가 존재한다. 본 연구는 밀도범함수이론(density functional theory, DFT) 계산을 기반으로 클러스터 전개법이 적용된 기계학습 프로그램인 'The Alloy-Theoretic Automated Toolkit (ATAT)'을 개선하고 분말 x-선 회절패턴예측 프로그램을 활용하여 촉매 표면 정보를 구축하여, 연료전지 산소환원반응(oxygen reduction reaction, ORR) 효율을 평가할 수 있는 지표(descriptor) 로써 신속하게 촉매 반응 효율을 평가하는 방법을 제시하였다. 또한, 이를 통하여 다양한 합금 조성비에 대하여 백금기반의 연료전지 환원전극 합금 촉매를 개발하였다.

우선, ATAT의 개선은 DFT 에너지 계산과정에서 magnetic moment 설정 값이 초기화 되는 문제와 계산결과 파일로부터 DFT 에너지 값을 추출하는 과정에서의 오류를 수정하였으며, 클러스터 전개법의 진행과정을 모니터링 할 수 없는 문제를 보완하였다.

또한, 백금 기반의 연료전지 환원전극 합금 촉매(Pt-skinned $Pt_{1-x}M_x$, M = Ni, Co, Mn, Ir) 개발에 있어서는 Shin et al. (2021)[1]의 선행연구를 통하여 ORR의 descriptor로 개발된 산소흡착에너지를 descriptor로 활용하였으며, 본 연구에서 도출된 다양한 합금 조성비에 대한 촉매 구조의 ORR 활성과 Shin et al. (2021)[1]의 연구결과와 비교 분석하였다. 분석결과 Shin et al. (2022)[1]에서 가장 높은 활성을 보인 $L1_0$-type Pt-skinned $Pt_{0.5}Ni_{0.5}$와 유사한 활성을 갖는 Pt-skinned $Pt_{0.583}Co_{0.417}$ 구조를 도출하였으며, 이외에도, Pt-skinned $Pt_{0.625}Ni_{0.375}$, Pt-skinned $Pt_{0.6}Mn_{0.4}$ 구조를 산소환원반응 고효율 촉매로 제시할 수 있었다. 본 연구에서 제안된 방법은 계산화학적 합금 촉매 개발 연구에서 다양한 합금 조성비에 대한 연구가 가능하게 할 것으로 판단된다.

Reference

1) Shin, D. Y., Shin, Y.-J., Kim, M.-S., Kwon, J. A., & Lim, D.-H. (2021). *Applied Surface Science, 565*, 150518.

Poster No.2

Magnetic force linear response theory for relativistic exchange interactions

Do Hoon Kiem[1], Hongkee Yoon[1] and Myung Joon Han[1]

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

Relativistic exchange interactions like anisotropic Heisenberg interactions as well as Dzyaloshinskii-Moriya (DM) or Kitaev interactions are important ingredients for establishing of magnetic phenomena such skyrmion or spin excitations. Magnetic force theorem is a useful first-principles approach to calculate Heisenberg interactions. However, it is not straightforward to obtain relativistic interactions due to spin-orbit couplings. In this presentation, we demonstrate the expansion of our code 'Jx' based on the magnetic force theorem for non-collinear spins (NC-MFT) with spin-orbit couplings. To check the reliability and applicability of NC-MFT, we apply our method on representative bulk materials CoPt, FePt, and B20 compounds as well as two-dimensional monolayer of Janus vanadium dichalcogenides within the fully relativistic density functional theory calculation. Our calculation results show the significant DM interaction in bulk and two-dimensional systems.

Poster No.3

DFT+U+V as an efficient method for GW

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

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

We show that the density functional theory with corrections from extended Hubbard interactions, DFT+U+V, is an efficient and accurate method for the computation of materials properties, can be regarded as an approximation of the GW method. We prove that the extended Hubbard interactions can map onto the local and nonlocal static self-energy of the GW approximation. This mapping suggests that the DFT+U+V, which is a parameter-free, self-consistent pseudohybrid functional method of with an appropriate implementation of the spatial variation of screenings, is a proper method for descriptions of physical properties of materials. We show that the DFT+U+V method is accurate in descriptions of energy band gap, effective mass, work function, absorption spectra, and renormalized optical phonon frequency for bulk silicon, monolayer black phosphorus, and NiO, relying on the precise description of the dielectric screenings of materials.

Poster No.4

Anharmonicity, vacancy disorder, and the lattice thermal conductivity of GeTe

Minjae Ghim[1], Seung-Hoon Jhi[1]

[1]*Department of Physics, Pohang University of Science and Technology, Pohang, 37673, Republic of Korea*

Anharmonic effect on the lattice thermal conductivity has been thoroughly investigated non-perturbatively based on molecular dynamics. However, the vacancy disorder has been treated perturbatively mostly at an extreme case of the phonon-isotope scattering. This simplification ignores the realistic features such as the non-bonding character and the random distribution of vacancies. In this study, we calculate the lattice thermal conductivity of GeTe by considering the anharmonicity and the vacancy disorder on the same footing using the machine-learned potential molecular dynamics. The random distribution of the vacancies is emulated adopting the special quasi-random structures. We find that Ge vacancy of about 9%, a typical concentration, gives a comparable effect on the lattice thermal conductivity to that by the anharmonic effect. We produce the unfolded phonon dispersion and analyze the scattering of each phonon mode by vacancies.

Poster No.5

Giant bulk photovoltaic effect driven by the wall-to-wall charge shift in WS2 nanotubes

Bumseop Kim[1], Noejung Park[1*], Jeongwoo Kim[2*]

1Department of Physics, Ulsan National Institute of Science and Technology, Ulsan, 689-798 Korea
2Department of Physics, Incheon National University, Incheon, 406-772 Korea

The intrinsic light–matter characteristics of transition-metal dichalcogenides have not only been of great scientific interest but have also provided novel opportunities for the development of advanced optoelectronic devices [1, 2]. Among the family of transition-metal dichalcogenide structures, the one-dimensional nanotube is particularly attractive because it produces a spontaneous photocurrent that is prohibited in its higher-dimensional counterparts. Here, we show that WS2 nanotubes exhibit a giant shift current near the infrared region, amounting to four times the previously reported values in the higher frequency range [3]. The wall-to-wall charge shift constitutes a key advantage of the one-dimensional nanotube geometry, and we consider a Janus-type heteroatomic configuration that can maximize this interwall effect. To assess the nonlinear effect of a strong field and the nonadiabatic effect of atomic motion, we carried out direct real-time integration of the photoinduced current using time-dependent density functional theory. Our findings provide a solid basis for a complete quantum mechanical understanding of the unique light–matter interaction hidden in the geometric characteristics of the reduced dimension.

[1] Mak, K. F., Lee, C., Hone, J., Shan, J. & Heinz, T. F. Atomically thin MoS2: a new direct-gap semiconductor. Phys. Rev. Lett. 105, 136805 (2010).
[2] Lopez-Sanchez, O., Lembke, D., Kayci, M., Radenovic, A. & Kis, A. Ultrasensitive photodetectors based on monolayer MoS2. Nat. Nanotechnol. 8, 497-501 (2013).
[3] Kim, B., Park, N., Kim, J., Giant bulk photovoltaic effect driven by the wall-to-wall charge shift in WS2 nanotubes. *Nat. Commun. accepted*

Poster No.6

Acceleration of Iterative diagonalization algorithm by Applying dynamic floating-point arithmetic

Seonghwan Kim

Department of Chemistry, KAIST, 291 Daehak-ro, Yuseong-gu, Daejeon 34141, South Korea

The Hamiltonian diagonalization process is one of the time-consuming processes in quantum mechanical calculations, and accelerating of the process does matter. Using single-precision for floating-point arithmetic is 2x faster on CPUs and 2x to 64x faster on GPUs, depending on the machine, than using double-precision. However, the use of single-precision in the entire computational process is limited by its high precision error compared to the required accuracy. We propose a method to dynamically use different precisions in a diagonalization algorithm. In our method, single- and double-precision are used in the preceding steps with large residuals and the subsequent steps, respectively, so both the same accuracy as double-precision and improved speed can be obtained. We confirmed the acceleration by our method for finite-difference Hamiltonian matrices in density functional theory and various randomly generated sparse symmetric matrices.

Poster No.7

Ab-initio thermodynamics study for phase separation of $Ce_{0.75}Zr_{0.25}O_2$ solid solution

Hyun-Kyu Kim[a], Seol Hee Oh[b], Jong-Ho Lee[b] and Yeong-Cheol Kim[a]

[a]School of Energy Materials and Chemical Engineering, KOREATECH, Cheonan, Republic of Korea
[b]Center for Energy Materials Research, KIST, Seoul 02792, Korea

Keyword

fuel electrode catalyst, solid solution, phase stability, computer simulation, first principles calculation

Since CeO_2 shows high oxygen storage/release capacity and this capacity can be further improved by adding ZrO_2, $Ce_{0.75}Zr_{0.25}O_2$ (CZO) has been studied for catalyst support of vehicles' catalytic converter and fuel electrode of solid oxide fuel cells. Phase separation, however, of CZO under reducing atmosphere at elevated temperatures has been observed experimentally. TEM with EDS shows oxygen-poor and pyro-like phases as intermediates before being completely separated to almost pure CeO_2 and ZrO_2; CeO_2 and ZrO_2 contain less than 1 % Zr and Ce, respectively. Ab-initio thermodynamics with density functional theory is employed to analyse the phase separation behavior of CZO.

Poster No.8

Impact of native defect on the magnetism in $EuTiO_3$

Inseo Kim[1)], Minseok Choi[1)*]

[1]*Department of Physics, Inha university, Incheon 22212, Korea*
[*]minseok.choi@inha.ac.kr

Perovskite $EuTiO_3$ has G-type antiferromagnetic (AFM) ground state with a Eu spin moment of $S = 7/2$ [1]. However, the competition between AFM and ferromagnetic (FM) ordering in the oxide is delicate and hence the FM phase can appear by mechanical deformation and carrier doping [2,3]. In this work, the impact of native defects on the magnetic ground state of $EuTiO_3$ was examined using the DFT+U calculation. Our results show that native defects stabilizes the FM phase more than the AFM phase. By combining with experiment, we proposed that the emergence of FM phase is attributed to the weakened Eu-Ti-Eu AFM super-exchange interaction and to the introduction of the Eu-O-Eu FM interaction [8].

[1] C-L. Chien, S. DeBenedetti, and F. De S. Barros, Phys. Rev. B **10**, 3913 (1974).
[2] H. Akamatsu *et al*., Phys. Rev. B **83**, 214421 (2011).
[3] Z. Gui and A. Janotti, Phys. Rev. Lett. **123.12**, 127201 (2019).
[4] J. B. Goodenough, Phys. Rev. **100**, 564 (1955).
[5] J. B. Goodenough, J. Phys. Chem. Solids **6**, 287 (1958).
[6] J. Kanamori, J. Phys. Chem. Solids **10**, 87 (1959).
[7] P. W. Anderson, Phys. Rev. **115**, 2 (1959).
[8] D. Shin *et al*., J. Am. Ceram. Soc. **104.9**, 4606 (2021).

Poster No.9

First-principles study on Li-doped BPhen in n-type charge-generation layer of organic light-emitting diodes

Jisu Kim[1], Suyeon Ju[1], Jaesun Kim[1], and Seungwu Han[1, *]

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

The tandem organic light-emitting diodes (OLEDs) are attracting great attention as promising devices for large displays. Vertical stacking of emission units ensures high efficiency and durability, but drive voltage increases with the number of emission units. Hence, it is important to improve the ability of charge generation and transportation at the charge generation layer (CGL) by alkali-metal doping. However, the underlying mechanism of doping remains unclear.
In this study, we propose a method for calculating the electronic structure of a metal-doped organic amorphous solid, for example, Li-doped Bathopenanthroline (BPhen). We introduce a series of calculations from generating amorphous solid with classical force-field to analyzing site energy distribution via density functional theory (DFT). Through this, it is possible to unveil how Li is doped into the amorphous organic solid and how it affects the electronic structure.

Poster No.10

First-principles calculation of the non-equilibrium quasi-Fermi levels in defective WSe_2 *p-n* junctions

Tae Hyung Kim, Juho Lee, and Yong-Hoon Kim*

School of Electrical Engineering, Korea Advanced Institute of Science and Technology, 291 Daehak-ro, Yuseong-gu, Daejeon 34141, Korea
(*Corresponding Author. Email: y.h.kim@kaist.ac.kr)

While the two-dimensional (2D) *p-n* junctions have been extensively studied for electronic and optoelectronic devices, the semiclassical approaches without considering atomistic details are still insufficient to describe its electronic structures, such as long depletion width and the role of defects. To overcome such limitations, we combine the multi-space constrained-search density functional theory (MS-DFT) formalism with the simulated doping method for describing the doped *p-n* junctions under finite-bias conditions. We introduce Se (W) vacancy in the depletion region and show that as the forward bias voltage increases, the depletion width of the *p*-doped (*n*-doped) WSe_2 region decreases faster than that of the *n*-doped (*p*-doped) WSe_2 region. Within the MS-DFT, we also extract the QFL profiles in the defective WSe_2 *p-n* junctions. Careful analysis of the QFL profiles shows that the asymmetrically varying depletion widths in defective WSe_2 *p-n* junctions originate from the asymmetrically penetrated QFL profiles mediated by the defect states.

Poster No.11

Moiré flat bands and interfacial charge polarization in lattice relaxed twisted bilayer hexagonal boron nitride

Fengping Li,[1] Dongkyu Lee,[1,2]Nicolas Leconte,[1] Jiaqi An,[1,2] Srivani Javvaji,[1] and Jeil Jung[1, 2]

[1]*Department of Physics, University of Seoul, Seoul 02504, Korea*

[2]*Department of Smart Cities, University of Seoul, Seoul 02504, Korea*

We simulate the electronic properties and the interfacial polarization of twisted bilayer hexagonal boron nitride by including the relaxation effects explicitly using an exact exchange and random phase approximation parametrized molecular dynamics force field in combination with a newly parametrized two-center approximation tight-binding model. The resulting lattice reconstruction induces a larger band gap than the one from the rigid structure while maximum localization of the flat band below 1° can be linked to the size of the deformed stacking domain regions. The band gap can be further engineered by applying an electric field leading to deformation of the moiré superlattice. The real space local density distribution indicates that interfacial charge polarization is sizeable for the parallel moiré stacking configuration between layers while it is negligible for the anti-parallel configuration under both relaxation effects and external electric fields.

Acknowledgments: We acknowledge grants NRF-2020R1A2C3009142 for F.L. and N.L., NRF-2020R1A5A1016518 for Y. P. D. L. and J.~A. were supported by the Korean Ministry of Land, Infrastructure and Transport (MOLIT) from the Innovative Talent Education Program for Smart Cities. J. J. acknowledges Samsung Science and Technology Foundation under project SSTF-BAA1802-06.

Poster No.12

Superconducting symmetries in Sr_2RuO_4 from first-principles using frequency-dependent vertex

Chang-Youn Moon[1]

[1]*Advanced Instrumentation Institute, Korea Research Institute of Standards and Science*

We investigate the superconducting gap functions in Sr_2RuO_4 by solving the linearized Eliashberg equation constructed within the DFT+DMFT method. We find that using frequency-dependent two-particle vertex moves the zero energy spin susceptibility peaks towards the Gamma point, compared with random-phase approximation which basically retains the peak positions closer to the Brillouin zone boundary as determined by the Fermi-surface nesting. d_{xy} orbital plays a central role here via its enhanced correlation strength. From this spin susceptibility, the prime candidate of the superconducting gap symmetry is a nodal s-wave, as well as a nearly degenerate d-wave solution, all in spin singlet. Furthermore, another set of degenerate spin singlet gap functions emerges, odd with respect to both k-point and orbital exchanges. We argue these gap symmetries are compatible with experimental observations.

Poster No.13

Predicting the activity of Multi-elemental catalyst for Hydrogen Evolution Reaction: A Machine Learning accelerated DFT study

Min Hee Park[1], Seung Jae Kwak[1], Yongjoo Kim[2], Won Bo Lee[1]

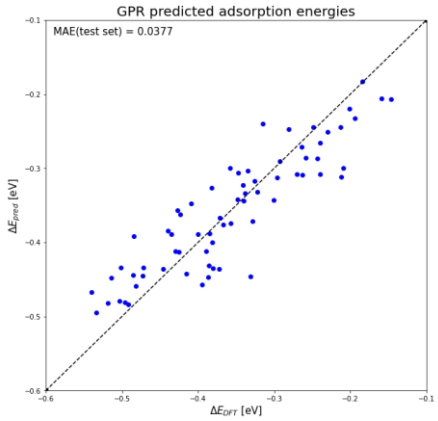
[1]*Seoul National University*
[2]*Kookmin University*

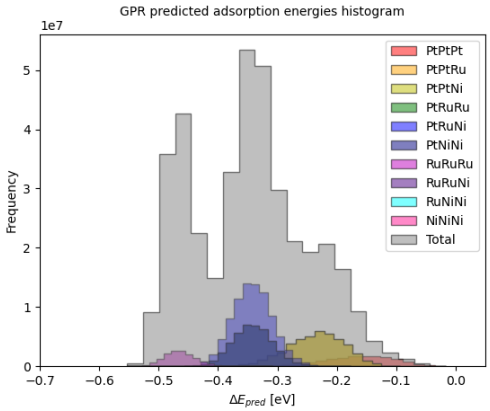
Introduction

Electrocatalytic processes have been long studied for their vital role in reducing the environmental pollution. The hydrogen evolution reaction (HER) is one of many electrocatalytic reactions that offers great potential to produce a sustainable energy source of hydrogen fuel. In order to achieve high efficiency of the catalytic reaction, it is necessary to develop a high-performance catalyst to minimize the overpotential required for the reaction. Multi-elemental catalysts are catalysts that contain three or more different chemical species. The main advantage of these catalysts is that mass production due to low fraction of noble metal. Also, the presence of randomly distributed metal elements has severe implications on the surface structure as well as the interactions between chemical elements within the catalyst. One of the most significant effects is the increase in unique surface sites. As the adsorption energy of the catalyst is determined by the element of the adsorption site and neighboring atoms, one can optimize the performance of the catalyst by adjusting the composition. Due to a large number of unique sites in Multi-elemental catalysts, there have been studies that apply Machine Learning method to analyze the activity of catalysts.

In this study, we aim to obtain the activity and stability of Multi-element catalyst toward hydrogen evolution reaction. First-principles-based density functional theory (DFT) calculations have been performed for approximately 400 Multi-elemental catalysts selected by Active Learning method. The DFT-calculated adsorption energies were used to train the Gaussian process regression model. By predicting the adsorption energies of all possible surface configurations, we have obtained the optimal ratio of Multi-elemental catalyst for HER.

Results and Discussion





The above figures show the result of Gaussian process regression predicted adsorption energies of hydrogen on the Multi-elemental catalysts. The MAE of the test set is 0.0377, which infers that the model has accuracy high enough to determine the overall activity of Multi-elemental catalysts. The model is applied to all available surface configurations consisting of three metals chosen, and the predicted distributions of adsorption energies are shown on a histogram. The color indicates the closest neighboring atoms of the adsorbate. With -0.27 eV as the optimal adsorption energy of hydrogen adsorption, we see that alloy catalysts outperform pure Pt catalyst. The predicted adsorption energies were than used to calculate the catalytic activity.

$$A = \sum_{i=1}^{Z} \left(\prod_{k}^{metals} f_k^{n_{ik}} \right) exp\left(-\frac{|\Delta E_i - \Delta E_{opt}|}{k_B T} \right)$$

Z is the total number of surface configurations, while f_k is the fraction of element k, n_{ik} is the number of element k in the surface configuration i. By using sequential least squares programming optimization method, the resulting maximum activity was 0.182 with atomic fraction of (f_{Pt}, f_{Ru}, f_{Ni}) = (0.75, 0.20, 0.05)

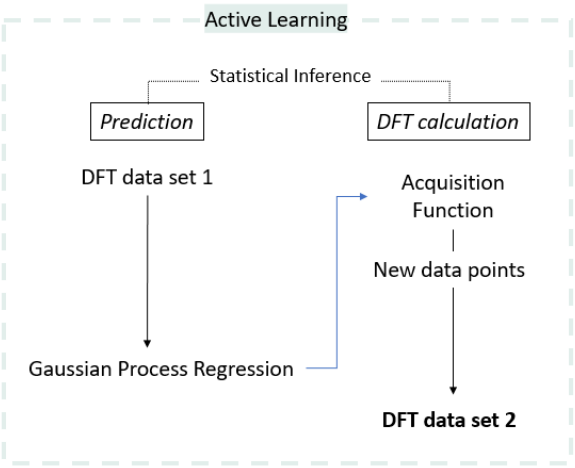
Methods

All DFT calculations were performed using Vienna Ab initio Simulation Package implemented in an Atomic Simulation Environment (ASE). The Revised Perdew-Burke-Ernzerhof (RPBE) functional form of generalized-gradient approximation (GGA) for electron exchange and correlation energies were used. The projector-augmented wave method was used with *k*-point grids of (x,y,z) = (4,4,1), and energy cutoff of 400 eV. Adsorption energies for training were calculated on 2x2, 4-layered slabs. The input for Gaussian process regression were expressed as array of length 15, which is comprised of number of each

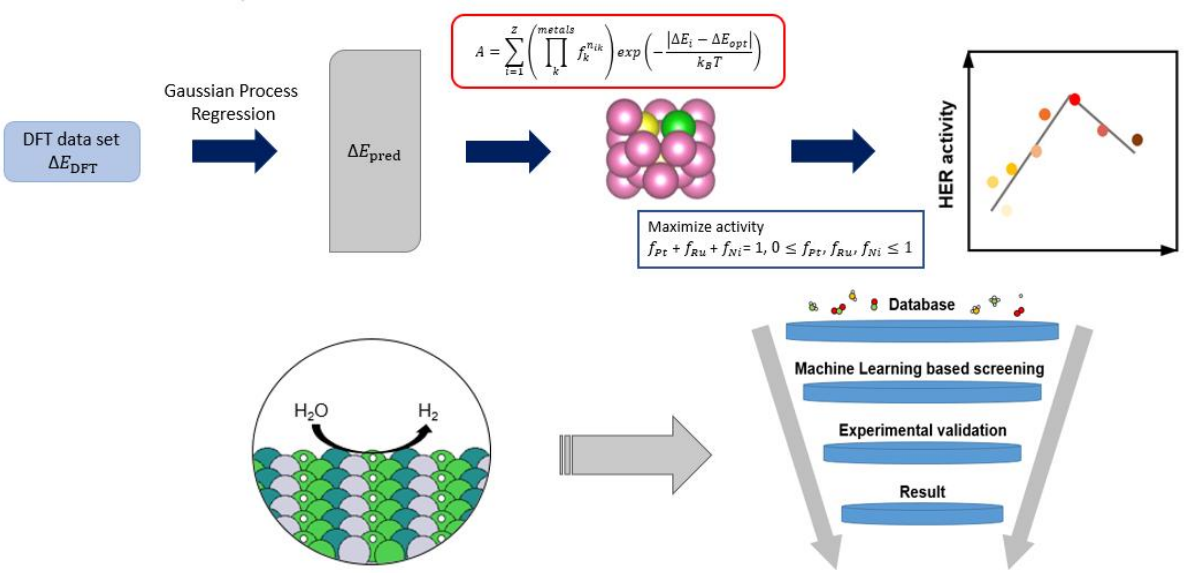
metal in each five surface sites.

Conclusion

Unique catalysts consisting of multiple chemical elements were observed with first principle calculations to illustrate the effect of randomly distributed elements. Adsorption energy prediction using



Gaussian Process Regression and Active Learning method established the possibility of fast and accurate screening of catalysts with numerous surface configurations.



References

Batchelor, Thomas AA, et al. "High-entropy alloys as a discovery platform for electrocatalysis." *Joule* 3.3 (2019): 834-845.

Tran, Kevin, and Zachary W. Ulissi. "Active learning across intermetallics to guide discovery of electrocatalysts for CO2 reduction and H2 evolution." *Nature Catalysis* 1.9 (2018): 696-703.

Miracle, Daniel B., and Oleg N. Senkov. "A critical review of high entropy alloys and related concepts." *Acta Materialia* 122 (2017): 448-511.
Kresse, Georg, and Jürgen Furthmüller. "Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set." *Physical review B* 54.16 (1996): 11169.
Kim, Minki, et al. "Searching for an Optimal Multi-metallic Alloy Catalyst by Active Learning Combined with Experiments." *Advanced Materials* (2022): 2108900.

Poster No.14

First-principles Study on the Phase Change Process in $GeTe/Sb_2Te_3$ Superlattices

Sunho Park[1], Chang Woo Lee[2], Mann-Ho Cho[2], Young-Kyun Kwon[1]

[1]Department of Physics and Research Institute for Basic Sciences,
Kyung Hee University, Seoul, 02447, Republic of Korea
[2]Department of Physics, Yonsei University, Seoul 120-749, Republic of Korea2

Facing limitations in the efficiency of memory devices, interfacial phase-change memory (IPCM) composed of Ge, Sb, and Te (GST) has been in the spotlight as a promising candidate for next-generation nonvolatile memory. It has been steadily reported that IPCM operates with great recyclability, low power consumption, and fast response time compared to other types of phase-change memories (PCMs). Despite these repetitive reports, however, not only its phase change mechanism, but even its metastable structure are also still debatable. To address this issue, we explored their structural and electronic properties by performing *ab initio* calculations based on the density functional theory (DFT). From their TEM images, we were able to find that the low resistance state (LRS) is a hexagonal structure of Ge_3Te_4-S_b2Te_3 superlattice, while the high resistance state (HRS) is a cubic structure with intermix and Ge vacancies. These structural characteristics are confirmed consistently in the experiments and calculations. The crystal structure is well-matched with the calculated and observed XRD, while the peak shift in XPS is explained by local atomic structures which are obtained by DFT calculations. We further proposed a possible phase change mechanism in which the Ge atoms diffusion plays an essential role in the transition between the most stable and metastable phases. To support this scenario, we evaluated the mobility of each atom and confirm that the Ge atoms are more diffusive in the system than the Sb atoms. Finally, we solved the Boltzmann transport equation to estimate the electric conductivities of both HRS and LRS, resulting in one or two orders of magnitude difference between them.

Poster No.15

Hybrid Density Functional Prediction of Diffusion of Mg Defects in Mg_2X (X = Si, Sn)

Sungjin Park and Byungki Ryu*

Energy Conversion Research Center, Korea Electrotechnology Research Institute (KERI), 12, Jeongiui-gil, Seongsan-gu, Changwon-si, Gyeongsangnam-do, 51543 South Korea
E-mail address: byungkiryu@keri.re.kr

Thermoelectric power generation technology generates electricity through the reversible and direct energy conversion of waste heat, and has attracted attention as an upcoming clean energy technology. Eco-friendly thermoelectric materials, such as $Mg_2Si_xSn_{1-x}$, have recently attracted interest because previously investigated Bi_2Te_3- and PbTe-based materials are toxic to the human body and environment. The thermoelectric figure of merit has reached 1.7 by co-doping $Mg_2Si_xSn_{1-x}$ with Bi and Cr [1]. Recently, by investigating the defect formation in Mg_2X (X = Si, Sn), it was found that Mg interstitials and Mg vacancies are the most stable intrinsic defects in Mg_2X [2]. Understanding the stability of Mg_2X requires investigating the diffusion of these defects. However, the diffusion mechanism of these defects within Mg_2X remains largely unresolved. In this study, we investigated the atomic diffusion of Mg defects in Mg_2X through hybrid density functional theory calculations. The charged defect formation energies of native point defects were revisited, and the migration path of Mg interstitials and Mg vacancies in Mg_2X was determined. Using the nudged elastic band method, migration barriers for Mg interstitials and Mg vacancies were obtained. As a result, the activation energies of diffusion were computed.

References

1. G. Goyal, S. Mukherjee, R. Mallik, S. Vitta, I. Samajdar, and T. Dasgupta, *ACS Appl. Energy Mater.* 2, 2139–2137 **(2019)**.
2. B. Ryu, E. Choi, S. Park, J. Chung, J. de Boor, P. Ziolkowski, E. Müller, S. Park, *J. Alloys Compd.* 853, 157143 **(2021)**.

Poster No.16

First-principles study on the enhancement of the oxygen diffusivity in La2−xSrxCuO4 by cation substitution

Sohee Park,† Young-Kyun Kwon,*,†,‡ and Changwon Park*,¶

†Department of Information Display, Kyung Hee University, Seoul 02447, Korea
‡Department of Physics and Research Institute for Basic Sciences, Kyung Hee University, Seoul 02447, Korea
¶School of Computational Sciences, Korea Institute for Advanced Study, Seoul 130-722, Korea

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

Ruddlesden-Popper phase oxides in the form of A2BO4, such as La2CuO4, are expected to have potential for cathode materials for solid oxide fuel cells. Among their several advantages, the high oxygen diffusivity within layered structures is regarded as the most important property for low-temperature operation. However, the systematic improvement has been limited due to the lack of atomic-level understanding of their oxygen diffusivity. Here, we show our density functional theory calculations and random walk simulations for Sr-doped La2CuO4 (La2-xSrxCuO4), which scrutinize the major hopping routes with low activation energies, as well as anisotropic diffusion coefficients of oxygen vacancies along the in-plane and out-of-plane directions. We discovered that Sr doping, which is commonly used for cathode materials' electronic conduction, not only accelerates the production of oxygen vacancies but also improves oxygen diffusivity. According to our random walk simulations, the improvement of oxygen diffusivity is the result of two competing effects of Sr atoms: (i) weakly binding to oxygen vacancies and (ii) promoting the vacancies to escape from the most stable places.

Poster No.17

A strong oxidant as a localized electron scavenger for realizing highly efficient halide perovskite photovoltaics: A first–principles study

Seulyoung Park,[1] Jun Zhu,[2] Oh Yeong Gong,[1] Chang Hwun Sohn,[1] Zijia Li,[2] Zhenru Zhang,[2,3] Bonghyun Jo,[2] Wooyul Kim,[3] Gill Sang Han,[1] Dong Hoe Kim,[4] Tae Kyu Ahn,[2] Hyun Suk Jung,[1] Jaichan Lee*[1]

*Corresponding author: jclee@skku.edu

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

[2]*Department of Energy Science, Sungkyunkwan University, Suwon 16419, Republic of Korea*

[3]*Department of Chemical and Biological Engineering/Research Institute of Global Environment, Sookmyung Women's University, Seoul 04310, Republic of Korea*

[4]*Department of Nanotechnology and Advanced Materials Engineering, Sejong University, Seoul 05006, Republic of Korea*

Formamidinium lead iodide ($FAPbI_3$)-based perovskites is considered as strong candidates for next-generation solar energy conversion materials due to their outstanding light absorption coefficient and long carrier diffusion lengths. However, despite these properties, primary intrinsic defects in $FAPbI_3$ (i.e. iodine vacancy) upon photoexcitation induce strong electron localization and become recombination centers which significantly deteriorate photovoltaic properties. Therefore, suppressing the electron localization in iodine vacancies has become a critical issue for realizing efficient solar cells. In this work, formamidine disulfide dihydrochloride (FASCl) is used as an electron scavenger. Since the FAS^{2+} ion in FASCl has been frequently used as a strong oxidant for gold dissociation, it could prevent the strong electron localization in the iodine vacancies. First-principles calculation shows that FASCl is successfully incorporated into the $FAPbI_3$ lattice, scavenges localized electrons, and consequently annihilates deep traps in $FAPbI_3$.[1] Calculation results are also confirmed by experimental results which show significant improvement of charge carrier lifetime, leading to remarkable power conversion efficiency, 23.11% of solar cells.

[1] *Energy & Environmental Science*, *14*(9), 4903-4914.

Poster No.18

Topology imprinted in laser-induced photoemission delay driven by quantum interference

Hyosub Park and J.D. Lee*

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

Electronic band structure and wavefunction determine Berry curvature and topology of a material. The signature of topology has been observed by various physical quantities like anomalous hall current, high-harmonic generation, circular dichroism, etc. In this research, we theoretically present a new fingerprint of topology through the photoemission delay in the high-energy XUV limit, which manifests the microscopic dynamics for the quantum phase. The photoemission delay is analytically obtained by the second-order time-dependent perturbation theory for two-photon (XUV and drive pulse) dynamics in the Haldane model. Resultant analytic calculations show that a photoelectron undergoing interband transition by the drive pulse has a transient laser-induced photoemission delay compared to a photoelectron directly emitted without interband transition. Furthermore, it is found that the interference between valence and conduction paths of a photoelectron causes an additional delay, which reveals the Berry curvature and topology of the system. The analytic photoemission delays are agreed with our numerical calculation for the attosecond streaking method, implying the feasibility of experimental observation. These results suggest that the photoemission delay can be utilized as a fingerprint of topology for 2D materials.

Poster No.19

Revealing Berry curvature of the unoccupied band

Gimin Bae, Youngjae Kim, and J. D. Lee*

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

Experimental determinations of the net Berry curvature have been made for the occupied band because they are basically available on the basis of electronic and magnetic responses of carriers occupying the band, for instance, through the measurement of the anomalous Hall effect or the magneto-optical Kerr effect. Here, we investigate the circular dichroism of the high-order harmonic generation (HHG) in the monolayer undoped MoS_2. Breaking the three-fold rotational symmetry of the pristine monolayer MoS_2 by applying the uniaxial strain and the external bias field, we find that the third order HHG signals deliver nonvanishing dichroic signatures. These signatures are essentially identical as the net Berry curvatures obtained from the monolayer electron-doped MoS_2 with the forementioned symmetry broken. This finding implies a new experimental challenge to observe the net Berry curvature of the unoccupied band, which should open another stage toward an advancement of the valleytronics.

Poster No.20

Nanoscale Seebeck domain junction in MoS_2 5|7 grain boundary

Authors: Seungil Baek[1], Eui-Cheol Shin[1], Jun Jung[1], Ho-Ki Lyeo[3], 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.*

[3]*Korea Research Institute of Standards and Science, Daejeon 34113, Republic of Korea.*

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

Abstract:.

Grain boundary is an unavoidable defect in the synthetic process, being a major obstacle for device application. In low dimensional systems, including transition metal dichalcogenides (TMD) family, its importance grows because of enhanced surface-volume ratio. However, it is proposed that grain boundary can improve thermoelectric properties by becoming a source of phonon scattering. Though the thermoelectricity originates from local electronic structure, conventional approach remained in a macroscopic viewpoint. Here, by using *ab initio* scanning Seebeck microscope (SSM) simulation, we demonstrate that nanoscale domain of local Seebeck coefficient could be created in the MoS_2 grain boundary system. Near the pentagon-heptagon 5|7 dislocation cores, local charge accumulation induces in-plane electric field and modifies the Seebeck profile, thereby leading to a domain of different magnitude or even different sign of Seebeck coefficient. Furthermore, sign of each domain could be readily tuned by appropriate doping condition. We expect that the delicate dislocation engineering in grain boundaries could open up a new field of controllable Seebeck coefficient domain for nanoscale device applications.

Poster No.21

Hybrid density functional theory calculation of orthorhombic cesium lead halide perovskite alloys

Youbin Song and Ji-Sang Park*

Department of Physics Kyungpook National University, Daegu 41566, Korea

Hybrid organic-inorganic perovskite (HOIP) has recently attracted much attention for solar cell applications because of its high absorption coefficient, tunable bandgap, and long carrier lifetime. To achieve better efficiency, halogen atoms are usually mixed to tune the electronic band gap. First-principles density functional theory (DFT) calculations also have been performed to investigate the electronic structure of HOIPs, however, there has been inconsistency between the DFT calculation and experiments on the band gap of $CsPbI_{3-3x}Br_x$.

To obtain the accurate bandgap, we performed hybrid DFT calculations. The atomic structure of orthorhombic $CsPbI_{3-3x}Br_{3x}$ and $CsPbBr_{3-3x}Cl_{3x}$ were optimized by using generalized gradient approximation (GGA) exchange-correlation functional [1] with a van der Waals correction. Spin-orbit coupling was included throughout the calculations. The thermal stability of mixed halide perovskites was examined by calculating with the consideration of mixing entropy. The bandgap calculated by using hybrid DFT [2] was in better agreement with experiments. The band gap of these materials was also cost-effectively obtained by using down-sampled *k*-point grid for Hartree-Fock (HF) exchange in hybrid DFT [3].

[1] J. P. Perdew, K. Burke, and M. Ernzerhof, Phys. Rev. Lett. 77, 3865 (1996).
[2] J. Heyd, G. E. Scuseria, and M. Ernzerhof, J. Chem. Phys. 118, 8207 (2003).
[3] J.-S. Park, Curr. Appl. Phys. **20**, 379 (2020).

Poster No.22

Cost-effective hybrid density functional theory calculation of point defects in diamond Si

Youbin Song, Seyeon Park, and Ji-Sang Park*

Department of Physics Kyungpook National University, Daegu 41566, Korea

Understanding defects in semiconductors is necessary for making semiconductor devices by controlling the electrical properties. Defects are can be either useful or detrimental: Shallow defects are used to modulate the Fermi level, but deep defects decrease efficiency by promoting non-radiative recombination. The hybrid density functional theory (DFT) [1] has been recently widely used to analyze the material properties of semiconductors. The heavy computation cost of the method has been a bottleneck for high-throughput studies, but recent studies show that its computation cost can be reduced without losing much accuracy by using the downsampled *k*-point grid for the Fock exchange [2]. Our study shows that the downsampling method can be used to investigate defects as well [3]. The stability and electrical properties of substitutional P defect, Si vacancy, and Si self-interstitial defects in diamond Si were cost-effectively calculated with respect to the conventional hybrid DFT calculation.

[1] J. Heyd, G. E. Scuseria, and M. Ernzerhof, J. Chem. Phys. **118**, 8207 (2003).
[2] J.-S. Park, Curr. Appl. Phys, **20**, 379 (2020).
[3] Y. B. Song, S. Y. Park, and J.-S. Park, Curr. Appl. Phys, **39**, 51 (2022).

Poster No.23

Theoretical investigation of Pt-skinned Pt-M alloys (M = Co, Ni, Mn, and Ir) for the oxygen reduction reaction in fuel cells

Dong Yun Shin, Yeon-Jeong Shin, Min-Su Kim, Jeong An Kwon, Dong-Hee Lim*

Department of Environmental Engineering, Chungbuk National University

Pt-based binary alloys (Pt-M, M = transition metal) with optimal electronic and geometric properties may be used to secure the economic feasibility of fuel cells by reducing Pt content and increasing cathodic efficiency. The oxygen reduction reaction (ORR) on Pt-M alloys (Pt_3M and PtM, M = Co, Ni, Mn, and Ir) was probed by density functional theory (DFT) calculations to reveal that the oxygen dissociation pathway (O_2* → O*+O* → O*+OH* → O*+H_2O(g) → OH*+$H_2O_{(g)}$ → *+2$H_2O_{(g)}$, * represents the state adsorbed on a surface) is optimal for Pt(111), Pt_3M(111), and PtM(111) surfaces. However, the above alloys showed the inferior ORR efficiency to Pt (onset potential = 0.60 V) catalysts. In order to solve this, Pt-skinned Pt-M alloys were designed by adding a single Pt skin layer to the top of Pt-M alloys, which enhanced ORR performance by decreasing the adsorption strengths of key intermediates (O* and OH*) in the potential limiting step to values below those observed for the Pt catalyst. Pt/PtNi (0.88 V) and Pt/PtCo (0.81 V) catalysts with the decreased Pt content, showed particularly high ORR performances. The results of electronic structure analysis demonstrated that the above decrease in adsorption strength was due to the inhibition of the high activity of the Pt-M(111) surface by the Pt skin layer. Finally, simple descriptors (optimal d-band center position and adsorption strength) were established to enable the further search for better fuel cell catalysts.

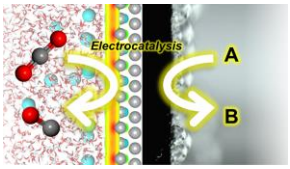
Poster No.24

A mean-field QM/MM study revealing the aqueous electric double layer structure and its importance on the electrocatalysis

Seung-Jae Shin[1], Dong Hyun Kim[2], Geunsu Bae[2], Stefan Ringe[3], Hansol Choi[4], Hyung-Kyu Lim[5], Chang Hyuck Choi[2], and Hyungjun Kim[6,*]

[1]*Department of Materials Science and Engineering, Yonsei University*
[2]*Department of Chemistry, Pohang University of Science and Technology (POSTECH)*
[3]*Department of Chemistry, Korea University*
[4]*School of Materials Science and Engineering, Gwangju Institute of Science and Technology,*
[5]*Division of Chemical Engineering and Bioengineering, Kangwon National University,*
[6]*Department of Chemistry, Korea Advanced Institute of Science and Technology,*
**email: linus16@kaist.ac.kr*

To design electrochemical interfaces for efficient electric-chemical energy interconversion, it is critical to reveal the electric double layer (EDL) structure and relate it with electrochemical activity; nonetheless, this has been a long-standing challenge. Of particular, no molecular-level theories have fully explained the characteristic two peaks arising in the potential-dependence of the EDL capacitance, which is sensitively dependent on the EDL structure. We herein demonstrate that a mean-field QM/MM simulation results reproduce the experimental capacitance peaks. The origin of two peaks emerging at anodic and cathodic potentials is unveiled to be an electrosorption of ions and a structural phase transition, respectively. We further find a cation complexation gradually modifies the EDL structure and the field strength, which linearly scales the carbon dioxide reduction activity. This study deciphers the complex structural response of the EDL and highlights its catalytic importance, which bridges the mechanistic gap between the EDL structure and electrocatalysis.



Poster No.25

Magnetic structure of oxygen-deficient perovskite nickelates with ordered vacancies

Yongjin Shin,[1,2] and James M. Rondinelli[1]

[1]*Department of Materials Science and Engineering, Northwestern University, Evanston, IL, 60208, USA*
[2]*Pritzker School of Molecular Engineering, University of Chicago, Chicago, IL 60637, USA*

The oxygen vacancy concentration in $LaNiO_{3-\delta}$ nickelate perovskites affects magnetic interactions and long-range magnetic order through changes in local electronic configurations, crystal field splitting energies, and polyhedral arrangements. Here we use density functional theory calculation to examine the magnetic structure of $LaNiO_{2.5}$ and $LaNiO_{2.75}$ with structural ordered oxygen-vacancies (OOV). These OOV phases exhibit columnar arrangements of NiO_4 square planar units, which adopt low-spin Ni^{2+} d^8 configurations with nominally zero magnetic moment (S=0), interconnected by NiO_6 octahedral units. The magnetic structure of the OOV phases are governed by the flexible charge state of the NiO_6 octahedral units, whose density and connectivity depends on the oxygen vacancy concentration. $LaNiO_{2.5}$ is stable in an insulating A-type antiferromagnetic (AFM) phase derived from octahedral units comprising Ni^{2+} in AFM chains. $LaNiO_{2.75}$ is a narrow-gap insulator with zigzag-type AFM order originating from weakly localized electrons in columnar breathing distortions to the NiO_6 units.Our results suggest that nanoscale OOV phases within single phase $LaNiO_{3-\delta}$ crystals can account for its reported complex magnetic ground state structure.

Poster No.26

Reliable *ab initio* local thermoelectric transport in the layered material

Eui-Cheol Shin[1] and 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

The Scanning Thermoelectric Microscope has proposed a notable quantum sensing technique for highly amplified energy differential of the local density of states in a coherent transport regime. The experimental thermoelectric voltage has been satisfactorily understood using the *ab initio* local Seebeck calculation based on density functional theory and Tersoff-Hamann approximation for single layer material. Unfortunately, due to the well-known delocalization problem in density functional theory, the appropriate description of coherent thermoelectric transport for the layered system is not fully guaranteed in the Tersoff-Hamann regime. Here, we will show a high-order scattering theory based on Bardeen's transfer matrix for the 1H-MoS_2 van der Waals layered systems. This method successfully demonstrates a reliable local Seebeck coefficient without artificial interlayer interaction of the inherent nature of density functional theory.

Poster No.27

First-principles study of the isomerization of cadmium sulfide magic-sized clusters

Doeun Shim[1], Juhyung Lee[1], and Joongoo Kang[1]*

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

Recently, magic-sized clusters (MSCs) of semiconductors have attracted much attention as key intermediates in the synthesis of colloidal quantum dots. So, it is essential to characterize and understand the atomic structures of MSCs and their structural transformations. The recent experimental finding of chemically reversible isomerization of CdS MSCs suggests that the cluster transformation simultaneously exhibits characteristics of two different length scales, namely, molecular isomerization and solid-solid transformation [1]. However, the microscopic mechanism of such multiscale isomerization is not understood. Here, using density-functional calculations, we reveal that when triggered by methanol adsorption and desorption, the $Cd_{41}S_{20}$ MSC undergoes a reversible isomerization through (i) the Cd-S bond exchanges at the bond-length scale (molecular isomerization) and (ii) the associated stacking-order changes at the cluster-size scale (solid-solid transformation). Our work thus sheds light on understanding the intriguing multiscale transformation of inorganic nanoclusters.

[1] C. B. Williamson et al. *Science* **2019**, 363, 731.

Poster No.28

Atomistic simulations of band gaps in graphene on hexagonal boron nitride

Jiaqi An,[1, 2] Nicolas Leconte,[1] Srivani Javvaji,[1] Youngju Park,[1] and Jeil Jung[1, 2]

[1]*Department of Physics, University of Seoul, Seoul 02504, Korea*

[2]*Department of Smart Cities, University of Seoul, Seoul 02504, Korea*

We present atomistic molecular dynamics simulations of graphene on hexagonal boron nitride (BN) to assess the impact of the substrate relaxation in the primary and secondary valence band gaps as a function of twist angle. Both primary and secondary gaps reduce their overall magnitude when twisted away from alignment yet they show quantitative differences depending on the specific profiles of the moire strains and molecular dynamics force fields. With commonly used reactive bond order (REBO2) potentials, the primary band gap near the charge neutrality for the zero twist aligned geometry undergoes reductions from 20 meV from suspended fully relaxed G/BN bilayers through 9 meV for rigid remote hBN, and 5 meV for rigid contacting hBN layer, down to 3 meV for completely rigid structures. For substrate supported relaxed G/BN we find a non-monotonic behavior of the primary band gap with a maximum around $\sim 0.8^{\circ}$ before it starts decreasing for larger twist angles. The secondary valence band gap is less sensitive to the relaxation schemes and drops from a value of $\sim$12 meV for aligned geometry to zero for twist angles below 1°. The reduction of the primary band gap by a factor of two and four respectively when we disallow the strains in the next nearest nearest neighbor hBN layer respectively shows the influence of substrate relaxation when modeling graphene based moire superlattices.

Acknowledgments: We acknowledge grants NRF-2020R1A2C3009142 for N.L., NRF-2020R1A5A1016518 for Y. P. J.~A. was supported by the Korean Ministry of Land, Infrastructure and Transport (MOLIT) from the Innovative Talent Education Program for Smart Cities. J. J. acknowledges Samsung Science and Technology Foundation under project SSTF-BAA1802-06.

Poster No.29

Interplay Between Twisting and Octahedral Chirality in Two-dimensional Magnetic Materials: Antiferromagnetic CrI_3 Bilayers

Kunihiro Yananose[1], Paolo G. Radaelli[2], Mario Cuoco[3],
Jaejun Yu[1], Alessandro Stroppa[4]

[1]*Center for Theoretical Physics, Department of Physics and Astronomy, Seoul National University, Seoul 08826, Republic of Korea*
[2]*Clarendon Laboratory, Department of Physics, University of Oxford, Parks Road, Oxford OX1 3PU, United Kingdom*
[3]*CNR-SPIN, Salerno, Italy*
[4]*CNR-SPIN, L'Aquila, Italy*

Two-dimensional materials are defining a new and exciting field in material science. The possibility of introducing twisting in bilayers could further increase the tunability of their physical properties. Twisting naturally introduces structural chirality in the system, thus defining two enantiomers, i.e., left- and right-handed bilayers depending on whether the twist is clockwise or counterclockwise. In this work, using density functional theory calculations combined with symmetry analysis and tight-binding model calculations, we focus on antiferromagnetic CrI_3 twisted bilayers. We discuss the interplay of twisting with an additional structural degree of freedom of the system, i.e. the octahedral chirality, which is defined for each Cr site by the local geometry of the bonds. The coexistence of the twisting and the octahedral chirality can lower the magnetic point group symmetry, thus activating, for example, the magneto-optical Kerr effect (MOKE) as well as the presence of the electric polarization, which would be otherwise absent in untwisted antiferromagnetic homo-bilayers. Interestingly, both electric polarization and Kerr angle reverse their sign when switching between the left- and right-twisting.

Poster No.30

Deep learning interatomic potentials for molecular dynamics simulations of the h-BN growth on Pt(111)

Kangmo Yeo, Karam Park, Sukmin Jeong*

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

In this study, we construct deep learning potentials for (B, N)/Pt(111) to simulate the atomistic processes of the hexagonal boron nitride (h-BN) synthesis on the Pt(111) surface, which is a versatile 2D material in applications. The deep learning potentials learn the training data produced by the active learning method [1]. The MD simulations reveal that B adatoms diffuse into the substrate while N adatoms stay on the substrate. Early in the h-BN synthesis process, the B and N adatoms combine to form BN chains, and then the BN chains become a Y-shaped structure when the B or N adatoms are attached to the side of the BN chains. As the MD simulation continues, the Y-shaped structures become hexagonal through a BN square structure. The Pt adatoms help this h-BN synthesis process by behaving as a surfactant. We also investigate the effect of cooling for the B segregation in the Pt substrate. The present results provide deep insights for the growth of 2D materials on the metal surface and expand the versatility of neural network potentials to the growth phenomena.

Keywords: Machine learning, Artificial neural network potential, Interatomic potential, Pt(111), h-BN, molecular dynamics.

[1] K. Yeo, K. Park, S. Jeong, Curr. Appl. Phys. **39**, 62 (2022)

Poster No.31

First-principles study of the functionalized-MXene for Li-ion battery application

Hyeonwoo Yeo and Yong-Hoon Kim*

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

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

Two-dimensional (2D) transition-metal carbides/nitrides (MXenes) have been highlighted as one of the promising battery anode materials due to their long cycle lifetime, low diffusion barrier, and controllable interlayer distance using surface functionalization. Tailored introduction of functional groups on the surfaces of MXenes can further enhance their physical and chemical properties, extending possible applications of MXenes to a wider set of fields. In this presentation, we carried out first-principles calculation and studied the effect of functionalization of MXene in the aspect of the anode application for Li-ion battery. Calculating the binding energy, diffusion barrier, and diffusion path of a Li atom, we first evaluate the Li-ion battery anode performance of pristine Ti_3C_2 as well as functionalized MXenes ($Ti_3C_2T_x$, T_x = -F, -O) and exhibited that the MXene-based anodes show better performance than conventional graphite anode. Next, we consider $Ti_3C_2O_2$ with nitrobenzene-termination ($C_6H_4NO_2$), which was experimentally obtained recently and demonstrated that the Li ion diffusion paths can be controlled using nitrobenzene-termination with low diffusion barrier heights. This study will offer promising strategies for the design of advanced MXene-based battery materials.

Poster No.32

Machine learning potential for reactions in atomic layer deposition

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

[1] *Seoul National University, Seoul 08826, Korea*
*e-mail: hansw@snu.ac.kr

With computing power increasing, machine learning methods are used in many fields such as social science, engineering, physics, chemistry, and material science.

In physics and material science, many researchers use this methods for physical property prediction, crystal structure prediction, machine learning potential and others.

Machine learning potential (MLP) is one of applications that can compute molecular dynamics as fast as classical force field with accuracy of ab initio computations. MLP can be used in many large systems that are difficult to compute with ab initio level due to their high cost.

In this research, we studied reaction mechanism of titanium nitride (TiN) atomic layer deposition process with TiCl4 and NH3 precursors due to its importance in semiconductor industry.

First, we investigate complex reaction mechanism of TiN atomic layer deposition and its thermodynamic properties. Density funcitonal theory (DFT) was used to calculate the reaction energies of possible pathway for reactions in atomic layer deposition process

Using results of DFT calculation, we trained machine learning potentials with neural network model to predict thermodynamic properties in untrained regions.

Finally, the test set was used to verify the accuracy of neural network potential(NNP) in predciting reaction energy.

These results help to study reactions in atomic layer deposition and accelerating large-scale simulations such as Kinetic Monte Calro .

Poster No.33

Efficient calculation of Coulomb energy and forces using atom-centered compensation charges in density functional theory

Jeheon Woo

Department of Chemistry, KAIST, 291 Daehak-ro, Yuseong-gu, Daejeon 34141, South Korea

We present a method for efficiently calculating Coulomb energy and Hellmann-Feynman (HF) forces in periodic and aperiodic systems using the atom-centered compensation charge (ACC). The long-range interactions of nuclear-nuclear and nuclear-electron cause a quadratic increase in computational cost for the number of atoms. Especially in the linear-scaling method, these interactions account for a large portion of the overall computation. The ACC compensates for the nuclear potential, making the nuclear-nuclear and nuclear-electron interactions short-range, allowing the calculation of Coulomb interactions with linear-scaling. In this work, we show newly derived equations of energy and HF force by using the ACC.
We applied the ACC method to density functional theory calculations in the real-space method and confirmed the dramatic acceleration of the Coulomb energy and HF force calculations.

Poster No.34

Ab initio calculation to unveil physical origin of electro-plasticity

Seungwoo Yoo[1], Sangmoon Yoon[2], Young-Kyun Kwon[1*]

[1]*Kyung Hee University*
[2]*Gachon University*

The plasticity of some metals enhances well under electric current. Industrially, this plasticity has been utilized when metals need to be bent and to transform their shapes. Originally, Joule heating was proposed as a possible origin of such phenomenon. In a recent study, however, it turned out that the temperature rise due to Joule heating was not sufficiently high to explain the increased plasticity. In this work, we explored the physical origin of such electro-plasticity using first-principle calculation. We investigated the effects of extra charges that could be supplied by the current on structural deformations and phonon behaviors. We found that bulk structures are not strongly affected by a small amount of supplied electric charges, whereas structures with imperfections such as surfaces, and structures with grain boundaries exhibit significant phonon softening. In addition, we figured out that extra charges can reduce the energy barrier of shear motions in various metal slabs. Finally, we revealed that an increase in plasticity under electric current originates from local charge accumulation or deficiency occurring in imperfect regions.

Poster No.35

Dual nature of ferromagnetic Hund's metal 1T-$CrTe_2$

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

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

A van der Waals ferromagnetic metal 1T-$CrTe_2$ is recently synthesized in thin-film form and gained substantial interest due to its room temperature intrinsic ferromagnetism. Despite this intriguing observation, its nature of electronic correlation and magnetic properties remained unclear. Here, through density functional theory plus dynamical mean-field theory (DFT+DMFT), we found that 1T-$CrTe_2$ belongs to the Hund's metal family, where Hund's coupling J_H comes to play an important role in the strong electronic correlation. Although all Cr-d orbitals are responsible for the metallicity, t_{2g} and e_g orbitals show localized and itinerant nature, respectively. Nevertheless, both orbitals contribute to the total magnetization, exhibiting the dual nature of ferromagnetism in 1T-$CrTe_2$. Further, comparison of Curie temperature (T_C) between bulk and monolayer structures indicates weak (strong) ferromagnetic interlayer (intralayer) interaction. We illustrate the significance of Hund's coupling 1T-$CrTe_2$, shedding light on the correlated and magnetic nature of the system.

Poster No.36

Accelerating density functional theory calculations by predicting charge density using convolutional neural networks

Ryong-Gyu Lee, and Yong-Hoon Kim*

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

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

Density functional theory (DFT) has been established as a standard methodology for describing the electronic and structural properties of solids and molecules in materials science. However, the practical use of the DFT is limited to systems containing less than a few hundred atoms, since the computational costs extremely increase with respect to the system size. Here we propose a machine learning (ML) approach based on the three-dimensional (3D) convolutional neural networks to accelerate the DFT calculation by predicting electronic charge density, which is one of the key ingredients for DFT calculation. Since we directly use the 3D grid-based physical properties as input feature vectors, the proposed model is simple and intuitive not requiring any artificial descriptors. Utilizing the CNN architecture, the model is transferable to translational and rotational variance and also can be applied to periodic systems, like polymer and DNA. We finally validate performance that the predicted charge density is accurate enough to capture the other electronic properties, such as the density of states. Our findings provide insight towards the future direction for accelerating the materials simulations based on the ML approach.

Poster No.37

Inverse design of nanoporous graphene/graphene heterobilayers for electric-field-tunable bandgaps

Byeoksong Lee[1] and Joongoo Kang[1]*

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

Nanoporous graphene (NPG) with periodic nanopores is a new multifunctional carbon material [1]. Depending on the size, shape, and periodicity of the nanopores in NPG, its electronic structure can be largely tailored for applications. This theoretical work reveals two mechanisms for the electric-field-tunable bandgap in NPG/graphene (Grp) bilayers: (i) type-I bandgap opening in graphene through 2D inversion symmetry breaking and (ii) type-II bandgap opening through the merging of Dirac cones of graphene [2]. An inverse design method based on the "upfolding" of low-energy effective Hamiltonian is developed to extract the design principles of NPG/Grp bilayers with the target functionality. First-principles calculations show that the inverse-designed NPG/Grp bilayers indeed exhibit the field-tunable bandgaps in graphene as predicted; the type-I bandgap opening is characterized by a linear field dependence of the bandgap, while the type-II bandgap opening exhibits a highly nonlinear field dependence of the bandgap. The distinct electric-field dependences of the bandgap in the type-I and type-II NPG/Grp bilayers could provide a way of building new types of graphene transistors.

[1] C. Moreno et al., Science 2018, 360, 199–203.
[2] B. Lee and J. Kang, Adv. Electron. Mater. 2022, 2200252.

Poster No.38

Flat imaginary phonon band-driven amorphization under compression in metal halide perovskite $CsPbI_3$

Seho Yi and Jung-Hoon Lee*

Computational Science Research Center, Korea Institute of Science and Technology, Seoul 02792, Republic of Korea

Due to their advantageous optoelectronic features and inexpensive cost, halide perovskites are a class of solar absorber materials being intensively investigated for photovoltaic applications. Several recent high-pressure experiments indicated that they generally undergo the reversible phase transitions between distinct crystalline phases and between crystalline and amorphous phases under an external pressure. In this study, using first-principles density-functional theory (DFT) and *ab-initio* molecular dynamics (AIMD) simulations, we investigate the origin of the pressure-induced amorphization in $CsPbI_3$. We find that the amorphous-like structures derived from AIMD calculations become more stable than the orthorhombic *Pbnm* phase above 6.66 GPa, in good agreement with experimental measurement (4.44 GPa). Intriguingly, we discover that an imaginary flat band appears in the phonon dispersion of the orthorhombic $CsPbI_3$ phase across the Brilliouin zone at a 10 GPa, leading to degenerated lattice instabilities. We further demonstrate that these energetically degenerated phonon modes are related to the PbI_6 octahedral tilting modes and provide random local distortion patterns without long-range order under compression leading to amorphization. Our findings contribute to a greater comprehension of the mechanism behind the pressure-induced amorphization of halide perovskites.

Poster No.39

The first principle calculation study of remote epitaxy on h-BN coated sapphire substrates

Youngjun Lee[1] , Seungjun Lee[1] and Young-Kyun Kwon[1,2]

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

[3]*Department of Information Display, Kyung Hee University*

Remote epitaxy, which grows materials crystallographically aligned to substrates despite existing an inserted 2D layered material in-between, has attracted much attention as a novel method that provides easy detachment and transfer for other various applications. Remote epitaxy in its original paper was explained by first-principles calculations showing the potential variation over an inserted layer is teleported from the substrate. We revisited such teleported potential profile to investigate the physical origin of remote epitaxy using various materials on sapphire substrate with an inserted 2D layer. Using the first-principles calculation based on density functional theory, we investigated the local potential distribution on the c-, m-, and r-sapphire planes with a 2D space material, such as graphene and hexagonal boron nitride, while changing the number of its layers from n=0 up to n=3. When n >= 2 of either h-BN or graphene, the local potential of the sapphire substrates is completely screened regardless of the surface orientation of the sapphire substrate. However, with a monolayer, the local potential pattern on the space layer somewhat resembles that of the sapphire substrate but its fluctuation becomes much weaker than that on the bare sapphire substrate. We further found that such observed resemblance of local potential distribution can be completely disappeared by changing supercell structure of the combined system. Therefore the teleported potential profiles over the 2D layer would be an artifact, thus the physical origin reported in the original remote epitaxy paper needs to be investigated. We proposed another epitaxy called thru-hole epitaxy to explain the real seemingly remote epitaxy situation.

Poster No.40

A Deterministic Approach to Find a Common Supercell between Two Similar Crystalline Surfaces

Weon-Gyu Lee[1] and Jung-Hoon Lee[1,*]

[1]*Computational Science Research Center, Korean Institute of Science and Technology (KIST), Seoul 02792, Republic of Korea*

Fundamental properties of two-dimensional (2D) heterojunctions are mainly determined by interface geometries and properties. Here, we propose a new numerical method which is capable of deterministically finding a common supercell between two similar crystalline surfaces such as square-square and rhombus-rhombus lattices. Using the complex plane, we can regard the 2D lattice as the 2D complex vector. Then, the relationship between two surfaces becomes the eigenvector-eigenvalue relationship where an operator corresponds to a transformation matrix. We show that this transformation matrix can be determined by the lattice parameters and rotational angle of two crystalline surfaces without scanning all possible cases. Thus, our method can find the transformation matrix forming the common supercell between two similar crystalline surfaces with $O(\log N_{\max})$ time complexity, where $N_{\max}$ is the maximum index of repetition matrix elements. This is much faster than the conventional algorithm with $O(N_{\max}{}^4 N_\theta)$ time complexity where N_θ is the maximum index of rotational angles. [1] We further find that our method successfully reproduces experimental 2D heterostructures and their moiré patterns. We believe that our deterministic approach can be used for helping to find hidden 2D heterostructures including new moiré patterns.

---

[1] D. Stradi, L. Jelver, S. Smidstrup, and K. Stokbro, *Method for Determining Optimal Supercell Representation of Interfaces*, Journal of Physics: Condensed Matter **29**, 185901 (2017).

---

* jhlee84@kist.re.kr

Poster No.41

First principle calculation insight of modified relaxation time and conductivity about surface boundary scattering

Jin Soo Lee[1], Youngjun Lee[1], Seungjun Lee[1] and Young-Kyun Kwon[1,2]

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

In modern semiconductor industry technology, downscaling for the integration of circuits is essential. It is also important to reduce the power consumption of circuits along with downscaling while keeping low resistivity of interconnects. Copper, the currently-used interconnect material, turns out to rapidly increase its resistivity as circuit integration becomes downscaled. Our research focuses on searching for new interconnect materials that may replace the existing copper. To evaluate the resistivity of various materials, we perform first-principles calculations that include the electron-phonon interactions explicitly. We also develop a new method, which takes into account the reduction of the electron mean free paths. This method predicts the resistivity values of various materials varying due to not only the thickness, and the surface and transport directions of interconnect materials, but also the anisotropicity of their Fermi surfaces. Such modified electrons mean free paths, which can be converted to modified relaxation times, and the group velocities obtained from their electronic structures are used to solve the Boltzmann transport equation. Our evaluated size- and direction-dependent resistivities of various materials are compared to the experimentally observed values available and the fitted values based on the FS theory. We believe that our method model provides a more sophisticated and theoretical exploration of new candidates for interconnect materials.

Poster No.42

First-principles investigation of electron-phonon coupling in superconducting Lacunar spinel GaTa4Se8

Chulwan Lee [1] , Min Yong Jeong [1] , Myung Joon Han [1]

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

GaTa4Se8 has attracted attention for its interesting physics, such as Jeff = 3/2 Mott insulating phase, insulator-metal transition, and superconducting phase under high pressure. Due to the intriguing spin-orbital coupled Jeff=3/2 ground state, pressure-induced superconductivity has been studied in the viewpoint of unconventional superconductivity [1, 2]. In this work, we calculated electron-phonon coupling and phonon-mediated superconducting critical temperature (TC) under pressure via the first-principles method. We found that the calculated TC by the Allen-Dynes equation yielded 8.4 K at 20 GPa, which is close to the experimental result [3]. This implies that the electron-phonon coupling can play the main role in the superconductivity of GaTa4Se8. Additionally, we examined the dynamical stability of the cubic structure and found that the cubic phase becomes stable at 20 GPa.

[1] M. J. Park, et al., npj Quantum Mater. 5, 41 (2020)
[2] M. Y. Jeong, et al., Phys. Rev. B 103, L081112 (2021)
[3] M. M. Abd-Elmeguid, et al., Phys. Rev. Lett. 93, 126403 (2004)

Poster No.43

Ferromagnetism in two-dimensional rhodium oxide

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

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

Minseok.choi@inha.ac.kr

The emergence of magnetism in two-dimensional (2D) materials has been attracted attention as an ideal platform to investigate exotic physical phenomena and technically promising for next generation device applications [1]. According to Mermin-Wagner theorem [2], the long-range magnetic order is unstable in 2D system due to the thermal fluctuation. However, the magnetic anisotropy is able to remove this restriction and hence stabilizes the long-range magnetic order in 2D system. In this work, we investigated the magnetic ordering in 2D RhO_2. Density functional $+U$ calculations and Monte Carlo simulations were employed by considering the various of 2D magnetic configurations including in-plane and out of plane magnetic ordering. The effects of mechanical strain on the magnetic property was also examined. Our results show that 2D RhO_2 prefers the out-of-plane ferromagnetic phase, providing the possibility for applications such as spintronic devices. In addition, magnetic anisotropy of 2D RhO_2 is enhanced by strain.

[1] K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, Y. Zhang, S. V. Dubonos, I. V. Grigorieva and A. A. Firsov, Science, 2004, **306**, 666.
[2] N. D. Mermin and H. Wagner, Phys. Rev. Lett. **17**, 1133 (1966)

Poster No.44

Electronic structure of solid energetic materials, from first principal calculations within TB-mBJ exchange potentials

Prathap kumar Jharapla[1] and G. Vaitheeswaran[2]

[1]*Department of Physics, University of Seoul, Seoul 02504, Korea*

[2]*School of Physics, University of Hyderabad, Hyderabad 500046, India*

The ease with which an energetic material (explosives, propellants, and pyrotechnics) can be initiated is a critical parameter in assessing their safety and application. Traditional methods for determining impact sensitivity characteristics include expensive and dangerous experiments. In order to forecast impact sensitivities for a variety of chemically, structurally, and energetically different materials, electronic band structure calculations were carried out. The idea is that the smaller the band gap for energetic materials, the easier it is for electrons to migrate from the valence band to the conduction band, and the more they decompose and burst. This work demonstrates the electronic band structure of the different classes of materials, i.e., alkali metal perchlorates, alkali metal 5-Aminotetrazoles, DBX-1, and Dinitramide-based compounds are all wide band gap insulators. We used the Generalized Gradient Approximation (GGA) for the structural optimization and the Tran-Blaha modified Becke-Johnson (TB-mBJ) potential for an improved description of the electronic band structure.

Acknowledgments: P. Kumar Jharapla has been partly supported by the Korean NRF grant number NRF-2020R1A2C3009142.

Poster No.45

Pseudospin rotation in graphene

Jiwon Jeon, Youngjae Kim, and J.D. Lee*

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

Pseudospin, a degree of freedom in a two-level quantum system of two sublattices, is a basic quantum number posing the fundamental symmetry prone to the electronic nature of graphene. We propose an extended Hamiltonian to involve the SU(2) rotation of pseudospin for the electron-phonon scattering, which has a significant merit over the conventional second-quantized polar coupling. A phonon satellite accompanied by an electron linearly pumped to the upper Dirac cone corresponds to a rotated pseudospin within a scheme of the time-resolved photoemission spectroscopy (TRPES), which is found to carry nonzero angular momenta and induce nonvanishing Berry curvatures through the dichroic mode of TRPES. A phonon bringing the pseudospin rotation is identified to be an elliptically polarized one, which compensates angular momenta delivered to the pseudospin. This is an indication of the chiral phonon excitation without the circularly polarized pulse pumping. Our findings suggest that a controlled generation of phonon build up a new roadmap for engineering the Berry curvature and topology in the Dirac semiconductors.

Poster No.46

Ferroelectric Polarization Effect of Perovskite ABO3 Substate on Magnetic Anisotropy Energy of Fe Layer

Dameul Jeong[1], Seoung-Hun Kang[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*

CMOS-based conventional semiconductor devices have recently come close to a 5nm or 3nm process. But, chip scaling is always accompanied by quantum mechanical problems. A quantum tunneling effect and excessive heat by narrow circuits are typical examples. Many researchers have tried to develop spin-based devices and spintronics over the past few decades to break limitations. Recently Intel proposed spin-based devices called MESO devices on two main mechanisms: spin-charge conversion and spin switching of a ferromagnetic made of La-doped BiFeO3, a multiferroic material. The key issue is replacing intractable multiferroic materials and how to control magnetic anisotropy energy to make switching easier. Using the first-principles density functional theory, we investigate the magnetic properties of Fe layers stacked on various ferroelectric oxides ABO3, where A is one of the alkaline earth metals (Ca, Sr, or Ba) and B is a transition metal in the titanium group (Ti, Zr, or Hf). We reveal the effects of the spontaneous polarization of ABO3 as well as of different elements A and B on the magnetic anisotropy energy of an Fe single layer. Such dependence effects on MAE can be universally described by a few descriptors obtained through machine learning.

Poster No.47

Topological Breathing Kagome Lattice Hidden in Hexagonal Transition Metal Dichalcogenides

Jun Jung[1] and 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*

A Kagome lattice, formed by triangles of two different directions with a star of David pattern, is known to host many emergent quantum phenomena. Breathing anisotropy of bond strength induces a non-trivial higher-order topological insulator (HOTI). Due to the mismatch between the atomic site and the Wannier center, topologically protected corner states emerge. Experimental realizations of topological breathing Kagome lattices have been reported for many artificial systems, but not for simple natural materials with an electronic breathing Kagome lattice. Here we show that a breathing Kagome lattice and HOTI are hidden inside the electronic structure of hexagonal transition metal dichalcogenides (h-TMD). Due to the trigonal prismatic symmetry, sp^2-like hybrid d orbitals form an electronic Kagome lattice with breathing anisotropy of inter-site and on-site hoppings. We demonstrate that h-TMD triangular nanoflakes host topologically protected corner states, which could be quantum-mechanically entangled with triple degeneracy. Because h-TMDs are easily synthesizable and stable with a large bandgap at ambient conditions, our findings open a new avenue for quantum physics based on simple condensed matter systems.

Poster No.48

Charge density phase diagram of a 2DEG in a confined ribbon through density functional theory calculations

Woon Hyung Cho[1,2], Jeil Jung[1,2,*]

[1] *Department of Physics, University of Seoul, Seoul 02504, Korea*

[2] *Department of Smart Cities, University of Seoul, Seoul 02504, Korea*

The negative compressibility and other instabilities in a 2DEG is expected at higher densities than in a 3DEG due to an effective strengthening of the Coulomb interactions in low dimensions. We discuss the charge density instability of a 2DEG in a confined 2DEG ribbon geometry by means of the Kohn-Sham density functional theory within the local spin density approximation. We obtain the phase diagram of the non-magnetic (NM), ferromagnetic (FM) and antiferromagnetic (AF) Kohn-Sham solutions as a function of average carrier density, and resolve the charge density profiles that accompany the ferromagnetic (FM) and antiferromagnetic (AFM) solutions. We find that for rs $\lesssim$ 6 the NM state has the lowest total energy, while the AFM phase is favored in all the other cases. We define a contrast function in the density maxima and minima to show that a charge density instability in either AFM or FM phase is triggered near rs $\sim$ 14 where the second derivative of the total Hartree energy with respect to rs goes to zero. Our self-consistent calculation suggests that the main driving force of the inhomogeneous charge density instability is the relative dominance of the Hartree over the band-kinetic energy, while a full treatment of the exchange-correlation beyond the local density approximation is desirable for a more reliable study of inhomogeneous density systems.

Acknowledgments: W.H.C. was supported by the Korean Ministry of Land, Infrastructure and Transport (MOLIT) from the Innovative Talent Education Program for Smart Cities, and J. J. acknowledges Samsung Science and Technology Foundation under project SSTF-BAA1802-06.

Poster No.49

Accelerating discovery of thermoelectric materials via machine learning

Yelin Joo[1], Minsu Choi[1], Seulyoung Park[1] and Jaichan Lee[*1]
*Corresponding author: jclee@skku.edu

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

Thermoelectric material, which converts thermal energy into electrical energy and vice versa, is considered outstanding energy-harvesting material. Despite various endeavors to discover a new thermoelectric (TE) material, Figure of Merit (ZT) of TE material has not yet reached desired state of 2.0 at 300K. Recently, emerging machine learning (ML) techniques to predict material property using relevant structure information has broaden the horizons for the ongoing pursuit of novel TE materials. In this work, we construct a TE database with 819 compounds and employ LightGBM algorithm with in-house feature engineering code to predict ZT. Our model shows a coefficient of determination larger than 0.85. Within the prediction model, we present an outstanding ZT prediction ML model with dramatically reduced computational cost compared to DFT.

Poster No.50

First-principles study of the rotation-compatible polar structures in perovskite $CaSnO_3$

Min Chul Choi [1] and Se Young Park[1*]

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

In many perovskite oxides, ferroelectricity is known to be intimately related with octahedron rotation patterns in which the polar distortions can be suppressed or enhanced, depending on the octahedral rotation patterns. Using first-principles density functional theory, we present a workflow to identify materials with switchable polar distortions. In the workflow, phonon dispersions are systematically calculated for each of the rotation patterns commonly observed in perovskite oxides to identify unstable polar modes, until the metastable polar structures are obtained. We apply the workflow to perovskite $CaSnO_3$ and find that materials with $a^+a^+a^+$, $a^-a^-a^-$, and $a^+a^+c^-$ rotation patterns have metastable polar structures. Further study of the polar $a^-a^-a^-$ structure having lowest energy among the identified metastable polar structures shows the polarization comparable to conventional ferroelectrics. Possible candidates of substrate materials on which the polar $a^-a^-a^-$ structure can be stabilized are discussed. Our work, identifying metastable polar phases by changing octahedral rotation patterns, provides guidelines for designing new ferroelectric materials in thin-film/substrate configurations utilizing interfacial coupling.

Poster No.51

Green-Kubo lattice thermal conductivity of phase-change material GeTe by machine-learning potential

Young-Jae Choi and Seung-Hoon Jhi*

Department of Physics, Pohang University of Science and Technology, Cheongam-ro 77, Pohang 37673, South Korea

* E-mail: *jhish@postech.ac.kr*

Machine-learning potentials (MLP) are proving their capabilities to calculate atomic structure and lattice dynamics of universal materials. Computation of phonon and thermal transport properties of materials at large scale is especially benefited from MLP simulations. The Green-Kubo formula, which relate the lattice thermal conductivity and the thermal fluctuation, applies to any material regardless of its anharmonicity and structural disorder. Here, we calculate the lattice thermal conductivity of the phase-change material GeTe by using Deep-potential (DeepPot-SE) package and the Green-Kubo formula to be about 2.8 W/mK at room temperature.

Poster No.52

Effects of Hubbard *U* and inter-site *V* interactions on magnetic ordering of monolayer 1T-VSe_2

Tran Van Quang[1,2], Miyoung Kim[3], and Hanchul Kim[1,3,*]

[1] *Institute of Advanced Materials and Systems, Sookmyung Women's University, Seoul 04310, Korea*
[2] *Faculty of Electronics and Telecommunications, VNU University of Engineering and Technology, Hanoi 100000, Vietnam*
[3] *Department of Applied Physics, Sookmyung Women's University, Seoul 04310, Korea*

Abstract. Monolayer (ML) 1T-VSe_2 has been of great interest due to its exotic properties, such as various charge-density waves, theoretically predicted ferromagnetism, and frustrated antiferromagnetic order. In this report, we study the correlation effects of ML 1T-VSe_2 on its magnetic properties by carrying out density functional theory (DFT) calculations with different descriptions of correlation: The conventional DFT with the Perdew-Burke-Erenzerhof generalized gradient approximation (GGA), DFT+*U* with both the empirical [1] and the self-consistent *U*, i.e. ACBN0 [2], and DFT+*U*+*V* with self-consistent *U* and *V*, where *U* and *V* stands for the on-site Hubbard *correlation* and the inter-site *V* Coulombic interactions [3]. For the DFT+*U* calculations with the empirical *U*, we have swept the *U* value from 0.0 to 2.5 *eV*. We find that all the four methods predict the stability of the ferromagnetic (FM) state over the paramagnetic (PM) state. The calculated magnetic moment (m) is 0.64 μ_B with GGA, which is in agreement with previous calculations [4]. For the DFT+*U* empirical *U*, m varies monotonically with *U* from 0.64 to 1.23 μ_B. The self-consistent *U* from the ACBN0 calculation is 2.1 *eV*, and the resulting m is 1.22 μ_B. The self-consistent DFT+*U*+*V* calculation yields *U*=1.7 eV for V-3d. Regarding the inter-site *V* parameters, *V* between V-3p and Se-4s and Se-4p orbitals are calculated to be the dominant one. The calculated m is 1.00 μ_B. The magnetization energies, which are the energy differences between the FM and the PM, $\Delta E \equiv E_{\mathrm{FM}} - E_{\mathrm{PM}}$, are -16.6, -290.5, -584.7, and -845.6 $eV/1 \times 1$, for GGA, DFT+*U* with empirical *U*=2.0 eV, ACBN0, and DFT+*U*+*V*, respectively. The magnetization energies obtained by GGA and DFT+*U* with empirical *U* are in agreement with previous calculations [4].

References

[1] M. Cococcioni and S. De Gironcoli, Phys. Rev. B **71**, 035105 (2005).
[2] L. A. Agapito, S. Curtarolo, and M. B. Nardelli, Phys. Rev. X **5**, 1 (2015).
[3] S. H. Lee and Y. W. Son, Phys. Rev. Res. **2**, 043410 (2020) (2020).
[4] M. Esters, R. G. Hennig, and D. C. Johnson, Phys. Rev. B **96**, 1 (2017).

---

* Email: hanchul@sookmyung.ac.kr

Poster No.53

DFT Study on the Local Atomic Arrangement Effect of CuZn Alloy on Ethylene and Ethanol Product Selectivity of CO2RR

Deokgi Hong[1], Yeji Baek[2], Hakhyeon Song[2], Sungwoo Lee[1], Young-Chang Joo[1], Jihun Oh[2], and Gun-Do Lee[1*]

[1] *Seoul National University*

[2] *Korea Advanced Institute of Science and Technology (KAIST)*

Electrochemical CO_2 reduction reaction (CO_2RR) using Cu-based catalyst has been actively studied as a way to alleviate the problems of global warming and energy shortage. Selectivity control of C_2 products such as ethylene and ethanol among CO_2RR products of Cu catalyst is an important issue due to their high economic efficiency and energy density. Among various approaches to improve the C_2 product selectivity in CO_2RR of Cu-based catalyst, alloying is promising method. However, the complex atomic structure of the active sites on the surface of Cu-based alloys and the limitations of the spatial and temporal resolution of the characterization technique impede our understanding of the origin of the enhanced C_2 product selectivity. In this situation, atomic simulations such as DFT calculations can play a big role. Here, we report a DFT study to understand the relationship between the local atomic arrangement and C_2 product selectivity of CuZn alloys.

Our group conducted electrochemical measurements with CuZn alloy with different Zn compositions and observed an increase in the ratio of ethanol production to ethylene production as the atomic composition of Zn increased. [1] We DFT calculations were performed to understand the change in C_2 product selectivity according to Zn composition and the effect of atomic arrangement on C_2 product selectivity. We classified the atomic arrangement on the CuZn alloy surface into three types of Cu-rich, Zn-rich and Cu-Zn interfacial sites and calculated the free energy change of CO_2RR on the three types of sites. Then we compared the energy changes at the step where the reaction pathways for ethanol production and ethylene production branched. As a result, it was confirmed that ethanol production was more dominant at Cu-Zn interface sites and ethylene production was more dominant at Cu-rich sites. Therefore, as the Zn content increased, the ratio of Cu-Zn interfacial sites increased, and accordingly, the ratio of ethanol production to ethylene production increased.

This study contributes to understanding the effect of the local atomic arrangement of CuZn alloys on C_2 product selectivity and provides insight into the rational design of high-performance CO_2RR catalysts.

[1] Y. Baek, H. Song, D. Hong, S. Wang, S. Lee, Y.-C. Joo, G.-D. Lee and J. Oh, J. Mater. Chem. A, 2022, 10, 9393–9401.

Poster No.54

Inverse Design of Surface Geometries using Generative AI Models

Jae-Yeong Hwang,[1] Weon-Gyu Lee,[1] Sang-Hoon Lee,[2] Young-Woo Son,[2] and Jung-Hoon Lee[1*]

[1]*Computational Science Research Center, Korea Institute of Science and Technology (KIST), Seoul 02792, Republic of Korea*

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

The material space needed to consider for designing new materials is almost infinite. Thus, it is labor-intensive and inefficient to manually find materials with desired properties. Materials development using artificial intelligence (AI) and materials database (DB) is able to overcome this problem. In particular, inverse design technology using generative AI models that can create new structures based on target physical properties will become a core technology in the field of materials design[1–5]. Herein we introduce our Si surface geometry DB generated using an extended Hubbard U+V approach[6] which can more accurately predict the ionization energy as well as the bandgap than semilocal and hybrid functionals. By using this high-quality surface geometry DB, we develop generative AI models and generate new Si slab geometries. We believe that our high-quality slab DB combined with our generative AI models will successfully generate new slab geometries with target surface properties such as the ionization energy.

[1] Sanchez-Lengeling and Aspuru-Guzik, Science **361**, 360 (2018).

[2] Noh, Kim, Stein, Sanchez-Lengeling, Gregoire, Aspuru- Guzik, Jung, Matter **1**, 1370 (2019).

[3] Kim, Lee, and Kim, Sci. Adv. **6**, 9324 (2020).

[4] Court, Yildirim, Jain, and Cole, J. Chem. Inf. Model. **60**, 4518 (2020).

[5] Kim, Noh, Gu, Aspuru-Guzik, and Jung, ACS Cent. Sci. **6**, 1412 (2020).

[6] Lee and Son, Phys. Rev. Res **2**, 043410 (2020).

* jhlee84@kist.re.kr