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제15회 고등과학원

전자구조 계산학회

일시 : 2019년 7월 4일 (목) - 7월 5일 (금)
장소 : 고등과학원 1호관 대강당

KIAS 고등과학원
KOREA INSTITUTE FOR ADVANCED STUDY

PROGRAM AND ABSTRACTS

제 15회 고등과학원

전자구조계산학회

2019년 7월 4일(목) ~ 7월 5일(금)

고등과학원 1호관 대강당

초청연사

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7월 4일 (목)		**7월 5일 (금)**	
8:30 – 9:20 등록		**8:30 – 9:30 등록**	
9:20 – 9:30 환영인사			
Session I: **기계학습응용** **(Applications of Machine Learning 1)** **좌장 장기주** **(한국과학기술원)**	**09:30 - 10:10** 한승우 (서울대) Neural network potential: fundamentals and applications **10:10 - 10:50** 이훈표 (강원대) Machine Learning in combination with many-body numerical approaches	**Session VII:** **상호작용 현상 2** **(Correlated Phenomena 2)** **좌장 김용성** **(한국표준과학연구원)**	**9:30 - 10:10** 민병일 (포항공대) Revisit to Rare-Earths : electronic structures and topological properties **10:10 - 10:50** 김흥식 (강원대) Ab initio dynamical mean-field study of spin-orbital-lattice interplay in correlated oxides and chalcogenides
10:50 – 11:10 휴식		**10:50 – 11:10 휴식**	
Session II: **상호작용 현상 1** **(Correlated Phenomena 1)** **좌장 이재찬** **(성균관대)**	**11:10 - 11:50** 최형준 (연세대) DFT+DMFT study of electron correlation in surface-doped FeSe layer **11:50 - 12:30** **김수란 (경북대)** Apical ion dynamics-Modulated In-plane Properties of Cuprate Superconductors	**Session VIII:** **방법론** **(Computational Methods)** **좌장 서호성** **(아주대학교)**	**11:10 - 11:50** 한명준 (한국과학기술원) Natural orbital, quantum entropy and the electronic structure of correlated materials **11:50 - 12:30** 류훈 (한국과학기술정보연구원) Million Atomic Simulations with a Tight-binding Approach: 10nm-scale Perovskite Optoelectronics
12:30 – 13:50 점심식사		**12:30 – 13:40 점심식사**	
Session III : **고성능 계산** **(High Performance Computing)** **좌장 이인호** **(한국표준과학연구원)**	**13:50 - 14:30** 염민선 (한국과학기술정보연구원) Electronic structure calculations on the KISTI supercomputer-5 **14:30 - 15:10** 신정호 (한국화학연구원) Infrastructure for Data-driven Materials Science: NOMAD Laboratory and FAIRmat	Session IX: 위상물질 (Topological Materials) 좌장 지승훈 (포항공대)	**13:40 - 14:20** 박철환 (서울대학교) Landau bands in Weyl and Dirac semimetals **14:20 - 15:00** 김정우 (인천대학교) Ferroelectricity-driven Berry curvature dipole with switchable charge and spin photogalvanic effect in the SnTe monolayer
15:10 – 15:30 휴식		**15:00**	
Session IV : **저차원물질** **(Low Dimensional Materials)** **좌장 박창원** **(IBS-CALDES)**	**15:30 - 16:10** 김한철 (숙명여대) Adatoms, Charge-Density-Wave, and Solitons in a Quasi-One-Dimensional Metal: In/Si(111)-4×1 **16:10 - 16:50** 황정운 (전남대학교) ZnO composite nanolayer with mobility edge quantization	**Session X :** **시상 및 폐회** **좌장 손영우** **(고등과학원)**	우수 포스터 시상식 및 폐회
16:50 – 17:10 휴식			
Session V: **기계학습응용 2** **(Applications of Machine Learning 2)** **좌장 조영미** **(삼성디스플레이)**	**17:10 - 17:50** 최윤석 (삼성종기원) Discovery of Organic Molecules with Artificial Intelligence **17:50 - 18:30** 이주형 (광주과기원) Massive screening for cathode active materials using deep neural network		
Session VI: **포스터 발표** **좌장 김세중** **(과학기술연합대학원대학교)**	**18:30 - 20:30** 포스터 발표 및 저녁식사		

Talk Abstracts

Talk No.1

Neural network potential: fundamentals and applications

Dongsun Yoo, Wonseok Jeong, Kyuhyun Lee, Dongheon Lee, Kyeongpung Lee,
Seungwu Han

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

Recently, machine-learning (ML) approaches to developing interatomic potentials are attracting considerable attention because it is poised to overcome the major shortcoming inherent to the classical potential and first-principles method, i.e., difficulty in potential development and huge computational cost, respectively. Favored ML models are the neural network and Gaussian process. In particular, the high-dimensional neural network potential (NNP) suggested by Behler and Parrinello is attracting wide interests with applications demonstrated over various materials encompassing metals, insulators, semiconductors, and molecular clusters. In this presentation, we first discuss on the fundamental aspect of ML potentials that enables the transferability of the potential.[1] We show that the transferable atomic energy can be defined within the density functional theory, which means that the core of machine-learning potentials is to deduce a reference atomic-energy function from the given set of total energies. By utilizing invariant points in the feature space at which the atomic energy has a fixed reference value, we examine the atomic energy mapping of neural network potentials. Examples on Si consistently supports that NNPs are capable of learning correct atomic energies. However, we also find that the neural network potential is vulnerable to 'ad hoc' mapping in which the total energy appears to be trained accurately while the atomic energy mapping is incorrect in spite of its capability. We show that the energy mapping can be improved by choosing the training set carefully and monitoring the atomic energy at the invariant points during the training procedure. The energy mapping in multi-component systems is also discussed. We also introduce our in-house code for training and executing NNP called SIMPLE-NN (SNU Interatomic Machine-learning PotentiaL packagE-version Neural Network) [2] and discuss its unique feature such as GDF weighting [3]. We present application examples on the oxidation of Si-SiO_2 interface, phase change behavior of GeTe and Sb_2Te_3, silicidation process of Ni.

[1] D. Yoo et al, arXiv:1903.04366 [physics.comp-ph]
[2] K. Lee et al, Computer Physics Communications, in press.
(doi.org/10.1016/j.cpc.2019.04.014)
[3] W. Jeong et al, Journal of Physical Chemistry C **122**, 22790 (2018)

Talk No.2

Machine Learning in combination with many-body numerical approaches

Hunpyo Lee[1]

[1]Department of Liberal studies, Kangwon National University at Samcheok

We would like to present two subjects. First, an acceleration of continuous time quantum Monte Carlo (CTQMC) methods is a potentially interesting branch of work as they are matchless as impurity solvers of a density functional theory in combination with a dynamical mean field theory (DMFT) approach for the description of electronic structures of strongly correlated materials. Here, we propose the CTQMC method in combination with a machine learning (ML) technique, which would eliminate the computationally time-consuming need for multiplication of the matrix with the non-interacting Green's function. We find that this method predicts the accurate double occupancy, impurity Green's function and four-points vertex function at low temperature, and also considers the physical properties of high Matsubara frequency in a much shorter computational time than the conventional CTQMC method.

Second, we would like to talk about the ML on semi-classical approximation (SCA) for 3D Hubbard model. In brief, even though the SCA approach ignores the charge and dynamical fluctuations, it can capture the long-range spin fluctuations given by the Hubbard-Stratonovich transformation. Therefore, it is adaptable to analyze the physical properties on the lattice systems beyond DMFT approximation. Here, we employ the convolutional neural network (CNN) and convolutional auto-encoder approaches on configurations of the spin fluctuations to classify the phases and to predict physical properties, respectively. Our results are comparable with those obtained by determinant quantum Monte Carlo in combination with ML.

Talk No. 3

DFT+DMFT study of electron correlation in surface-doped FeSe layer

Hyoung Joon Choi

Department of Physics, Yonsei University, Seoul, Korea

The single-unit-cell-thick electron-doped FeSe layer has been attracting enormous attention for high-temperature superconductivity and strong electron correlation that is enhanced with the doping. Since the doping makes Fe 3d orbitals away from half filling, the enhancement is quite anomalous. Here we investigate electronic structure of potassium-dosed FeSe layers using the density functional theory combined with the dynamical mean-field theory. We show that K dosing induces the charge transfer from K atoms to the topmost FeSe layer, and subsequently, ionized K atoms generate a strong local electric field. Role of this charge-transfer induced electric field is discussed with emphasis on its impacts on the electronic structure and electron correlation among Fe 3d orbitals. By controlling the concentration of K atoms, we systematically investigate the evolution of the electronic structure of both FeSe mono- and bilayers. Notably, K dosing reduces bandwidths of the Fe 3d bands near the Fermi level and significantly enhances electron correlation. We also discuss the structural changes of FeSe layers due to K dosing. Our results illustrate that charge transfer from external agents to FeSe layers can have substantial effects other than electron doping and account for their enhanced electron correlation. This work was supported by NRF of Korea (Grant No. 2011-0018306) and KISTI supercomputing center (Project No. KSC-2017-C3-0027).

[1] Young Woo Choi and Hyoung Joon Choi, Role of Electric Fields on Enhanced Electron Correlation in Surface-Doped FeSe, Phys. Rev. Lett. 122, 046401 (2019).

Talk No. 4

Apical ion dynamics-Modulated In-plane Properties of Cuprate Superconductors

Sooran Kim[1,2], Xi Chen[2], William Fitzhugh[2], and Xin Li[2]

[1]*Department of Physics Education, Kyungpook National University, South Korea*
[2]*John A. Paulson School of Engineering and Applied Sciences, Harvard University, USA*

For copper-based superconductors, the maximum superconducting transition temperature $T_{c,max}$ of different families measured from experiment can vary from 38 K in La_2CuO_4 to 135 K in $HgBa_2Ca_2Cu_3O_8$ at the optimal hole doping concentration. We demonstrate herein, using *ab initio* computations, a new trend suggesting that the cuprates with stronger out-of-CuO2-plane chemical bonding between the apical anion (O, Cl) and apical cation (e.g., La, Hg, Bi, Tl) are generally correlated with higher $T_{c,max}$ in experiments. We then show the underlying fundamental phenomena of coupled apical charge flux and lattice dynamics when the apical oxygen oscillates vertically. This triggers the charge flux among the apical cation, apical anion, and the in-plane CuO4 unit. The effect not only dynamically modulates the site energy of the hole at a given Cu site to control the in-plane charge transfer energy, but also can modulate the in-plane hole hopping integral simultaneously in a dynamic way by the cooperative apical charge fluxes.

[1] S. Kim, X. Chen, W. Fitzhugh, and X. Li, Physical Review Letters, 121, 157001 (2018)

Talk No. 5

Electronic structure calculations on the KISTI supercomputer-5

Han Seul Kim and Min Sun Yeom

[1]*Center for Supercomputing Applications, Div. of National Supercomputing, Korea Institute of Science and Technology Information, 245 Daehak-ro, Yuseong-gu, Daejeon, Korea 34141*

KISTI-5 system is the world's 13th-fastest supercomputer with a computation speed of 25.7 petaflops. Through the KISTI-4 system, we supported about 1,500 creative R&D projects and 86 grand challenge projects to create numerous outstanding scientific results. 108 creative R&D projects had already been selected for KISTI-5 systems, and 5 grand Challenge projects that use at least 1700 KNL nodes exclusively had been selected. KISTI staffs are supporting optimization and parallelization technologies in order to successfully carry out these projects. Calculation tasks that use more than 4,096 CPU cores account for about 68% of the total computational work. And more than 300,000 calculations per month are being done on KISTI-5 systems. KISTI also provides customized technical support to about 40 small-medium businesses every year. This reduced development time by 61% and development costs by 78%. The KISTI-5 system is also used to resolve national social issues such as Disaster, Traffic, Climate change, Fine dust and so on. Researchers should apply for computing resources via the web page (https://enables.ksc.re.kr).

Talk No. 6

Infrastructure for Data-driven Materials Science: NOMAD Laboratory and FAIRmat

Jungho Shin[1]

[1]*Chemical Data-driven Research Center, Korea Research Institute of Chemical Technology*

As the people in the NOMAD project (https://nomad-coe.eu) have often mentioned “Data is a crucial raw material of the 21st century.”, most important big-data projects in the world focus on a data infrastructure of processing raw data and using information from them for data-driven materials design. For the implementation, collecting data should be promoted as the central role since in the computational materials science field, data have been scattered everywhere in this planet. Such data has never been integrated into one united place and therefore have been used less powerfully. For the last 5 years, there have been enormous efforts to construct huge databases and file repositories such as AFLOW, Materials Projects and OQMD. The NOMAD laboratory is one of those and obviously only a data hub which contains raw data files from all of them: the biggest repository in the world. Since 99 % of the amount of the data are open access, researchers in this community has used them freely with comprehensive big-data services on the web-based data infrastructure; uploading, downloading and sharing data in code-independent format (Repository and Archive) system, searching materials and display of properties (Encyclopedia), analysis tools including machine learning methodology (Big-data Analytics), and remote visualization service and virtual reality (Advanced Graphics). They all are supported by high performance computing usage. Currently, FAIRmat (https://fairdi.eu/fairmat), as its new phase, implements the FAIR data concept: data which meet standards of findability, accessibility, interoperability, and reusability.

Talk No. 7

Adatoms, Charge-Density-Wave, and Solitons in a Quasi-One-Dimensional Metal: In/Si(111)-4×1

Hanchul Kim[1]

[1]*Department of Applied Physics, Sookmyung Women's University, Seoul 04310, Korea*

Indium (In) atomic wires self-assembled on the Si(111) surface is a prototypical quasi-one-dimensional (quasi-1D) system undergoing a structural phase transition from the room-temperature (RT) 4×1 to the low-temperature 8×2 structure at ~120K, which is known to be a charge density wave (CDW) condensation. In this presentation, we will deliver the results on this intriguing system obtained by the combined study of scanning tunneling microscopy experiments and density-functional-theory calculations. Frist, we will briefly introduce the structural and electronic feature of the RT quasi-1D In wires, In/Si(111)-4×1 and its LT CDW phase. Then, we will present the atomic structure of different adatom defects including H, O, and In and their effect on the phase transition. Finally, we will address recently debated issue on solitons (domain walls between degenerate CDW phases), the localized *vs*. extended solitons, and discuss about the intertwinement between In adatoms and solitons which is attributed to the two-dimensional nature of the quasi-1D system.

Talk No. 8

ZnO composite nanolayer with mobility edge quantization

Jeongwoon Hwang[1], Myung Mo Sung[2], and Kyeongjae Cho[3]

[1]*Department of Physics Education, Chonnam National University, Gwangju 61186, Republic of Korea*
[2]*Department of Chemistry, Hanyang University, Seoul 04763, Republic of Korea*
[3]*Department of Materials Science and Engineering, University of Texas at Dallas, Richardson, TX 75080, USA*

In a recent study, we proposed a quantum confined transport phenomenon in a composite zinc oxide (ZnO) nanolayer consisting of quantum dots (QDs) and amorphous domains. In an amorphous semiconductor such as a-Si, the mobility edge defines the practical band gap where electron transports are suppressed. Distinct from those homogeneous amorphous, the composite ZnO nanolayer generates quantized conducting states at the mobility edge due to the quantum confinement phenomenon of QDs. The unique quantized conducting state at the mobility edge, which we refer to as *"mobility edge quantization"*, is attributed to a synergistic effect of localized states within the amorphous domain and quantized states of QDs. The conducting state with mobility edge quantization has low density of states and can effectively limit the number of available carriers, which enables well-defined intermediate current states for multi-value logic transistor applications.

[1] Lee *et al*., Nature Communications **10**, 1998 (2019)
[2] Hwang *et al*., *in preparation*

Talk No. 9

Discovery of Organic Molecules with Artificial Intelligence

Youn-Suk Choi[1]

[1]*Samsung Advanced Institute of Technology*

Discovery of high-performance functional materials is crucial for overcoming various technical issues in modern industries. However, conventional trial-and-error type approach is time-consuming and costly, thus extensive efforts have been devoted toward accelerating and facilitating the development process not only experimentally but also from the viewpoint of materials design. Recently, machine learning has attracted considerable attention, as it can exploit the inherent knowledge in materials database and provide rational guidelines without resorting to prior human knowledge. In this regard, we have developed various deep learning-based molecular discovery techniques such as active learning with exhaustive enumeration, molecular structure optimization, and inverse design to accelerate the materials exploration. These fully data-driven methodologies extracted design rules from previous libraries and, eventually, reduced the time and effort of human researchers to search enormous chemical space by proposing not only target molecules but also rational design paths. This innovation in chemistry, previously unimaginable, was possible with the advent of high-performance computing and artificial intelligence. And their synergistic effect is expected to connect to the field of experiment and further accelerate the materials development.

Talk No. 10

Massive screening for cathode active materials using deep neural network

Joo-Hyoung Lee[1]

[1]*School of Materials Science and Engineering, Gwangju Institute Science and Technology*

The demand for high capacity batteries is ever increasing for various applications including portable electronics, electric zero-emission vehicles and stationary energy storage systems. Tremendous research efforts have been devoted to discovering next-generation battery cathode materials, but finding a magic chemical compound that satisfies all design criteria such as high energy density, flat voltage curve, minimal volume change and low ion migration barrier makes a highly complex problem due to the vast materials space to explore. In this talk, I will describe our recent development that implements an efficient and accurate deep neural network (DNN) model to address this important issue, and results of a massive, accelerated screening of more than 32,000 candidate compounds. A total of three alternative cathode active materials for Mg-ion batteries are identified through DNN and further investigated with *ab initio* density functional theory calculations. Our calculations demonstrate that the proposed candidates not only attain higher energy density than known cathode materials but also maintain low ion-migration energy barrier as well as minimal volume change. These results will shed a new light on designing beyond-Li cathode active materials in future battery applications.

Talk No. 11

Revisit to Rare-Earths : electronic structures and topological properties

Byung Il Min

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

Recent attention to the topological nature in *f*-electron systems greatly revives the research interest in the rare-earth systems. Many studies have been reported to search for nontrivial topological materials, where the Kondo hybridization gap exists, e.g., CeNiSn, $CeRu_4Sn_6$, $Ce_3Bi_4Pt_3$, SmB_6, SmS, and YbB_{12}. However, the topological nature of their mother elements, Ce, Sm, and Yb, supplying the correlated f-electrons to the above Kondo insulator compounds, has not been explored yet. We have investigated the electronic structures of γ and α phases of Ce, based on the dynamical mean-field theory (DMFT) approach combined with density functional theory (DFT). We have found that a narrow *f*-band metal α-Ce has the non-trivial topology of topological-insulator and topological-crystalline-insulator-type nature, and the topological phase transition and the Lifshitz electronic transition occur concomitantly with the γ–α volume collapse transition in Ce [1].

[1] Junwon Kim, Dongchoon Ryu, Chang-Jong Kang, Kyoo Kim, Hongchul Choi, T.-S. Nam, B. I. Min, "Topological Phase Transition in an archetypal *f*-electron Correlated System: Ce" (2019).

Talk No. 12

Ab initio dynamical mean-field study of spin-orbital-lattice interplay in correlated oxides and chalcogenides

Heung-Sik Kim

Department of Physics, Kangwon National University

Thanks to recent developments of electronic structure calculation methods and computational power, the dream of true 'first-principles' study of correlated materials has become even closer. Especially, the combination of ab-initio density functional theory and the so-called dynamical mean-field theory (DFT+DMFT) has been successfully applied for the research of correlated materials and their heterostructures [1]. Furthermore, the achievement of full charge-self-consistency condition in DFT+DMFT, which has been recently implemented [2], enables computational investigation of the spin, orbital, and lattice degrees of freedom correlated materials on an equal footing. In this talk I will briefly introduce our recent results on the spin-orbital-lattice interplay manifested in a deficient spinel chalcogenide compound GaV_4S_8, which has been actively studied for its magnetoelectric coupling and magnetic skyrmion crystal phase [3]. By employing DFT+DMFT method for the V_4 cluster we clarify the nature of the Mott insulating phase to be originated from the V_4 clustering and the resulting tetrahedral molecular orbital formation. Furthermore, from DFT+DMFT structural optimizations, an intriguing relation between the V_4 spin state and the degree of V_4 clustering is revealed, implying a possible nontrivial role of Hund's coupling in determining the crystal structure and magnetoelectric coupling [4]. At the end of the talk I will briefly mention about iridium oxide superlattices which show even more interesting coupling between the charge and crystal structure [5].

References:
[1] G. Kotliar et al., Rev. Mod. Phys. 78, 865 (2006).
[2] K. Haule, J. Phys. Soc. Jpn. 87, 041005 (2018).
[3] I. Kézsmárki et al., Nat. Mater. 14, 1116 (2015).
[4] H.-S. Kim, K. Haule, and D. Vanderbilt, arXiv:1810.09495.
[5] X. Liu, M. Kotiuga, H.-S. Kim et al., submitted.

Talk No. 13

Natural orbital, quantum entropy and the electronic structure of correlated materials

Myung Joon Han[1]

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

Calculating correlated electron materials has been a great challenge in the first-principles methodology, and many different approaches have been suggested for the last decades. In a widely-used framework of so-called LDA+U (local density approximation plus U; or DFT+U) and LDA+DMFT (local density approximation plus dynamical mean-field theory or DFT+DMFT), the still challenging issues include the double-counting problem, analytic continuation and the choice of local subspace projectors. In this talk, after presenting an overview of our recent progress in this field of research, I will focus on the two topics. First, I will report our recent implementation of DFT+DMFT by adopting natural atomic orbitals as a local projector. This new projector not just shows the reasonable description for electron number counting and the local feature, but also has some promising aspects in terms of computation efficiency [1]. In the second part, I will briefly discuss our newly-suggested ideas for analytic continuation problem [2, 3]. By introducing quantum relative entropy, we successfully extend the applicability of maximum entropy method to the off-diagonal matrix elements, which can serve as a useful tool to study, for example, the distorted oxides and the large spin-orbit coupling materials [2]. We also try to use modern machine-learning technique to perform the continuation of imaginary Green's function [3].

[1] J.-H.Sim and M. J. Han, "DFT+DMFT with natural atomic orbital projectors" (submitted)
[2] J.-H.Sim and M. J. Han, "Maximum quantum entropy method" Phys. Rev. B 98 205102 (2018)
[3] H .Yoon, J.-H.Sim and M. J. Han, "Analytic continuation via domain-knowledge free machine learning" Phys. Rev. B 98 245101 (2018)

Talk No. 14

Million Atomic Simulations with a Tight-binding Approach: 10nm-scale Perovskite Optoelectronics

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Electronic structure simulations of realistically sized atomic structures are important as they can not only predict properties of physically realizable novel materials, but accelerate potential designs of advanced nanoscale devices. This talk covers discussion of (1) the performance of our in-house code for tight-binding simulations of large-scale electronic structures including up to 10^7 atoms, which has been accelerated with a parallel computing on P100 GPU clusters [1] and the Intel® KNL-based NURION system [2], and (2) the latest research work done with the code, which proposes ways to design metal-halide-perovskite (MHP) materials that are robust to the phase-separation-induced red-shift, demonstrating a potential blueprint for stable light-emitting source designs with MHPs [3].

References

[1] H. Ryu *et al.*, Fast, energy-efficient electronic structure simulation for multi-million atomic systems with GPU devices, *Journal of Computational Electronics* **17**, 2, 698-706 (2018)
[2] H. Ryu, Massively scalable computing method to tackle large eigenvalue problems for nanoelectronics modeling, *Intel® eXtreme Performane User Group Meeting* (2019)
[3] H. Ryu *et al.*, Role of Quantum Confinement in 10 nm Scale Perovskite Optoelectronics, *Journal of Physical Chemistry Letters* **10**, 2745-2752 (2019)

Talk No. 15

Landau bands in Weyl and Dirac semimetals

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In this presentation, I will discuss the Landau band structures of Weyl semimetals [1] and Dirac semimetals [2]. The focus will be two folds: (1) the coupling between the Weyl or Dirac nodes due to the magnetic field and (2) our k.p method based on first-principles maximally-localized Wannier functions.

[1] P. Kim, J. H. Ryoo, and C.-H. Park, "Breakdown of the Chiral Anomaly in Weyl Semimetals in a Strong Magnetic Field," Phys. Rev. Lett. 119, 266401 (2017).
[2] P. Kim, J. H. Ryoo, and C.-H. Park, unpublished

Talk No. 16

Ferroelectricity-driven Berry curvature dipole with switchable charge and spin photogalvanic effect in the SnTe monolayer

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The concept of Berry curvature (BC) is becoming important due to its unique behaviors in various topology- and transport-related phenomena. In symmetry-broken crystalline solids, BC is established from the quantum geometry hidden in the electronic structure. For example, the monopole component of the BC is created by the time-reversal symmetry breaking, and the BC dipole arises from a lack of inversion symmetry, thereby giving rise to the anomalous Hall and nonlinear Hall effects, respectively. In this talk, I will show the ferroelectricity in a van der Waals monolayer of SnTe develops an intriguing BC structure, which offers charge- and spin-controllable photocurrents by manipulating the photon handedness and the ferroelectric polarization. Even with the sizable band gap of the SnTe monolayer, the BC dipole is comparable to those of small-gap or gapless topological materials. I will also discuss that the fundamental origin of the ferroelectrically driven BC is closely related to an orbital angular momentum texture, referred to as the orbital Rashba effect.

Poster Abstracts

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제 15회 고등과학원 전자구조계산 학회

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Poster 1

Designing high-performance CdSe nanocrystal thin-film transistors based on one-step process of ligand exchange and simultaneous doping

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We investigate a simple, solution-based, and post-synthetic process for ligand exchange and simultaneous doping of CdSe nanocrystals (NCs) to design high-performance field-effect transistors (FETs). Indium plays a crucial role in enhancing the mobility of $InCl_3$-treated CdSe NCs as donors [1]. Using the first principle calculation, we have proved that halogen, as well as indium, have a significant influence on mobility. The halogen states are formed closer to the valence band edge as the atomic number of halogens increases. Therefore, electron carriers can be easily trapped in these acceptor states, inhibiting efficient intra-nanocrystal charge transport and leading to low mobility in InI_3-treated CdSe NC FETs. This result not only matches well with our experiments but also provides a fundamental understanding of the electronic structure and charge transport behavior of quantum dots.

[1] Sayevich, V, *et al., Adv. Funct. Mater.* **26**(13), 2163 (2016).

Poster 2

First-principles study of pressure effect on electronic properties of few layer Y_2C elecctride

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Di yttrium carbide(Y_2C) is a two-dimensional electride, which is an ionic material where electrons behave anions. Recently, Y_2C has been successfully synthesized.

We study pressure effects on the electronic properties of few-layer Y_2C. We consider 2 and 4% compression, 2 and 4% stretch in the direction of normal to the layer.

Our calculations were based on density functional theory. For the study, we employed the Vienna Ab initio Simulation Package (VASP). The cutoff energy was 600 eV and the generalized gradient approximation was used for the exchange-correlation functional.

The compression (stretch) causes higher (lower) electron density at the interstitial space, and shift the energy bands up (down) by ~0.1 eV in band structures. Our results show that the Fermi velocity is also decreased (increased) when interlayer gap becomes narrower (wider).

Poster 3

First-principles-based calculation of branching ratio for 5*d*, 4*d*, and 3*d* transition metal system

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X-ray techniques have been established as one of the most standard approaches for physics research and its calculations are conducted by various methods such as independent particle approximation, Bethe-Salpeter equation, real-space multiple scattering theory, and time-dependent density functional theory. A new first-principle computation scheme to calculate ‘branching ratio’ has been applied to various 5*d*, 4*d*, and 3*d* transition metal elements and compounds. This recently suggested method is based on a theory which assumes the atomic core hole interacting barely with valence electrons [1, 2]. While it provides an efficient way to calculate the experimentally measurable quantity without generating spectrum itself, its reliability and applicability should be carefully examined especially for the light transition metal systems. Here we select 32 different materials which cover not only elements but also Mott insulators and compare the calculation results with experimental data. We also check the dependency of branching ratio about orbital basis. It is found that our scheme well describes 5*d* and 4*d* transition metal systems whereas, for 3*d* materials, the difference between the calculation and experiment is attributed to the neglect of core-valence interaction which is not well described in multi-d valence orbital system in any other methods.

[1] J.-H. Sim, H. Yoon, S. H. Park, and M. J. Han, *Physical Review B* 94, 115149 (2016)
[2] B. T. Thole and G. van der Laan, *Physical Review A* 38, 1943 (1988)

Poster 4

Prediction of superconductivity in hole-doped perovskite oxyhydride

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We study the superconductivity of a series of oxyhydrides ATiO2H (A=K, Rb, Cs), new hydride superconductor candidates, under hole-doping rather than high pressures. These materials have rich hydrogen states just below the Fermi-level. Thus, the hydrogen-vibration can contribute to the superconductivity under the hole doping condition. The Wannier interpolation scheme is used to calculate the phonon dispersion and the electron-phonon coupling accurately combined with the optimized-tetrahedron method. We found that the critical temperature reaches about 10 K in the optimal doping condition. We showed that 2D-like and quartic dispersion enhanced the softening of the hydrogen vibration and thus the superconductivity.

Poster 5

Releasing the hidden shift current in TTF-CA organic molecular solid by symmetry lowering

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The bulk photovoltaic effect, characterized by the excitation-driven spontaneous photocurrent in the absence of external bias, has attracted significant attention mainly owing to its potential for harvesting solar energy. Here, we investigate the photovoltaic characteristics of organic molecular solids, particularly focusing on the association between the photocurrent and the crystal symmetry in the exemplary case of the tetrathiafulvalene-p-chloranil (TTF-CA). We perform comprehensive first-principles calculations, including the direct evaluation of the excited-state current through the real-time propagation of the time-dependent density functional theory. We find that the charge shifting in the low-temperature phase is mainly driven by the intrachain ferroelectricity, which gives rise to the photocurrent not only at the visible-light range but near the band-edge infra-red region. We discuss that the shift current locked in the symmetry of the high-temperature phase can be released by introducing a potential asymmetry in the perpendicular direction to the chain. We suggest that the photovoltaics of organic molecular solids can be exploited even in high temperatures through an appropriate engineering to lower the symmetry.

Poster 6

Screening Phase-Change Materials by High-Throughput Ab Initio Calculations

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Phase-change material (PCM) has been considered as candidate for next-generation non-volatile memory. These materials have distinct physical properties between amorphous and crystalline phases. PCM operation by detecting the electrical resistance difference between the amorphous and crystalline stats is utilized to encode digital information. However, the key issue of commercial using PCM is its low crystallization speed, which is insufficient to satisfy the requirement of dynamic random access memory (DRAM). Various studies have been conducted to overcome slow crystallization rate. In order to find PCM with a fast crystallization rate, we choose new descriptors and use a massive database for screening method. To identify promising PCM, we screen various compounds of arsenides, nitrides, sulfides, phosphides, chlorides, antimonides, and tellurides, through automated ab initio calculations.

Poster 7

Phosphorus clustering behavior in silicon from First-Principles calculations

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In silicon semiconductor industry, ion implantation is the most common method for improving charge carrier concentration of silicon. However, it is generally true that not all the injected atoms are electrically activated. Thus, ion implantation normally follows by an annealing process that activates the implanted ions. However, electrically inactivated dopant clustering can generate in this process. Therefore, it is necessary to study the phosphorus clustering behavior to control clustering generation. In this study, first-principles density functional theory calculation was employed to identify phosphorus clustering behavior. Our research has focused on energy perspective of phosphorus clustering, in order to identify conditions that make clustering of phosphorus under certain conditions. Based on our understanding, this study will be helped in finding optimal process conditions to minimize clustering.

Poster 8

Atomistic origins of low-resistance metal contacts to phase-engineered MoS_2

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In realizing high-performance electronic devices based on transition metal dichalcogenides (TMDCs), the high contact resistance at the metal-TMDC interface remains a major obstacle to overcome. Recently, the phase engineering of TMDCs has been demonstrated as a promising scheme to achieve low-resistance contacts for ultrathin TMDC transistors, but its atomistic mechanism remains unclear. Here, carrying out density functional theory (DFT) and DFT-based matrix Green's function calculations, we systematically explore the roles of 1T MoS_2|2H MoS_2 and metal/1T MoS_2 interfaces in lowering contract resistance for phase engineered TMDCs by considering different electrode metal species (In, Pd, Au) and the top and edge contact configurations. We demonstrate that the improved charge injection mainly results from the lower contact resistance of the extrinsic metal|1T MoS_2 interface rather than the intrinsic 1T MoS_2|2H MoS_2, counterpart.

Poster 9

First-principles study of quasiparticle energies of bulk and few-layer $PdSe_2$

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We studied the electronic band structure of $PdSe_2$ using the density functional theory (DFT) and the GW method. It is known that $PdSe_2$, a material with stacks of pentagonal layer structure, has a semiconducting band structure experimentally. However, DFT calculations show that bulk $PdSe_2$ has a semi-metallic band structure because of DFT underestimation of the band gap of the material. To obtain the band gap of $PdSe_2$ correctly, we calculated the quasiparticle band structure of bulk $PdSe_2$ using the one-shot GW method and obtained a band gap which is consistent with experimental results. Then we calculated the electronic structure of two-dimensional $PdSe_2$ to investigate the layer-number dependence on the energy gap. We discuss band-to-band transition energies and other physical properties obtained from band structures of $PdSe_2$. This work is supported by the NRF of Korea (Grant No.2011-0018306). Computational resources have been provided by KISTI Supercomputing Center (Project No. KSC-2018-CRE-0097).

Poster 10

Design of two dimensional hetero-structure electrodes via machine learning model

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The importance of rechargeable battery is dramatically increasing since secondary batteries are essential in most of the current and upcoming technologies such as electric vehicle, mobile devices, IoT and renewable energies. However, since the performance of conventional Li-ion battery has been saturated, the next-generation battery is required that has higher capacity and efficiency. A further enhancement for rechargeable battery requires an introduction new electrode materials. Recently, 2D hetero-structure has arisen as a next generation electrode material aiming enhanced capacity, cell potential and stability.[1] By using first-principles calculation based on density functional theory (DFT), those properties of 2D hetero-structure could be predicted in atomic scale. However, massive computational cost is required to screen various 2D hetero-structures as electrode materials, since a huge number of combinations of 2D hetero-structures are possible. Therefore, introduction of machine learning model can greatly enhance the efficiency of searching promising 2D hetero-structure electrodes. In this study, various types of 2D materials combined with graphene, the most widely used anode material, are calculated to find stable Li-ion intercalation sites and the theoretical capacity. From the obtained data, we succeed to develop a machine learning model for intercalation energies for various 2D hetero-structures.

[1] Bediako, D. K., *et al. Nature*, **558**, 425–429 (2018).

Poster 11

Theoretical investigation of α-GeTe phases observed in TEM image

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α-GeTe, which is characterized by the R3m space group in the trigonal crystal system, is the stable equilibrium configuration among various GeTe phases. At the same time, α-GeTe can be classified by the Cm space group, in the monoclinic crystal system containing the trigonal system. Definitely, mentioning the R3m symmetry as the Cm symmetry is symmetry misrepresentation happening when selecting its unit cell differently. It is concerned that this would happen during experimental characterizations. Using various TEM images of GeTe materials and model structures obtained using density functional theory, we carefully characterize the structural symmetries. Our investigation propose that structural characterization would misguide observers to regard the α-GeTe as different phase of GeTe. Finally, we carry out the polarization calculation to explain polarization experiment.

Poster 12

A new insight into the catalytic activity in carbon-based two-dimensional materials *via* bond characteristic analysis

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Due to its high electrical conductivity, light weight, large surface area, stability in both acidic and alkaline media, abundance, and other unique properties carbon-based two-dimensional (2D) materials and their derivatives have been actively studied as one of the most promising candidates. However, these developments are still in an early stage compared to catalytic reactions such as hydrogen evolution reaction, oxygen reduction (or evolution) reaction because of chemically inert properties: very low density of states at Fermi level and no free chemical bonds. For a significant activity improvement, various routes to tune the electronic states are developed and understanding the mechanism also become very important. For this perspective, the density functional theory (DFT) calculations has been highlighted for accelerating the discovery of origin in catalytic reactions.

Based on DFT performing the crystal overlap Hamilton population (COHP) analysis, which provides a framework that effectively connects the local bonding chemistry with the electronic structure, we clarify that the origin of catalytic activity in carbon-based 2D materials is highly related to bond characteristic between active site atom and its adjacent neighboring atoms. These findings are expected to facilitate the understanding the catalytic activity and give a excellent insight for future potential applications such as automated and high-throughput massive calculation.

Poster 13

The origin of n-type 2DEG in the $LaAlO_3/SrTiO_3$ (111) interface

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The emergent discovery of two-dimensional electron gas (2DEG) at the $LaAlO_3/SrTiO_3$ (LAO/STO) heterostructure has attracted considerable attention over the past decade. Recently, unlike LAO/STO (001) interface, a wide n-type 2DEG distribution is reported at the LAO/STO (111) interface (K. Song et al., Nat. Nanotechnol. 13, 198 (2018)). According to the polar catastrophe scenario, the LAO/STO (111) interface consisting of $[Ti]^{4+}$ and $[LaO_3]^{3-}$ layers is expected to exhibit the p-type characteristics. Despite controversies, the origin of n-type 2DEG at the LAO/STO (111) interface has not been revealed yet. Here, we carry out first-principles density functional theory calculations to explore the 2DEG distribution and its origin in the LAO/STO (111) interface. We find that the n-type 2DEG originates from extra electrons created by the oxygen vacancy in the $[LaO_3]^{3-}$ terminated LAO (111) surface, and oxygen vacancies significantly suppress the octahedral rotations in LAO layers. The presence of oxygen vacancy and reduction of octahedral rotations in the vicinity of LAO (111) surface are clearly confirmed by annular dark-field scanning transmission electron microscope image at the atomic scale.

Poster 14

Initial step for hexagonal boron nitride: precursor gas and transition metal surfaces interaction

Garam Park

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Recently two-dimensional (2D) layered materials are very attractive in various fields because of their interesting properties. For this reason, the study for interaction between catalytic metal surface and a precursor molecule such as borazine($B_3H_3N_3H_3$) or benzene(C_6H_6) has been one of the intensive topics of low-dimensional materials. Inevitably, experiments for growth of 2D materials have been influenced by surface atom, the atomic structure of surface and precusor molecules. a computational study of the interaction between molecules and various surfaces can contribute to growth of 2D materials of good quality. In this study, we investigate the adsorption structure and density of states of borazine on the copper, platinum, nickel and iron(111) surface using generalized gradient approximation functional (PBE) including dDsC(density dependent dispersion correction) vdW approximation. As a result, the boron and nitrogen atoms of the molecule are strongly adsorbed on the Ni(111) and Fe(111) surface compared to other surfaces. On the Pt(111) surface, the molecule make only Pt-N pairs with surface atoms and this type of bonding maintains the inherent planar structure of the molecule. The Fe(111) surface has different adsorption sites from other surfaces and the Cu surface has very weak bonds with molecules. We present our analysis for the trend and different behaviors depending on surfaces

Poster 15

Zeeman-splitting induced topological nodal structure and anomalous Hall conductivity in ZrTe5

Yichul Choi, John W. Villanova, and Kyungwha Park

Virginia Tech

Among various three-dimensional (3D) topological materials, ZrTe5 is unique in many aspects. The material exists very near a phase boundary between weak to strong topological insulator (TI), and it showed intriguing transport properties such as chiral magnetic effect and large anomalous Hall effect despite non-magnetic nature of the system. Very recently, the three-dimensional quantum Hall effect has been observed in bulk ZrTe5. Inspired by the recent experiment on the large anomalous Hall effect, we investigate topological nodal structure in 3D ZrTe5 driven by Zeeman splitting as a function of the direction of external magnetic field. We use Wannier-function-based tight-binding model obtained from first-principles calculations including spin-orbit coupling. Depending on the direction of magnetic field, type-I and type-II Weyl nodes or nodal rings are formed. The Hall conductivity arising fromBerry curvature is also computed as a function of the magnetic field direction and chemical potential near the Fermi level. We compare our results with experimental data.

Poster 16

First-Principle Study on the Edge Reconstruction Process in Hexagonal Boron Nitride Sheet in the Strong Electric Field

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Using the first-principles density functional theory and the GW approximation, we investigate the equilibrium edge structures of hexagonal boron nitride (hBN) and their electronic and optical properties. It is found that the armchair edge is the most stable edge structure, and the zigzag edge can be stabilized by the 5-7 reconstruction. Intriguingly we find that the electric field can expedite the reconstruction of the boron-terminated zigzag edge due to the B-N bond polarity, but not of the nitrogen-terminated zigzag edge. Our calculation further shows that boron-terminated zigzag edge exhibits certain gap states, the gap of which corresponds to the near ultraviolet (NUV) luminescence observed in an experiment. We further discuss the correlation of the defect states of various point defects observed in hBN with experimentally-observed luminescence.

Poster 17

Role of Indium in phase change mechanism of Ag- and In-doped Sb-rich SbTe: First Principle Study

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[2]Institute of Physics and Applied Physics, Yonsei University

Among phase change materials for next generation memory device elements, GeTe-Sb_2Te_3 pseudo-binary alloys and Sb-rich alloys have been widely investigated for real applications. Especially, $Ge_2Sb_2Te_5$ has attracted a lot of attentions and been studied intensively on various phase change properties such as recrystalization mechanism. On the other hand, even though they exhibit enhanced performances in phase change behaviors, Sb-rich alloys have been much less studied. Especially Ag-In-Sb-Te alloy exhibiting excellent phase change properties are waiting to reveal their phase change mechanism, such as the roles of Ag and In atoms. Performing intensive molecular dynamics simulations based on *ab initio* density functional theory, we investigate the local structures and phase transition properties of $AgInSb_{18}Te_4$ selected as an exemplary model configuration. We identify its crystalline structure by considering a number of atomic configurations and its amorphous phase through melt-quenching MD simulation. To figure out more specific role of each atoms, we also design and evaluate the phase of $Ag_8In_8Sb_{144}Te_{32}$ forming a 2×2×2 supercell of $AgInSb_{18}Te_4$. Evaluating and analyzing its radial distribution function, angle distribution function, and solid angle distribution, we find that the In atom plays an important role not only in phase transition process, but also in retaining or stabilizing amorphous phase.

Poster 18

First-principles studies of the HfO_2-based ferroelectric tunnel junction

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Owing to the recent advances in the oxide growth technology, ferroelectricity has been stabilized even in a few nm-thick films, which makes it possible to realize the oxides-based ferroelectric tunneling junction (FTJ) combining the quantum-mechanical tunneling phenomena and switchable spontaneous polarization into novel device functionality. Among various ferroelectric oxides, HfO_2 is the most promising material for FTJ devices since it has the great advantage of complementary metal-oxide-semiconductor (CMOS) process compatibility. Despite this considerable attention, the tunneling current mechanism on HfO_2-based FTJ has not been clearly understood yet. Here, using first-principles density functional theory calculations, we explored the tunneling current in the TiN/HfO_2/TiN devices at the atomic scale. From a comparison of experimental results with our calculation, we estimate the atomic structure of experimental results.

This work was supported by the MOTIE (Ministry of Trade, Industry & Energy (#10080643) and KSRC (Korea Semiconductor Research Consortium) support program for the development of the future semiconductor device.

Poster 19

Nature of Symmetry Protected Magnetic Weyl Nodal Loops in $5d^n$ Cubic Double Perovskites

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Recently, topological semimetals, possessed the Dirac (Weyl) nodes near the Fermi level, have been extensively studied theoretically and experimentally due to their exotic properties. When these Dirac(Weyl) nodes form lines, these lines are called the Dirac (Weyl) nodal lines (D(W)NLs). The nodal line leads to a dispersionless surface band connecting two nodal points, dubbed the drumhead states. These drumhead states give rise to the large surface density of states, which is a potential ingredient for the surface superconductivity and magnetism with a high critical temperature. No WNLs without the time-reversal symmetry (TRS) has been realized yet. Thus, it is highly required to find robust magnetic WNLs.

In this presentation, using both *ab initio* approaches and the tight-binding (TB) model Hamiltonian analysis, we will address the nature of topological characters in the fcc-like cubic double perovskites (DPs) with $5d$ orbitals. Our TB model indicates that $dd\sigma$ and $dd\pi$ hoppings lead to nodal lines on the mirror planes of the Brillouin zone. In contrast to TRS preserved cases, where SOC breaks all Dirac nodes, the magnetic Weyl nodal lines protected by the mirror symmetry are robust. These results appear in the cubic DP materials with $5d^1$ ($5d^2$) states. According to our *ab initio* results, the mirror symmetry protected magnetic WNLs are robust in the $5d^2$ state. Due to the strong magnetic anisotropy, these WNLs remain only on the $k_z = 0$ plane, which is perpendicular to the direction of SOC (001). Remarkably, in our calculated anomalous Hall conductivity, this magnetic anisotropy results in a single sharp peak at the energy of WNLs, suggesting these WNLs to be measureable. More detailed analyses about our results will be discussed.

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Poster 20

Development of global optimization algorithm and its application to the study of chemical reaction pathways

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Abstract: We propose a general framework that runs global optimization algorithm. This algorithm utilizes several global minimization methods (e.g. genetic algorithm (GA), conformational space annealing (CSA) and particle swamp optimization (PSO)) to find a target material with several acceleration methods (e.g. Crystal generation using Wyckoff positions and neural network potential (NNP) acceleration). This is an object-oriented code implemented under the framework Atomic Simulation Environment (ASE). To improve the efficiency of this global optimization algorithm, we have tested and implemented the GA-CSA with symmetry constraint (under the Wyckoff space group technique). Further, we embed the NNP algorithm that builds the energy surface based on the data sets that have been conducted during global optimization process. We will check its accuracy with various size of the training data before we apply the method to the study of chemical reaction pathways

Poster 21

First principle predictions for screening low stacking fault energy of $SiVCrMn_{0.3}Fe_{0.5}CoNi$

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In metals or alloys, the planar defect known as stacking fault energy(SFE) is important for improving mechanical properties of these materials. Especially in low-SFE materials, dissociation into partial dislocations is more energetically favorable, and the spacing between the partial dislocations results in twinning. It is generally believe that the twinning increases dislocation storage capacity, strain hardening rate, and ductility, so the low SFE can solves the strength-ductility paradox in structure materials. Recently, it was reported that the specific high entropy alloys(HEAs) have much smaller SFE than conventional alloys. However, due to a number of cases in which HEAs have various kinds of elements and atomic compositions, experimental limitations exist. Overcoming these limitations, the more effective method to screening low-SFE alloys is required.

In this study, we carried out *ab-initio* calculations to investigate the SFE of HEAs. Among these various HEAs, we focus on $SiVCrMn_{0.3}Fe_{0.5}CoNi$ systems. In order to calculate stacking fault energy, the stability of fcc structure is compared with that of hcp structure. According to our results, compositions of the lowest-SFE system are close to $Fe_{0.5}Mn_{0.3}Co_{0.1}Cr_{0.1}$(TRIP-DP HEA), which has extremely high mechanical behavior[1]. Finally, we construct the SFE map of our calculated systems. It can help to select proper alloys in our SFE map.

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Poster 22

First-Principle Study of Charge Transfer at Ta_2O_5/RuO_2 Interface

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RuO_2 is used as catalyst for chlorine evolution reaction (CER) and oxygen evolution reaction (OER). In the mechanism of these reaction, anion adsorption on electrode catalyst is the rate determining step.[1] We assume that electron transfer from RuO_2 to Ta_2O_5 induces higher oxidation state of RuO_2 and it increases adsorption of anions and catalytic activity. In this research, we study the interface structure of Ta_2O_5/RuO_2 by calculation of surficial free energy. And we investigate charge transfer at this interface through work functions based on first-principle calculations in the level of density functional theory. Our research will suggest the better structure of RuO_2 electrode to increase catalytic activity.

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Poster 23

Theoretical understanding on the growth and stacking-fault mechanism of GaAs nanowires grown by catalyst-free method

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The precise control in the growth of GaAs nanowire on commercial Si substrate has been developed to integrate the novel functionalities originated from the one dimensional geometry as well as intrinsic properties. Dislocation and crack caused by the mismatch in lattice constant and thermal expansion coefficient have been effectively reduced by the small contact area between the nanowire and Si substrate. The last remaining difficulty to grow perfect nanowires is the stacking-fault, which is shown to be abundant and randomly distributed to date. In this study, the growth and stacking-fault mechanism in GaAs nanowire is theoretically explained using the nucleation model during the growth of GaAs nanowire using catalyst-free methods. The changes in adsorption behavior and interface energy during the growth are calculated as a function of temperature and pressure using ab-initio thermodynamics [1]. By considering the variation in Gibbs energy of nucleation depending on growth conditions, the reason why the GaAs crystal grows preferentially in one direction is confirmed to be the preferential adsorption on the growing surface. In addition, the origin of experimental observations about stacking-fault behavior depending on growth conditions and direction is thoroughly explained.

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Poster 24

Effects of the molecule-electrode contact configurations on the single-molecule diode performance: A finite-bias first-principles study

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ABSTRACT

Being the fundamental building block of semiconductor devices, realizing large and robust diode effects has been a major goal in the field of single-molecule electronics. Particularly, while the molecule–electrode contact configurations should play a critical role in determining the rectification behavior, their atomistic understanding has been so far incomplete. Herein, carrying out finite-bias first-principles quantum transport calculations based on the multi-space constrained search density functional theory (MS-DFT) we have recently developed [1], we study the correlations between the S–Au linkage coordination numbers [2] and the diode effects in single molecular junctions by analyzing the electrochemical potentials or quasi-Fermi level profile across the channel that are uniquely produced within MS-DFT. We firstly studied the rectification behavior of the junctions with insulating molecule core, in which the molecular core energy levels are much farther away from fermi level and thus the role of Au−S contacts is maximized. Moreover, we deal with the device with non-insulating molecule core and again find out the relationship between the rectification behavior of the junctions and the S–Au linkage coordination numbers.

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Poster 25

Ab initio study of intrinsic anomalous Hall conductivity in ferromagnets

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ABSTRACT

We study intrinsic anomalous Hall conductivity (AHC) of 3d ferromagnetic materials such as Fe, Co and Ni, based on the noncollinear-spin density function theory (DFT) calculation including spin-orbit coupling. We implement the AHC calculation to the SIESTA code which uses localized pseudoatomic orbitals to expand electronic wavefunctions, and test the convergence of AHC with respect to various parameters of the DFT calculation including real-space grids and k-point grids. We also test the dependence of AHC on different types of pseudopotentials, exchange-correlation functionals, and pseudoatomic orbital basis sets. Since the electrostatic repulsion among 3d electrons is underestimated in the local density approximation or the generalized gradient approximation, we also consider the Coulomb interaction parameters, U and J, for 3d electrons and examine their influence on AHC values. We analyze the energy and momentum dependences of the Berry curvature, and compare our AHC values and their temperature dependence with previous theoretical results as well as experimentally measured results. This work was supported by NRF of Korea (Grant No. 2011-0018306) and KISTI supercomputing center (Project No. KSC-2018-CRE-0097).

Poster 26

Atomic energy mapping of neural network interatomic potential

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Machine-learning interatomic potentials are becoming a popular method for large scale simulations that gives nearly the accuracy of ab initio calculations with the cost of classical force-fields. Among many models proposed to date, neural network potential (NNP) and Gaussian approximation potential are the two most popular models. Most machine-learning potentials approximate the total energy of a system as a sum of local atomic energies, which depend on the local chemical environment. They infer underlying atomic energy function from the total energy and atomic forces of ab initio calculations. However, little attention has been paid to the atomic energy function that is actually learned by machine-learning potentials. In this presentation, we will first show that the transferrable atomic energy can be defined in density functional theory. Then, by utilizing invariant points in the feature space where the atomic energy is uniquely defined, we examine the atomic energy mapping of neural network potentials. It is shown that neural networks are capable of learning correct atomic energy which is transferrable. However, we also note that neural network potential is vulnerable to 'ad hoc mapping' where total energies are trained accurately but atomic energy mapping is incorrect. The atomic energy mapping of the multi-component system will be also discussed.

Poster 27

Theoretical study for chemical principles of p-type oxides via high-throughput approach

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High performance p-type semiconducting oxides are required to realize high efficient transparent electronic devices. However, known p-type oxides still have limitations to use for consumer electronic devices despite tremendous effort to discover them. In the recent study, we showed that hole effective mass and branch point energy are inappropriate descriptors for p-type oxides and suggested hydrogen descriptor as a new reliable descriptor which can clearly classify the known p-type and n-type oxides.[1] However, the hydoren desciptor is too expensive to conduct high-throughput screening for all oxides so limited material space was used in the previous study. For the extend screening space, we should find cost efficient new descriptors.

In this study, we identify more simplified descriptors that correlate to the hydrogen descriptor. Using these simplified descriptors, we screen most of oxide compounds (~17,000 oxides) in Aflow database. As a result, we identify more one hundred p-type candidates including most of known p-type oxides and many unreported candidates. Then, we classify the survived p-type candidates according to their valence band character. From the candidates, we identify the chemical principle of p-type oxides, which can help to discover new p-type materials.

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Poster 28

Jx: An open-source software for calculating magnetic interactions based on magnetic force theory

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We describe our recently developed software named by **Jx**, to perform magnetic force linear response calculations [1]. **Jx** is a user-friendly and efficient tool to calculate the magnetic interaction in solids and molecules. Based on the magnetic force theory (MFT) [1-6], in a one-shot calculation, the MFT computes the short- and long-range interactions without multiple supercell total energy calculation. It is also possible to calculate an orbital-resolved matrix form of magnetic couplings [5, 7-9]. In spite of these useful features, MFT has not been used as widely as the total energy approach. It is largely due to the absence of user-friendly software. In **Jx**, we also support local axis rotation, to allows one to analyze the orbital-resolved magnetic coupling even when a well-defined global coordinate axis is absent. As an input, full DFT Hamiltonian from OpenMX [4,10] and also Wannier Hamiltonians (Wannier90 [11], OpenMX Wannier [12]) are available. Additionally, our code is efficiently parallelized and modularized for further extensions.

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Poster 29

Neural Network Potential for Sb_2Te_3

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Phase-change materials (PCMs) are in the spotlight due to their unique properties, so-called contrast of optical and electrical property. Optical contrast enables the PCMs to be used as an optical storage medium such as blue-ray disc, while electrical contrast is recently exploited to commercialize non-volatile storage-class memory devices. The bottleneck of improving the current PCM and utilizing it as a non-volatile DRAM-class device is, for example, resistance drift and slow crystallization.

DFT calculations have been performed to find the reasons of these problems in atom-scale resolution. However, due to the limitation of computational cost, the DFT can only simulate up to 1000-atom simulation box for a few nanoseconds, which is insufficient to observe long-range order or phase-change kinetics. Classical MD is a representative example for simulating larger system, but functional form of a force field for PCMs remains unknown. Machine-learned force field can be one solution to this problem, owing to its ability to learn the accurate results from reference data and grasp the potential energy surface without knowing the exact functional form.

In this study, we have developed the classical potential of Sb_2Te_3, which consists of pseudo-binary Ge-Sb-Te system, a representative phase-change material. Gaussian density function (GDF) as well as principal component analysis (PCA) and whitening is utilized for uniform force training, implemented in SIMPLE-NN code. The developed potential is operated at about 1,000 times faster than the DFT, and the results including both small and large size simulations were closely compared with those of the DFT. The ternary Ge-Sb-Te system will be the next target of machine learning potential.

Poster 30

SIMPLE-NN: an efficient package for training and running neural network interatomic potentials

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Recently, machine-learning (ML) potentials are gaining attentions because they can reproduce the potential energy surface at the level of the first-principles calculations with much lower computational costs. ML potentials have flexible functional forms and therefore can cover a wide range of interaction types. Therefore, efficient codes for training ML potential and applying the potential to atomic simulation are in high demand. In this presentation, we introduce our open-source package, SNU Interatomic Machine-learning PotentiaL packagE – version Neural Network (SIMPLE-NN) which support the ML potential based on the artificial neural network with the symmetry function as the environment descriptor. SIMPLE-NN is designed to interface with the atomic simulation environment (ASE) package and Google Tensorflow for expandability and efficient training. SIMPLE-NN also provides LAMMPS interface for the fast molecular dynamics simulation. In this presentation, we will explain key features of SIMPLE-NN and demonstrate its performance on various systems.

Development of Neural Network potential: A case study of GeTe

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Phase change random access memory (PRAM) is one of the promising candidates for the next generation non-volatile memory and has lots of advatages such as low power consumption, long-term memory retention, and reversible phase transition between amorphous and crystalline phase. However, technical bottlenecks like resistance drift and slow crystallization speed remain unsolved.

Although ab-initio molecular dynamics (MD) have so far provided useful insights into its fundamental physics, demanding computational costs are required to investigate such phenomenon. Classical MD simulations can be performed on large scale, but is less reliable for systems with complex bond characters. Recently, developing a neural network potential (NNP) is a viable and attractive approach to overcome limitations in both. NNP is fitted to a large number of ab-initio data with a small number of parameters. Other NNPs have successfully been developed for various systems such as silicon, carbon, and GeTe.

In this work, we developed the NNP of GeTe using an in-house code, SIMPLE-NN.[1] It is demonstrated that the NNP describe the structural properties of the crystalline, liquid, and amorphous phase of GeTe and the large-scale melt-quench process is performed successfully. Gaussian density function (GDF) weighting scheme was applied during force training, which prevents unphysical configurations from occurring during MD. In addtion, costs for training NNP is significantly reduced by applying PCA whithening to symmetry functions. MD simulations using the NNPs are about 1,000 times faster than AIMD. Our future work will be extended to developing the NNP of the ternary phase change material, $Ge_2Sb_2Te_5$.

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Poster 32

Analytic continuation of imaginary Green's function using neural network

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We present a machine learning (ML) approach to the analytic continuation, which is the notorious problem in quantum many-body physics [12]. The development of new methods for this problem ill-conditioned problem of obtaining a spectral function from an imaginary time Green's function has been focused for past decades [1-11]. Here we present efforts on an extension of our work for noise robust neural network method [12]. We examined the possible expandability of the neural network method at various temperature. We found that also in various temperature, neural network method showed noise robustness, and fast analytic continuation.

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Poster 33

First-principles approaches of two-dimensional magnetic materials

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We performed charge density functional theory plus U (CDFT+U) calculations of CrOX (X=Cl, Br) and MnF_3 monolayers. Our calculation shows that the CrOX monolayers have the antiferromagnetic (AFM) ground state while the previous DFT+U study based on spin-density functionals predicted these materials as high Curie temperature ferromagnets [1, 2]. Based on the analysis of the energy level splitting, it is demonstrated that magnetic phase diagram obtained from CDFT+U are more reliable than those from spin DFT+U. Furthermore, it is shown that the MnF_3 monolayer has the AFM insulating phase on the contrary to the previous report which theoretically suggested the system as a Dirac half metal [3]. We found that the Jahn-Teller distortion is crucial to describe the broken degeneracy of e_g orbital. It is the main reason of the antiferromagnetism and insulating phase.

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Poster 34

Quasi-Fermi level profiles across molecular junctions from multi-space constrained-search density functional theory

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ABSTRACT

While the quasi-Fermi level (or *imref*) is a standard concept in semiconductor physics employed to describe the finite-bias non-equilibrium operations of electronic and optoelectronic devices, its first-principles determination has not been achieved previously. Herein, based on the multi-space constrained-search density functional theory (MS-DFT) formalism we have recently developed [1], we calculate the non-equilibrium electronic structure of molecular junctions under a finite bias voltage and extract the quasi-Fermi level profiles across molecular device systems. Comparing with the conventional non-equilibrium Green's function (NEGF) calculations based on DFT, we first confirm the practical equivalence between MS-DFT and DFT-NEGF. An important feature of MS-DFT that differentiates it from DFT-NEGF is that it relies on the determination of the quasi-Fermi level or *electrochemical* potentials across the channel, which are not explicitly provided within DFT-NEGF unlike their *electrostatic* potential counterparts. Analyzing the spatial profiles of electrochemical potentials of molecular junctions based on different electrode-molecule contact geometries [2] at varying bias voltages, we extract important insights into the nature of nonequilibrium quantum transport at the nanoscale.

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Poster 35

Diffusion behaviors of nickel atoms in graphene-covered silicon thin foil: A First Principle Study

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Using the first-principles density functional theory, we study the diffusion process of Ni atoms in graphene-covered silicon surface. We calculate the binding energies of a Ni atom on various sites in the bulk Si to find the possible diffusion paths of the Ni atom. We find that the triangle site(TA) composed of 3 Si atoms belonging to an octahedron is the most stable site. The nudged elastic band (NEB) method to estimate the diffusion barriers between any two of local minimum sites. It is found that Ni atoms may diffuse mainly along the [111] direction by going over two diffusion barriers with ~20 meV and ~70 meV, respectively. We also consider the Ni atom diffusion processes on Si(110) surfaces by evaluating the diffusion coefficients using the harmonic transition state theory. Due to the strong anisotropy of the surface geometry of the Si(110) surface, the surface diffusion of Ni atoms exhibits a significant directional dependence. Furthermore graphene capping reduces the Ni diffusivity on the surface, but enhances the diffusion anisotropicity even stronger. Our result may explain the role of graphene capping layer of Ni diffusion observed at the interface of Si-Ni thin foil.

Poster 36

Evolution of kink in $NiS_{2-x}Se_x$ system:
Hund's coupling effect and coherence energy scale

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Strong electron correlation is traditionally believed to arise from the repulsive Coulomb interaction in the vicinity of Mott insulating state. In the last decade, however, there has been remarkable progress in the understanding of the Hund's coupling effect on the correlated systems. Due to the Hund's coupling, the strong correlation can arise even with relatively small Coulomb interaction in the non-single-occupied and non-half-filled multi-band systems such as iron pnictides/chalcogenides and ruthenates. These materials are classified into Hund's metal and have been studied intensively by both experimental and theoretical approaches.

The Hund's coupling effect in half-filled multi-band systems, however, is rarely discussed although it is well understood that the Hund's coupling also enhances the correlation strength in this case. For an investigation of the Hund's coupling effect in the half-filled multi-band systems, $NiS_{2-x}Se_x$ is probably the most suitable multi-band system to study.

In this presentation, we provide the insight of the Hund's coupling effect near the Mott transition in $NiS_{2-x}Se_x$ system using DFT+DMFT calculation and ARPES measurement. The kink originated from the Hund's coupling becomes clear and moves toward to lower energy scale as the system becomes close to the Mott insulating state. This kink behavior can be understood by the suppression of the coherence energy scale, T^* (or Kondo temperature, T_K).

Poster 37

Microscopic understanding of magnetic interactions in bilayer CrI_3

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We performed the detailed microscopic analysis of the inter-layer magnetic couplings for bilayer CrI_3. As the first step toward understanding the recent experimental observations and utilizing them for device applications, we estimated magnetic force response as well as total energy. Various van der Waals functionals unequivocally point to the ferromagnetic ground state for the low-temperature structured bilayer CrI_3 which is further confirmed independently by magnetic force response calculations. The calculated orbital-dependent magnetic forces clearly show that e_g-t_{2g} interaction is the key to stabilize this ferromagnetic order. By suppressing this ferromagnetic interaction and enhancing antiferromagnetic orbital channels of e_g-e_g and t_{2g}-t_{2g}, one can realize the desirable antiferromagnetic order. We showed that high-temperature monoclinic stacking can be the case. Our results provide unique information and insight to understand the magnetism of multi-layer CrI_3 paving the way to utilize it for applications.

Poster 38

Spin-orbit coupling and insulator-to-metal transition in $GaTa_4Se_8$: DFT+DMFT study

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The lacunar spinel compound $GaTa_4Se_8$ is known as the molecular Mott insulator, exhibiting insulator-to-metal transition (IMT) and superconductivity at near 5GPa and 10GPa [1-3]. With first-principles density functional theory (DFT) study shows that the spin-orbit coupling (SOC) induces the $J_{\text{eff}} = 3/2$ ground state in 4*d*/5*d* series of lacunar spinel compounds [4]. Recent resonant inelastic X-ray scattering (RIXS) experiments established the spin-orbit entangled $J_{\text{eff}} = 3/2$ electronic structure [5].

For understanding pressure-induced properties, it is necessary to figure out the stability of $J_{\text{eff}} = 3/2$ ground state under the high pressure. Dynamic mean field theory combined with DFT (DFT + DMFT) is one of the most powerful methods to study strongly correlated systems and IMT. In this study, we performed DFT + DMFT calculations with exact diagonalization (ED) solver [6] to understand IMT under the pressure and role of the SOC.

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Poster 39

Decoupling of Metal Insulator Transition and Structural Phase Transition of VO_2: *Ab-initio* Design

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In correlated materials, the metal-insulator transition (MIT) accompanies the structural phase transition (SPT) due to the coupling of electron and lattice distortion. We focused on phase transition of the vanadium dioxide (VO_2), one of the representative correlated materials that occurs near room temperature from insulating monoclinic to metallic rutile. Using the first principles density functional theory calculation and experiments, we demonstrate the purely electronic MIT without accompanying SPT.[1] From the phase coexistence during the first order phase transition of VO_2, we designed the rutile/monoclinic heterogeneous interface with which the electron-electron interaction of monoclinic VO_2 region was successfully reduced without crystal structure changing. First principles calculation predicts that metastable metallic monoclinic phase can be successfully stabilized by this interface design. MIT without SPT was also confirmed by experimental verification i.e., the growth of heterostructure and structural/electrical characterizations. Our results clarify that the long-time controversy about the origin of the phase transition in VO_2 is due to the Mott transition. We expect that this isostructural MIT will be applied to the high-speed functional devices.

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Poster 40

How to prepare neural network potentials for advanced bond breaking and forming materials simulations.

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For modeling dynamic bond-breaking and bond-forming processes, classical molecular dynamics (MD) simulations provide many valuable information in atomistic scale. Recently there has been an increasing interest in neural network based interatomic potentials (NNP) for next generation classical potential. It is particularly useful for systems with complex bonding natures since it has no prefixed functional form, and purely mathematical functions are automatically optimized through the machine learning on the reference ab initio data. In this work we present very dynamic NNP MD simulation of metal-silicon interface system which has both covalent and metallic bond, along with complex mixtures of them. Preparing a NNP for such complex system is not a trivial job, where it needs a deep understanding on conceptual foundation of NNP. In this presentation we demonstrate some of our recent works including the studies on atomic energy mapping of NNP.[1] We also introduce an on-the-fly indictor for examining the feasibility of NNP simulations which is built on our understanding of NNP atomic energies.

[1] arXiv:1903.04366

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Strain effect on electronic and Magnetic Properties on Non-van Waals 2D antiferromagnetic material C r_2Se_3

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Non-van der Waal magnetic materials have recently been of great interest for the research community with the possible novel application. Cr2Se3 as being a Non-van der Waal magnetic 2D material is a promising candidate for the future applications magnetism in 2Dmatetials. Here we tried to study the magnetic and electronic properties of Cr2Se3 bulk crystal using first principle calculations. The ground magnetic state was investigated and the corresponding electronic band structure is found to be half-metallic in which one spin is metallic and the other with a clear band gap. The effect of unidirectional strain on half-metallic property and electronic has been studied. The antiferromagnetically coupled layers of Cr atoms were closely carefully considered for a detailed picture of the magnetism in which directional strain along the c-axis of the crystal is used as a tuning control. The results of the insight we got in the coupling of magnetic layers are all discussed.

Poster 42

First-principles study of magnetic properties in hole-doped two-dimensional $PdSe_2$

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ABSTRACT

Doping induced magnetism in two-dimensional materials has drawn great interest. Previous density functional theory (DFT) calculations showed that decrease of the total number of electrons can induce Stoner-type ferromagnetism in $PdSe_2$ monolayer (ML) due to very high density of states near the valence band maximum. In our present work, we perform DFT calculations using virtual crystal approximations and supercell calculations to study dependence of magnetism in $PdSe_2$ ML on doping methods. We consider different atomic species of dopants and different spatial distributions of dopant atoms and analyze their effects on induced magnetic properties in $PdSe_2$ ML. We discuss Stoner-type ferromagnetism and localized magnetic moments to understand magnetic properties in hole-doped $PdSe_2$ ML. This work was supported by NRF of Korea (Grant No. 2011-0018306) and KISTI supercomputing center (KSC-2018-CRE-0097).

Poster 43

Screening of Transition-Metal Dichalcogenide Monolayers for CO_2 Reduction Reaction on Basal Plane

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Increasing energy demand and extreme climate change are two challenges for a sustainable society, and the electrochemical conversion of CO_2 into carbon-neutral fuels can be a promising solution to those problems. The conversion of CO_2 to more reduced chemical species is called CO_2 reduction reaction (CO_2R), and transition-metal catalysts, such as Au and Cu are suggested for the catalyst of this reaction. Recently, MoS_2 monolayer, which is well-known for hydrogen evolution reaction catalyst, was reported to produce 1-propanol as a major CO_2R product. Although the clean basal plane of MoS_2 monolayer is known to be inert, the reaction occurred at the basal plane, implying that defects were the active site. However, the selectivity of MoS_2 monolayer was very low for practical use. To find catalysts with good efficiency and selectivity, 39 transition-metal dichalcogenide (TMD) monolayers were screened for CO_2R on the basal plane. First, by analyzing defects on TMD basal plane, we found the most stable defect for each TMDs. Evaluating catalytic activity for many reaction pathways, there were several candidates that showed good catalytic properties. Suggesting possible active sites and catalytic performance of TMDs, this study can give a higher understanding of TMD catalysts and guidance to future TMD catalyst design.

Poster 44

First-principles studies of flexoelectric effect in corrugated two dimensional materials

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The flexoelectricity, the spontaneous electrical polarization induced by a strain gradient, is one of the very exotic physical phenomena because it can develop huge piezoelectricity even in centrosymmetric materials. Here, by combining density functional theory calculation and mathematical analysis, we find that the great flexoelectricity-related spontaneous out of polarization can be generated in the corrugated two-dimensional materials. The flexoelectricity in 2D materials is highly sensitive to the corrugation strength and tunable by adjusting the curvature at the nm scale. The correlation between curvature, flexoelectricity and resulting out of plane polarization will be presented from many different 2D materials and associated underlying mechanism will be addressed in detail.

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Poster 45

Structural classification of transition metal binary alloy with simple and predictable descriptor

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Structure prediction based on machine learning has appeared by combining with database and learning algorithm. With physically meaningful descriptor, machine learning can predict the properties with only several hundreds of data [1]. As expansion of our previous work [2], we use n_d and σ_d as descriptor to classify structural phase of training set, 1862 disordered binary alloys with support vector machine (SVM) algorithm [3,4]. As a result, 87.81 % of crystal structures are classified correctly. To reduce computational cost significantly, we suggest $< n_d >$ and $< \sigma_d >$ descriptor, which can be obtain from DFT calculation from pure transition metal, still have the prediction accuracy with 80.92 % for the binary alloys. It is expected that structural phase with complex alloy such as ternary alloy and high entropy alloy (HEA).

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Poster 46

Effects of point defects on electronic properties of dicalcium nitride (Ca_2N) monolayer and bilayer from first principles

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Dicalcium nitride (Ca_2N) is a two-dimensional electride an ionic crystal in which electrons act as anions. Using ab initio calculations based on density functional theory, we have investigated effects of vacancies and substitutional phosphorus (P) defect on geometric and electronic properties. In the present study, we employed Vienna Ab Initio Simulation Package (VASP). The wave functions were expanded using a plane wave basis set. According to our calculation, in the Ca_2N monolayer with a Ca vacancy, N atoms near the vacancy push each other whereas Ca atoms near vacancy pull each other. In contrast, in the Ca_2N monolayer with an N vacancy, Ca atoms near vacancy push each other. The tendency maintains even in the Ca_2N bilayer.

Interestingly, Vacancies and substitutional defect give to some changes in the electronic structure near -1.5 eV. We will also provide the simulated STM images of the defective Ca_2N layers.

Poster 47

Selective energy transfer through resonated amplifications of molecular vibrations: the case for H_2 production

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The resonated amplifications are the common phenomena in nature occurred by wind, voice, etc, and the resonance is one of selective energy transfer (SET), transference energy from one state onto another specific state, method. We have focused on this phenomenon on the molecular scale and suggested that the resonated amplification of molecular vibration can accelerate the chemical reaction without catalyst.

In this study, we have investigated on the hydrogen dissociation and hydrogen molecular production from methane via resonance effect. We implemented the external vector potential term into the QUANTUM ESPRESSO source code, and this term can describe the resonance effect by applying alternative vector potential. We simulated the Born-Oppenheimer molecular dynamics (BOMD) for the hydrogen dissociation process from two methane molecules and demonstrated the dissociated hydrogens and methane radicals are reborn as hydrogen and ethene molecules, respectively, by calculating radial distribution functions. Also, we calculated the real-time time-dependent density functional theory to compare resonated amplification of molecular vibration and thermal effect. Furthermore, we applied circular-polarized laser to distinguish the chiral molecules such as CHClBrI. From that results, we suggest that the novel selective energy transfer method through resonance frequency and this resonance phenomenon can accelerate the chemical reactions.

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Atomic and Electronic Structure of Twisted Graphene Layers

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Twisted graphene layers have become new experimental platform for exploring correlated electron physics with various tunable degrees of freedom as demonstrated by the recent observations of superconductivity and correlated insulating states in magic-angle twisted bilayer graphene (MA-TBG) and twisted double bilayer graphene (TDBG). As a starting point to understand the rich physics emerging in these moiré superlattices, it is crucial to determine accurate atomic and electronic structures as well as their interplays. In this work, we investigate electronic and phononic properties of twisted graphene layers obtained from atomistic description of the system including more than 10,000 atoms in the moiré supercell. Electronic structure, phonon spectrum, and electron-phonon coupling strength λ are obtained before and after atomic-position relaxation both in- and out-of-plane. We find that the lattice relaxation strongly affects the low-energy electronic structure, and λ is very large for the low-energy flat bands owing to the enhanced density of states. Furthermore, we show that the layer-number degrees of freedom offers additional tunability to the low-energy electronic structure through the sensitivity to the external electric fields. Our results provide fundamental understanding of electron-phonon interaction in twisted graphene layers and serve as a theoretical guide for exploring correlated electron physics in these versatile moiré superlattices. This work was supported by NRF of Korea (Grant No. 2011-0018306) and KISTI supercomputing center (Project No. KSC-2018-CRE-0097). Y.W.C. acknowledges support from NRF of Korea (Global Ph.D. Fellowship Program NRF-2017H1A2A1042152).

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Poster 49

Construction of Training Set for Machine-Learning Potential-Energy-Surface

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ABSTRACT

For the past decade, several machine-learned potential-energy-surface (ML-PES) models have been developed to perform accurate and fast computations of systems inaccessible by first-principles methods. [1, 2] While successful predictions of specific physical properties based on ML-PES model have been reported for many cases, discussion about the accuracy and reproducibility of these predictions is not well established. In machine learning processes for obtaining successful ML-PES, construction of good training sets with reliable strategies constitutes the most significant part. We have tested a model so-called randomly-arranged-atomic-system generator (RAG), which constructs training sets more effectively than MD simulations. We also utilized the t-SNE method, which helps to project the high dimensional potential energy surface to hypothetical two-dimensional potential energy surface, to analyze the RAG model in reproducing the ML-PES. [3]

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Poster 50

Origin of the robust out-of-plane polarization in TMDCs monolayer

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Out-of-plane polarization is rare phenomena in atomically thin film due to the depolarization fields, which are inversely proportional to the sample thickness. To achieve atomically thin ferroelectric film, the improper ferroelectrics such as in $YMnO_3$ have attracted great attention [1, 2]. The improper ferroelectrics refer to the ferroelectricity induced by the secondary mode of the transition, which cannot exist alone and should be coupled with the primary mode to drive the transition. Dependence of the polarization on both the primary and the secondary modes, however, has not been properly clarified in previous studies on improper ferroelectrics. In this study, we investigated the electronic origin of the ferroelectricity in distorted $1T$ ($d1T$) MoS_2 monolayer and overcoming mechanism of the depolarization field using first-principles calculations and the Landau theory of phase transition. We studied the stability of the ferroelectricity in $d1T$-MoS_2 monolayer from the energy-polarization curves in ferroelectric switching and to external electric fields. We also presented a possible mechanism of controlling the energy barrier in ferroelectric switching using mechanical strains.

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Poster 51

Enhanced Carrier Mobility of MoS_2 Nanoribbons: *Ab-initio* Study

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The one-dimensional (1D) hexagonal nanostructures, such as nanotubes, wires, rods and nanoribbons have been intensively investigated in recent decades due to their diverse physical properties. Monolayer MoS_2 is a semiconductor with a decent bandgap and regarded as a promising candidate for field effect transistor (FET) with a high on/off ratio but low mobility at room temperature limited their practical application. In this study, we investigated the mobility of monolayer MoS_2 nanoribbon under various conditions, i.e. tensile strain along the ribbon direction, i.e., armchair direction, and transverse external electric field perpendicular to the ribbon direction. Deformation potential theory was used to calculate the mobility of the MoS_2 nanoribbon along with the first-principle calculation. We found that mobility of MoS_2 nanoribbon has significantly enhanced by applying the strain and electric field simultaneously, and at room temperature carrier mobility of electron reaches up to 2,000 $cm^2/(V\cdot s)$ and hole mobility around 450 $cm^2/(V\cdot s)$. Our study suggests that strain with electric field provide a promising route for improving the transport properties of MoS_2 nanoribbons, which may make them a suitable candidate for a channel layer in FET.

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Effect of nano-enclosure on the $AlCl_4$ intercalation mechanism in 2D electrodes

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Graphite-based Al-ion battery has gain large attention due to extremely fast charge/discharge rate. However, the understanding on how the intercalation mechanism happen in this system is still vague. The concern comes with the size of $AlCl_4$ molecule as intercalated ion which is 5.28 Å in the form of tetragonal structure while the experimentally observed gallery height for graphite-based Al-ion battery is ~5.7 Å. In the recent theoretical studies, the computational models are mostly represent intercalation of $AlCl_4$ ion in tetragonal form which resulted in large expansion of graphite intercalation gallery, 8~9 Å. Thus, it cannot explained the smaller gallery distance which observed in experimental studies. We performed first-principles calculations which shows that the c-lattice parameter of graphite structure can tune the intercalation form of $AlCl_4$. On a certain intercalation gallery distance we found that $AlCl_4$ shows a metastable state in the planar form with intercalation gallery height is closer to the experimental data. This founding will explain the Van der Waals compressive interaction in experimental 2D structures on the ion intercalation mechanism which is represented by the c-lattice parameter in our calculation model.

Structure stability and dielectric constant of (Be,Mg)O solid solution

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As the size of DRAM shrinks, the leakage current in gate oxide becomes crucial. Therefore, the demand for materials having both high dielectric constant and high bandgap increases. Unfortunately, these two properties are in a trade off. Recently, the rocksalt structure BeO was expected as the novel high-κ (~275) dielectric materials with high bandgap (~10.1 eV) [1]. However, the stable structure of BeO at normal temperature and pressure condition is the wurtzite structure. On the other hand, the rocksalt structure is observed only at high temperature and high pressure condition [2,3], which is not desirable for the gate oxide materials. Thus, the solid solution of the rocksalt structure (Be,Mg)O is proposed whose dielectric constant becomes lower than that of pure rocksalt BeO but higher than MgO, keeping its bandgap to that of BeO. It is based on the idea that the rocksalt structure (Be,Mg)O is stabilized by the stable rocksalt structure MgO in the MgO-rich composition. In this study, the properties of (Be,Mg)O is investigated by density functional theory calculations. The instability of the rocksalt structure (Be,Mg)O is observed and explained according to the Pauling's rule [4] on the coordination number of Be. The dielectric constant and bandgap varies depending on the configuration as well as the composition. Therefore, the composition where the phase transition occurs is investigated based on the energetics of various (Be,Mg)O structures. In addition, the method to expand the composition range for the stable rocksalt structure (Be,Mg)O is proposed.

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Poster 54

Mechanism of doping in borophene

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ABSTRACT

We elucidate the structural transition, electronic and vibrational properties in borophene, when doped with nitrogen. During doping, the sp^2 orbitals are responsible arranging themselves to accommodate the electron of nitrogen atom to form planar *h*-BN. In the process metallic nature of borophene changes to insulating *h*-BN. We unravel the doping mechanism and extended it to doping of non-metallic and metallic ad-atoms on borophene. We hope, our findings will help to design boron based 2D materials.

Memo