초청연사

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김용훈 (한국과학기술원 전기및전자공학부)

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이현용 (고려대 디스플레이반도체물리학과)

지승훈 (포항공대 물리학과)

한상수 (한국과학기술연구원 계산과학연구센터)

자문위원회

김용현 (한국과학기술원), 김용훈 (한국과학기술원),
권영균 (경희대학교), 박철홍 (부산대학교),
심지훈 (포항공과대학교), 유재준 (서울대학교),
이승미 (한국표준과학연구원), 조준형 (한양대학교),
정유성 (한국과학기술원), 최형준 (연세대학교),
한명준 (한국과학기술원), 한상수 (한국과학기술연구원),
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제16회 고등과학원

전자구조 계산학회

일시 : 2020년 8월 27일 (목) – 8월 28일 (금)
장소 : 온라인 학회

KIAS 고등과학원 KOREA INSTITUTE FOR ADVANCED STUDY

시간표		
	8월 27일 (목)	8월 28일 (금)
9:30 ~ 10:10	학회 준비	학회 준비
	Session I: Correlated Systems 좌장 김흥식 (강원대)	Session IV: Energy Application 좌장 김수란 (경북대)
10:00 ~ 10:40	민병일 (포항공대) Electronic structures and physical properties of Rare-Earth systems: Past and Present	이정훈 (한국과학기술연구원) Role of organic cations in fundamental properties of hybrid halide perovskites
10:40 ~ 11:20	이현용 (고려대) Tensor network application to many-body physics	서동화 (울산과학기술원) First principles study on the reaction mechanisms of the electrode materials for Li-ion batteries
11:20 ~ 11:40	휴식	휴식
	Session II: Nanomaterials and Defects 좌장 황정운 (전남대)	Session V: Two Dimensional Materials 좌장 김정우 (인천대)
11:40 ~ 12:20	박지상 (경북대) Reconstruction of grain boundaries and defect accumulation	이근식 (울산과학기술원) Electrical control of interlayer exchange coupling in metallic 2D magnet
12:20 ~ 13:00	방준혁 (충북대) Excited state dynamics and carrier multiplication in graphene nanoribbons	김영국 (성균관대) Higher-order topological instanton tunneling oscillation in twisted bilayer graphene
13:00 ~ 14:30	점심식사	점심식사
	Session III: Method Development 좌장 김한철 (숙명여대)	Session VI: Machine Learning 좌장 이훈표 (강원대)
14:30 ~ 15:10	김용훈 (한국과학기술원) Multi-space excitation picture for nonequilibrium quantum transport: Progress and prospects	지승훈 (포항공대) *Ab initio* machine learning of chalcogenide phase change materials
15:10 ~ 15:50	송종원 (대구대) Development of DFT functional applicable to large molecular and periodic systems	한상수 (한국과학기술연구원) Pattern learning electronic density of states of metallic systems
15:50 ~ 16:30	이상훈 (고등과학원) Efficient First-principles approach with a pseudohybrid density functional for extended Hubbard interactions	김지한 (한국과학기술원) Artificial design and prediction of porous materials

Talk No. 1

Electronic structures and physical properties of Rare-Earth systems: Past and Present

Byung Il Min

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

In the beginning, pioneers in the solid state and electronic structure theory in Korea are quickly introduced. Then the interesting physical properties of rare-earth systems in the past and at present are briefly surveyed, which include Permanent magnets, Kondo behavior, Heavy fermion, Valence fluctuation, and Topological Kondo insulator. Our recent studies on Ce and Sm compounds are also presented.

Talk No. 2

Tensor Network Application to Many-body Physics

Hyun-Yong Lee[1,2]

[1]*Department of Applied Physics, Graduate School, Korea University, Sejong 30019, Korea*

[2]*Division of Display and Semiconductor Physics, Korea University, Sejong 30019, Korea*

Tensor networks have emerged as a powerful and useful language to describe many-body systems in recent years. The scope of its application covers from the evaluation of the partition function of the classical many-body systems to representing strongly entangled quantum many-body states. One of the most successful applications of the tensor network is the celebrated "density matrix renormalization group", which have been attempted to apply for the first principle calculations and to study the electronic structures. In addition, higher dimensional applications of tensor networks are also successful providing intuitive pictures of the exotic quantum ground states such as the quantum spin liquid in compact and efficient representations. The tensor network has attracted a lot of attention even in the research area of the field theory.

In this talk, I will give a brief introduction to the tensor network in the condensed matter physics. The fundamental ideas behind that will be discussed: why it should work, how efficient it is for many-body systems. Then, if time allows, I will discuss the Kitaev spin liquid in the spin representation which is represented by the tensor network in a compact way.

Talk No. 3

Reconstruction of grain boundaries and defect accumulation

Ji-Sang Park[1]

[1]*Department of Physics, Kyungpook National University, Daegu, 41566, South Korea*

Imperfections are categorized into point defects and extended defects depending on whether the translational symmetry is locally broken or not, respectively. The rapid development of the first-principles density functional theory (DFT) calculation methods enabled the accurate calculation of the physical properties of point defects. Extended defects in three-dimensional bulk semiconductors, however, need more fundamental studies to overcome difficulties such as large degrees of structural freedoms and the heavy computational cost.

In this presentation, we discuss how to investigate grain boundaries in semiconductor materials [1,2]. First, we propose a strategy based on a modified genetic algorithm to find the stable atomic structure of grain boundaries [1]. Our study shows that grain boundaries can be stabilized and self- passivated by reconstructions. Second, taking the grain boundaries in a halide perovskite as an example, the effect of the defect accumulation at the grain boundaries on the electrical and recombination properties will be discussed [2].

[1] J.-S. Park, *Stabilization and self-passivation of symmetrical grain boundaries by mirror symmetry breaking,* Phys. Rev. Materials **3**, 014602 (2019).
[2] J.-S. Park, J. Calbo, Y.-K. Jung, L. Whalley, and A. Walsh, "*Accumulation of Deep Traps at Grain Boundaries in Halide Perovskites*", ACS Energy Lett. **4**, 1321−1327 (2019)

Talk No. 4

Excited State Dynamics and Carrier Multiplication in Graphene Nanoribbons

Junhyeok Bang[1] and Joongoo Kang[2]

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2Department of Emerging Materials Science, DGIST, Daegu 42988, Republic of Korea

External perturbations such as light irradiation and applied voltage can excite electrons in materials and lead to a series of dynamic processes such as carrier thermalization, transfer, and recombination. Among these excited-state dynamics, carrier multiplication (CM) is an interesting process that generates multi-electron-hole pairs from a single photon absorption and thus can enhance optoelectronic device efficiency. However, CM is rather inefficient in conventional semiconductors because of strong restrictions on electronic transitions imposed by the energy and momentum conservation. Here, using time-dependent density functional theory, we show that CM occurs in armchair graphene nanoribbons due to the existence of subbands to release the strong restriction. The CM mechanism is different from the ones suggested for quantum dots and graphene. Furthermore, the band gap of AGNR is significantly modulated depending on nanoribbon width, and thus it provides the way to control the carrier dynamics and carrier multiplication in AGNRs.

Talk No. 5

Multi-space excitation picture for non-equilibrium quantum transport: Progress and prospects

Yong-Hoon Kim

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필자는 2017년 제13회 고등과학원 전자구조계산학회에서 우리 연구실에서 다년간에 걸쳐 개발을 진행하여 마무리 단계에 있던 다공간 제한탐색 밀도범함수론(multi-space constrained search density functional theory, MS-DFT)에 대해 설명한 바 있다 [1]. 현재 비평형 양자수송 현상의 제1원리 계산의 표준적인 기법이 되고 있는 란다우어(Landauer) 관점 및 이에 기반을 둔 비평형 그린 함수(non-equilibirum Green's function, NEGF) 방법론의 대안이 될 수 있는 MS-DFT 이론은 특히 "비평형 에너지"가 잘 정의된다는 점에서 란다우어-NEGF 방법론의 한계를 벗어나는 여러가지 활용성과 응용성을 가진다 [2]. 이번 발표에서는 초기 아이디어로부터 [3] 10년 이상의 고난한 연구를 통해 최근 성공적으로 마무리 된 MS-DFT 이론 및 소프트웨어의 개발을 간략히 정리하고 후속 연구 방향에 대해 설명하고자 한다. 한편, 2017년 발표에서 필자는Psi-k 뉴스레터 그해 4월호의 데이터에서 보이듯이 [4] 중국 등의 부상에 반비례해 아시아권에서마저 미약해지고 있는 우리나라 제1원리 계산 분야의 위상에 대해 걱정 어린 지적을 한 바 있다. 이번 발표에서도 이러한 위기 상황의 극복을 위한 집단적인 노력의 필요성을 강조하고 관련된 몇가지 화두를 던지고자 한다.

[1] H. S. Kim and Y.-H. Kim, *Bull. Am. Phys. Soc.* **60**, abstr. T23.0015, https://meetings.aps.org/link/BAPS.2015.MAR.T23.15 (2015); *ibid*. **61**, abstr. K31.0005, https://meetings.aps.org/link/BAPS.2016.MAR.K31.5 (2016); *ibid*. **62**, abstr. Y32.0003. http://meetings.aps.org/link/BAPS.2017.MAR.Y32.3 (2017); arXiv preprint, arXiv:1808.03608 [cond-mat.mes-hall] (2018).
[2] J. Lee, H. Yeo, and Y.-H. Kim, Proc. Natl. Acad. Sci. U. S. A. **117**, 10142 (2020); J. Lee, H. S. Kim, Y. H. Kim, Adv. Sci. DOI: 10.1002/advs.202001038 (2020).
[3] Y.-H. Kim, S. S. Jang, Y. H. Jang, and W. A. Goddard III, Phys. Rev. Lett. **94**, 156801 (2005).
[4] https://psi-k.net/download/highlights/Highlight_135.pdf

Talk No. 6

Development of DFT functional applicable to large molecular and periodic systems

Jong-Won Song[1,2]

[1]*Chemistry Education, Daegu University, 201 Daegudae-ro, 38453 Republic of Korea*

Nowadays, density functional theory (DFT) is a strong work-horse applicable to biomolecule and material sciences. In particular, hybrid DFT functionals which include Hartree-Fock (HF) exchange in exchange functional initiated active chemical applications of DFT, in that it can reproduce energy and property of finite systems within chemical accuracy as well as with low computational. However, in spite of its high applicability, DFT has shown severe inappropriateness of producing some following basic properties: inter- and intra-molecular van der Waals interaction, inter- and intra-molecular charge transfer excitation energy and its oscillator strength, (hyper-)polarizability, isomerization energy of organic molecules, core-excitation energy, HOMO-LUMO gaps of molecules, and so on. As a result of our commission to solve these problems, we proposed a new hybrid functional named long-range corrected (LC) DFT and showed successful improvement on the problems mentioned above [1].
However, still high demanding of time cost to evaluate long-range HF exchange is an obstacle for LC-DFT to be applied to large molecular systems and solid-state materials. Unlike acceleration methods for Coulomb integration, developing acceleration methods for the HF exchange is still a pioneering area. Upon this problem, we studied on developing a new linear-scaling method of HF exchange integration, in particular, for LC-DFT hybrid functional [2]. Then, we successfully applied our accelerated LC-DFT to the adsorption energy calculations of CO molecule on Cu periodic surface [3] and found LC-DFT functionals can reproduce the experimental adsorption energies with high selectivity on binding site, not to mention surface energies and lattice energies.

References

[1] Jong-Won Song, Tsuyoshi Hirosawa, Takao Tsuneda, and Kimihiko Hirao, J. Chem. Phys. 126, 154105 (2007).
[2] Jong-Won Song and Kimihiko Hirao, J. Chem. Phys. 143, 144112 (2015).
[3] Kenji Mishima, Masanori Kaneko, Jong-Won Song,* Hiroki Kawai, Koichi Yamashita, and Kimihiko Hirao, J. Chem. Phys. 152, 104105 (2020).

Talk No. 7

Efficient First-Principles Approach with a Pseudohybrid Density Functional for Extended Hubbard Interactions

Sang-Hoon Lee, and Young-Woo Son

Korea Institute for Advanced Study, Seoul 02455, Korea

For fast and accurate calculations of band gaps of solids, we present an ab initio method that extends the density functional theory plus on-site Hubbard interaction (DFT+U) to include intersite Hubbard interaction (V). This formalism is appropriate for considering various interactions such as a local Coulomb repulsion, covalent hybridizations, and their coexistence in solids. To achieve self-consistent evaluations of U and V, we adapt a recently proposed Agapito-Curtarolo-Buongiorno Nardelli pseudohybrid functional for DFT+U to implement a density functional of V and obtain band gaps of diverse bulk materials as accurate as those from GW or hybrid functionals methods with a standard DFT computational cost. Moreover, we also show that computed band gaps of few layers black phosphorous and Si(111)-(2×1) surface agree with experiments very well, thus meriting the new method for large-scale as well as high throughput calculations with higher accuracy.

Talk No. 8

Role of organic cations in fundamental properties of hybrid halide perovskites

Jung-Hoon Lee

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

Hybrid halide perovskites have been under intense investigation due to their high-power conversion efficiencies and low cost for solar cell applications. To further improve the efficiency of the perovskite solar cell, we need to find and understand control parameters for tuning fundamental properties of hybrid halide perovskites. Herein, we investigate the effect of methylammonium (MA) on the electronic structure, mechanical properties, and thermodynamic stability of hybrid halide perovskites using van der Waals (vdW)-corrected density functional theory (DFT) calculations. According to our calculations, hydrogen bonding between an organic MA cation and the halide frame induces the octahedral tilting which affects the optical band gap and carrier effective masses. In addition, we show that the MA cation improves the material's resistance to deformation. For example, the orientationally-averaged Young's modulus of orthorhombic $MAPbI_3$ increases by about 19% compared to the equivalent inorganic series of structures. We further show that the MA cation is mainly responsible for the pressure-induced phase transition in $MAPbI_3$. Taken together, these results can help guide the optimization of the fundamental properties of perovskite-based solar cell materials.

Talk No. 9

First principles study on the reaction mechanisms of the electrode materials for Li-ion batteries

Dong-Hwa Seo[1]

[1] *School of Energy and Chemical Engineering, Ulsan National Institute of Science and Technology (UNIST)*

Electrochemical energy storage devices are attracting tremendous interest due to the recent growing importance of sustainability and environmental concerns. The Li-ion batteries are one of the most advanced energy storage systems and serve as a major power source for various small electronic devices. With the growing interest in power sources for large applications such as the HEV (hybrid electric vehicle) or PHEV (plug-in hybrid electric vehicle), Li-ion batteries are finding new opportunities in this emerging area. Intensive research efforts are focused on developing suitable electrode material, the key component of Li-ion batteries, for these applications. The new electrode materials for Li-ion batteries for use in HEVs and PHEVs require high stability, high power, high energy, and low cost. In this talk, I will present the first-principles results on the oxygen redox activity in Li-excess cathode materials [1] and the reaction mechanism of $Li_{4+x}Ti_5O_{12}$ anode materials [2]. Fundamental understanding of the electrode properties based on first principles can accelerate to develop new electrode materials.

[1] D.-H. Seo et al., "The structural and chemical origin of the oxygen redox activity in layered and cation-disordered Li-excess cathode materials", Nature Chem., 8, 692 (2016)
[2] D.-H. Seo et al., "Kinetic Pathways of Ionic Transport in Fast Charging Lithium Titanate", Science, 367 (6481) 1030 (2020)

Talk No. 10

Electrical control of interlayer exchange coupling in metallic 2D magnets

In Kee Park[1], Geunsik Lee[1]

[1]*Department of Chemistry, Ulsan National Institute of Science and Technology, 44919, Ulsan, South Korea*

Downscaling the device size in silicon based technology is almost saturated these days and a new feasible technology is highly needed for next generation of technology. In the charge based devices the dielectric environment coupling is unavoidable and it needs to keep charging all the time, thus the spin based devices are more desirable for stable and low-energy processing of information. Recently reported magnetism in vdW layered materials provides great opportunity towards such direction, as weak coupling between atomically thin layers provides flexibility for various types of heterostack and low-energy tunability. Here we present DFT studies on electrical tuning of interlayer exchange coupling in Fe based 2D ferromagnets Fe_3GeTe_2. From electronic structure analysis in comparison with Fe_4GeTe_2 and Fe_5GeTe_2, the underlying mechanism is suggested as that Fe d electrons near the Fermi level with negligible hopping across the vdW gap provides a way to control electrically the magnitude of the itinerant type interlayer exchange coupling, thus the net exchange type can be switched by applying the out-of-plane electric field.

Talk No. 11

Higher-Order Topological Instanton Tunneling Oscillation in twisted bilayer graphene

Youngkuk Kim[1]

[1]*Department of Physics, Sungkyunkwan University, Suwon 16419, Korea*

A second-order topological insulator is a novel topological phase of matter, characterized by localized states at higher-dimensional lower boundaries. Here we argue that twisted bilayer graphene can realize a second-order topological insulator phase. We first show our first-principles calculations that diagnoses the higher-order topological phase based on both the mirror Zak phase and the second Stiefel-Whitney number [1]. Then, we argue that the topological corner states support an instanton tunneling, leads to a novel quantum oscillation in the energy spectrum [2]. We suggest that a second-order topological insulator generically features the instanton tunneling oscillation. The instanton tunneling oscillation is exemplified in twisted bilayer graphene. Our results suggest an opportunity to identify the higher-order topological phase in twisted bilayer graphene.

[1] “Higher-Order Topological Insulator in Twisted Bilayer Graphene“, Moon Jip Park, Youngkuk Kim, Gil Young Cho, and SungBin Lee, Phys. Rev. Lett. 123, 216803 (2019)
[2] “Higher-order topological instanton tunneling oscillation”, Moon Jip Park, Sunam Jeon, SungBin Lee, Hee Chul Park, and Youngkuk Kim, in preparation.

Talk No. 12

ab-initio Machine Learning of Chalcogenide Phase Change Materials

Seung-Hoon Jhi

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

Chalcogenide-based phase-change materials (PCMs) have attracted great attraction for their fast transition between crystalline and amorphous phases. Beside the fast transition behavior, PCMs have variety of intriguing phenomena such as topological insulator, Weyl semimetals, thermoelectricity, and multiferroicity. PCMs are also considered as promising materials for neuromorphic computing that is essential for neural network-based machine learning. The abundance of physical interests and industrial applications is originated from the structural peculiarity of PCMs, especially their unique bonding character and the vacancy disorders. Yet, no comprehensive frame of the phase-change process is established. One biggest issue in understanding the phase transition is that few theoretical tools are available for non-periodic disordered systems. Direct numerical simulations using state-of-the-art first-principles calculations are very limited for non-periodic systems at large scales. We study the vacancy disorder and chemical bonding in a frame of octahedral p-bonding network. We also utilize a machine-learning model to simulate the crystalline-amorphous phase transition of PCMs. For efficient training process, we develop a scheme named randomized atomic-system generator to construct training sets that cover the potential energy surface as even as possible. Constructed machine-learning potential simulates successfully the molecular dynamics of melting and crystallization processes of PCMs in a level similar to first-principles simulations.

Talk No. 13

Pattern Learning Electronic Density of States of Metallic Systems

Byung Chul Yeo,[1] Kihoon Bang,[2] Donghun Kim,[1] Hyuck Mo Lee,[2] and Sang Soo Han[1]

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2Department of Materials Science and Engineering, Korea Advanced Institute of Science and Technology (KAIST), 291 Daehak-ro, Yuseong-gu, Daejeon 34141, Republic of Korea

Electronic density of States (DOS) is a key factor in condensed matter physics and materials science that determines the properties of metals. First-principles density-functional theory (DFT) calculations have typically been used to obtain the DOS despite the considerable computation cost. Herein, we report a fast machine learning method for predicting the DOS patterns of not only bulk structures but also surface structures in mutli-component alloy systems by a principal component analysis (PCA). Within this framework, we use only four feature to define the composition, atomic structure, and surfaces of alloys, which are the d-orbital occupation ratio, coordination number, mixing factor, and the inverse of miller indices. Despite the success of this approach for representing DOS patterns of metallic systems in bulks and slab structures, it suffers from representation of nanoparticle (NP) structures. To overcome the issue, we have recently combined the PCA method with the crystal graph convolutional neural network (CGCNN). By applying PCA, one can covert a mathematically high-dimensional DOS image to a low-dimensional vector. The CGCNN plays a key role in reflecting the effects of local atomic structures on the DOS patterns of NPs with a few of materials features that are easily obtained from a periodic table. The PCA-GCNNN model is applicable for all pure and bimetallic NPs, in which a handful DOS training sets that are easily obtained with the typical DFT method, such as bulk, slab, and small-sized NPs, are considered. Although there is a small loss of accuracy with the PCA-CGCNN method compared to DFT calculations, the prediction speed is much faster than that of DFT methods and is not nearly as affected by the system sizes of NPs.

Talk No. 14

Artificial Design and Prediction of Porous Materials

Jihan Kim[1]

[1]*KAIST, Department of Chemical and Biomolecular Engineering*

In this presentation, I will explore the new trend of designing novel porous materials using artificial designs. Specifically, I will talk about using our in-house developed generative adversarial network (GAN) software to artificially create porous materials for the first time. Moreover, we have successfully implemented inverse-design in our GAN prompting ways to train our AI to create porous materials with user-desired capacity. Next, we extend from this paradigm to integrate machine learning with genetic algorithm to screen over trillions of materials to find optimal materials for methane storage.