The 21st Asian Workshop on First-Principles Electronic Structure Calculations (ASIAN-21)

October 29 — 31, 2018
Fusion Hall, KI Building
KAIST
Daejeon, Korea

KAIST

APCTP
Asia Pacific Center for Theoretical Physics

International Organizing Committee

Chang, Kee Joo (KAIST)
Chou, Mei-Yin (Academia Sinica)
Fang, Zhong (Chinese Academy of Sciences)
Gong, Xin-Gao (Fudan University)
Guo, Guang-Yu (National Taiwan University)
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Chul Hong Park (Busan National University)	
Noejung Park (UNIST)	
Young Woo Son (KIAS)	

Timetable

10/29 (Monday)	10/30 (Tueday)	10/31 (Wednesday)
9:00 – 9:45 **(Louie)**	9:00 – 9:45 **(Gonze)**	9:00 – 9:30 (Watanabe)
9:45 – 10:15 (Chou)	9:45 – 10:15 (Togo)	9:30 – 10:00 (Suzuki)
10:15 – 10:45 (30-min Break)	10:15 – 10:45 (30-min Break)	10:00 – 10:30 (Park)
10:45 – 11:15 (Quek)	10:45 – 11:15 (Matsushita)	10:30 – 10:45 (15-min Break)
11:15 – 11:45 (Mahadevan)	11:15 – 11:45 (Han)	10:45 – 11:15 (Chang)
11:45 – 12:15 (Sun)	11:45 – 12:15 (C. Kim)	11:15 – 11:45 (Wan)
12:15 – 14:00 (Lunch)	12:15 – 14:00 (Lunch/IOC Meeting)	11:45 – 12:15 (Lin)
14:00 – 14:45 **(Marzari)**	14:00 – 14:45 **(Wei)**	12:30 – 18:00 (Lunch/Tour) Baekje UNESCO Heritage tour
14:45 – 15:30 **(Blum)**	14:45 – 15:15 (Seo)	
15:30 – 16:30 (Photo/Poster)	15:15 – 16:15 (Poster)	
16:30 – 17:00 (D. Kim)	16:15 – 16:45 (Zhang)	
17:00 – 17:30 (Morikawa)	16:45 – 17:15 (Ishii)	
17:30 – 18:00 (Jungsuttiwong)	17:15 – 17:45 (Huang)	
	18:00 – 21:00 (Banquet)	

Homepage

http://events.kias.re.kr/AES21

Program

Oct. 29 (Monday)

(Registration @ Fusion Hall, KI Building, KAIST)
8:30 – 18:00

(Welcome Session)
8:50 – 9:00 Opening Remark – Prof. Yong-Hoon Cho (Associate Vice President of Academic Affairs, KAIST, Korea)

(Session 1): Physics of Low-Dimensional Materials - Chair: Prof. Kee Joo Chang (KAIST, Korea)

9:00 – 9:45
Prof. Steven G. Louie (UC Berkeley, USA)
Title: Topological and Interaction Effects in Atomically Thin 1D & 2D Materials

9:45 – 10:15
Prof. Mei-Yin Chou (Academia Sinica, Taiwan)
Title: Topics of Two-Dimensional Materials and Their Heterostructures

(30-min Coffee Break)
10:15 – 10:45

(Session 2): Novel 2D Materials - Chair: Prof. Suhuai Wei (Beijing Computational Science Research Center, China)

10:45 – 11:15
Prof. Su Ying Quek (National University of Singapore, Singapore)
Title: Electronic and Optical Properties of 2D-material-based Heterostructures

11:15 – 11:45
Prof. Priya Mahadevan (S. N. Bose National Centre for Basic Sciences, India)
Title: Engineering spin-valley physics in bilayers of $MoSe_2$

11:45 – 12:15
Prof. Jiatao Sun (Chinese Academy of Sciences, China)
Title: First-principles investigations of nonequilibrium states of periodically driven black phosphorous

(Lunch)
12:15 – 14:00
* Plenary/Invited speakers and local/international committee members are invited to the lunch at the Faculty Club.

(Session 3): State-of-the-Art Computation - Chair: Prof. Jisoon Ihm (POSTECH, Korea)

14:00 – 14:45
Prof. Nicola Marzari (EPFL, Switzerland)
Title: 2D, or not 2D?

14:45 – 15:30
Prof. Volker Blum (Duke Univ., USA)
Title: All-electron electronic structure theory for new materials for light harvesting and light emission

(Session 4): Recent Progress in Electronic Structure Calculations
15:30 – 16:30 Photo session/Poster presentation

(Session 5): Energy Materials - Chair: Prof. Isao Tanaka (Kyoto Univ., Japan)

16:30 – 17:00
Dr. Donghun Kim (KIST, Korea)
Title: Novel Materials for Ferroelectric Photovoltaics

17:00 – 17:30
Prof. Yoshitada Morikawa (Osaka University, Japan) – Oct. 29 or 30
Title: First-principles theoretical study of catalytic reactions at surfaces and interfaces

17:30 – 18:00
Prof. Siriporn Jungsuttiwong (Ubon Ratchathani Univ., Thailand)
Title: DFT Mechanistic Study of Carbon-Doped Boron Nitride Nanosheet as Highly Efficient Metal-Free Catalyst for NO Reduction

Oct. 30 (Tuesday)

(Registration @ Fusion Hall, KI Building, KAIST)
8:30 – 18:00

(Session 6): Phonon Effect - Chair: Prof. Jaejun Yu (Seoul National Univ., Korea)

9:00 – 9:45
Prof. Xavier Gonze (Uni. Cath. Louvain, Belgium)
Title: Vibrational effects in electronic structure: Temperature dependence, zero-point motion, spectral functions

9:45 – 10:15
Prof. Atsushi Togo (Kyoto university, Japan)
Title: High-throughput first-principles phonon calculation and phonon database

(30-min Coffee Break)
10:15 – 10:45

(Session 7): Electron Correlation - Chair: Prof. Tamio Oguchi (Osaka Univ., Japan)

10:45 – 11:15
Prof. Yu-ichiro Matsushita (Tokyo Institute of Technology, Japan)
Title: Quasiparticle spectra based on wave function theory: Application of coupled-cluster theory and self-energy functional theory

11:15 – 11:45
Prof. Myung Joon Han (KAIST, Korea)
Title: Toward the Better First-principles Description of Correlated Materials: Old Functionals and New Concepts

11:45 – 12:15
Dr. Choong H. Kim (IBS, SNU, Korea)
Title: Spin-orbital-entangled J_{eff}=1/2 state in 3d transition metal oxide CuAl2O4

(Lunch/IOC Meeting)
12:15 – 14:00
* Plenary/invited speakers and local/international committee members are invited to the lunch at the Faculty Club.
** The IOC meeting will take place at the conference room in the Faculty Club.

(Session 8): Defects in Semiconductors - Chair: Prof. Chul Hong Park (Pusan National Univ., Korea)

14:00 – 14:45
Prof. Suhuai Wei (Beijing Computational Science Research Center, China)
Title: First principle investigation of defect properties in energy materials

14:45 – 15:15
Hosung Seo (Ajou Univ., Korea)
Title: First-principles theory of defect-based qubits in heterogeneous semiconductors

(Session 9): Recent Progress in Electronic Structure Calculations
15:15 – 16:15 Poster presentation (continued)

(Session 10): Novel Electronic States - Chair: Prof. Atsushi Oshiyama (Nagoya Univ., Japan)

16:15 – 16:45
Prof. Dong-Bo Zhang (Beijing Computational Science Research Center, China)
Title: Strain-Induced Half-Metallic States in Graphene: Application of Generalized Bloch Theorem

16:45 – 17:15
Prof. Fumiyuki Ishii (Kanazawa University, Japan)
Title: First-principles study of Berry-phase-mediated thermoelectric effects

17:15 – 17:45
Prof. Li Huang (Southern University of Science and Technology, China)
Title: Origin of high thermoelectric performance in n^{-} and p^{-}type SnSe crystals

(Banquet @ The Academic Cultural Center)
18:00 – 21:00
* All participating principal investigators are invited to the banquet.

Oct. 31 (Wednesday)

(Session 11): Machine Learning & TDDFT - Chair: Prof. Young-Woo Son (KIAS, Korea)

9:00 – 9:30
Prof. Satoshi Watanabe (The University of Tokyo, Japan)
Title: Atom dynamics in solids studied by machine-learning techniques

9:30 – 10:00
Prof. Yasumitsu Suzuki (Tokyo University of Science, Japan)
Title: TDDFT study of electron scattering processes

10:00 – 10:30
Noejung Park (UNIST, Korea)
Title: Band topologies and spin-phonon dynamics of spin-orbit coupled insulators: a study with the real-time TDDFT

(15-min Coffee Break)
10:30 – 10:45

(Session 12): Topological Materials - Chair: Prof. Guang-Yu Guo (National Taiwan Univ., Taiwan)

10:45 – 11:15
Prof. Tay-Rong Chang (National Cheng Kung University, Taiwan)
Title: Topological crystalline insulator: from symmetry indicators to material discovery

11:15 – 11:45
Prof. Xian-Gang Wan (Nanjing Univ., China)
Title: Towards ideal topological materials: Comprehensive database searches using efficient symmetry indicators

11:45 – 12:15
Prof. Hsin Lin (Academia Sinica, Taiwan)
Title: Topological Materials

(Closing Session)
12:15 – 12:20 Closing Remark - Prof. Kee Joo Chang (KAIST, Korea)

(Tour)
12:30 – 18:00 Baekje UNESCO Heritage Tour
* Gathering place: Bus Stop by The Duck Pond

Posters

PO-1 Soungmin Bae (KAIST)
Density functional study of phonon-induced photocarrier capture in defective $MoSe_2$

PO-2 Xiangyan Bo (Nanjing University)
withdrawn

PO-3 Iulia Emilia Brumboiu (KAIST, KTH)
The Influence of Electron Correlation on the Electronic Structure of Transition Metal Phthalocyanines

PO-4 Sanggyun Byeon (Sungkyunkwan University)
withdrawn

PO-5 Seongjae Byeon (KAIST)
Computational study of strain effect on the electronic properties of Cu-doped CdSe nanoplatelets

PO-6 Supparat Charoenphon (Kasetsart University)
Energetics and optical properties of carbon impurities in rutile TiO_2

PO-7 Yifeng Chen (National University of Singapore)
Defect induced exciton states in transition metal dichalcogenide WSe_2 monolayer from first principles

PO-8 Young-Jae Choi (POSTECH)
Phonon-calculation validity of neural-network-potential

PO-9 Ji-Hae Choi (POSTECH)
Emergence of Out-plane Ferroelectricity in Atomically Thin $A_{0.5}B_{0.5}X_2$ (A=W Mo; B=Re Tc; X=S Se Te) Monolayer

PO-10 Min Choi (Ulsan National Institute of Science and Technology)
Excited electron dynamics in the 2H/1T heterophase of monolayer MoS_2 and its phase engineering: real-time time dependent density functional theory study

PO-11 Young Woo Choi (Department of Physics, Yonsei University)
Structural relaxation electronic structure and electron-phonon coupling in magic-angle twisted bilayer graphene

PO-12 Feng-Chuan Chuang (National Sun Yat-sen University)
withdrawn

PO-13 You Kyoung Chung (SungKyunKwan University)
The structural and electronic properties of $Mo_6S_3I_6$ nanowires by theoretical compositional arrangement

PO-14 Klichchupong Dabsamut (Kasetsart University)

First-principles Calculations of Stacking Stability of C_2N Bilayer Nanosheet

PO-15 Igor Di Marco (APCTP)
Standard model of the Rare-Earths analyzed from the Hubbard I approximation

PO-16 Alexey Dyachenko (Russian Academy of Sciences)
DFT+DMFT study of phase transitions with a large volume collapse in MnSe under pressure

PO-17 Yoshiyuki Egami (Hokkaido University)
First-Principles Study on Electron Transport Properties of Halogenated Graphene

PO-18 Liang Ying Feng (National Sun-yat Sen University)
Predicting topological insulators in hydrogenated transition metal dichalcogenide monolayers: A first-principles study

PO-19 Masahiro Fukuda (Project researcher of Institute for Solid State Physics, University of Tokyo)
Structure exploration for AB_2 type monolayers by high-throughput DFT calculations

PO-20 Pankajkumar Gajjar (Gujarat University)
withdrawn

PO-21 Hui-Jun Gu (Fudan University)
Intermediate-phase Method for Computing the Natural Band Offset between Two Materials with Dissimilar Structures

PO-22 Satoshi Hagiwara (National Institutes for Quantum and Radiological Science and Technology)
Theoretical study on positronium formation at metal surfaces based on two-component density functonal theory

PO-23 Woo Hyun Han (KAIST)
A hybrid approach combining artificial neural network potentials with first-principles calculations

PO-24 GyuSeung Han (KIST)
Phase Diagram of Ga (As Sb) and (In Ga)As by Cluster Expansion and DFT Calculations

PO-25 Koki Harada (Tokyo University Of Science)
Water droplet affects charge distribution of carbon nanotube

PO-26 Xin He (Jilin University)
Swarm-Intelligence Guided Computational Design of Novel Silicon Allotropes

PO-27 Keiya Hiraoka (ISIR-SANKEN, Osaka University, Japan)
A first-principle study on the magnetism of Fe/Bi/MgO multilayers

PO-28 Hikaru Horii (Tokyo University of Science)
Tunable Thermoelectric Effects of Bilayer Graphene by Vertical Electric Field

PO-29 Bao-Huei Huang (Department of Physics, National Central University)
Noncollinear Spin Torque Effect in Magnetic Heterojunctions: Combined First-Principles Calculation and TB-NEGF Method

PO-30 Jun Inagaki (TamKang University)
Polarization dependent optical response and layer-controlled band gap of group IV monochalcogenides

PO-31 Keisuke Ishizeki (Tokyo University of Science)
Electronic transport simulation in nitrogen-doped carbon nanotubes focusing on disappearance of Anderson localization due to phonon scattering

PO-32 Seung Woo Jang (KAIST)
Microscopic understanding of magnetic interactions in bilayer CrI_3

PO-33 Sunam Jeon (Sungkyunkwan University)
Type-I and Type-II nodal lines in a magnetic hexagonal InC sheet

PO-34 Min Yong Jeong (Department of Physics, KAIST)
DFT+DMFT study of Pressure dependent Insulator-to-Metal transition in molecular J_{eff} = 3/2 Mott insulator $GaTa_4Se_8$

PO-35 Jaemo Jeong (SungKyunKwan University)
Topological Phase Transition in $NaZnBi_xSb_{1-x}$

PO-36 Il-Seok Jeong (GIST)
withdrawn

PO-37 Hyo Sun Jin (Korea Univ.)
Weyl and Triple Nodal Points in half-metallic ferrimagnets

PO-38 Minwoong Joe (SKKU)
Dominant in-plane cleavage direction of $CrPS_4$ monolayer

PO-39 Jong Hyun Jung (Seoul National University)
A Simple Method to Calculate the Exfoliation Energies of Layered Materials

PO-40 Sirichok Jungthawan (Suranaree University of Technology)
First-Principles Study of Alkali Metal Intercalated MoS_2

PO-41 Sungmo Kang (Seoul National University)
Quantum Anomalous Hall Effect with Higher Chern Numbers in Electron-Doped $CrSiTe_3$: A First-Principles Prediction

PO-42 Narissa Kanlayakan (Chiang Mai University)
Path Integral Molecular Dynamics Simulations for Muoniated Thioformaldehyde Radicals

PO-43 Mitsuaki Kawamura (The Institute for Solid State Physics)
Benchmark of density functional theory for superconductors in elemental materials

PO-44 Muhammad Ejaz Khan (KAIST)
Semimetallicity and Negative Differential Resistance from Hybrid Halide Perovskite Nanowires

PO-45 Yeil Kim (Yonsei Univ.)
Non-Covalent Interactions in Density Functional Calculations

PO-46 Hu Sung Kim (KAIST)
Odd-even phonon transport effects in strained carbon atomic chains bridging graphene nanoribbon electrodes

PO-47 Min-Cheol Kim (KIST)
Abnormalities in Density Functional Calculations on Ions and Radicals and its solution: Density-Corrected Density Functional Theory

PO-48 Do Hoon Kim (KAIST)
First-principles-based calculation of branching ratio for 5d, 4d and 3d transition metal systems

PO-49 Hyun Woo Kim (KRICT)
Comparing two mapping formalisms for mixed quantum-classical simulations of complex systems

PO-50 Eunmi Kim (UNIST)
withdrawn

PO-51 Tae Hyung KIM (KAIST)
Atomistic origins of low-resistance metal contacts to phase-engineered MoS_2

PO-52 Dongwook Kim (Sungkyunkwan University)
Z 2 monopole nodal lines in ABC graphdiyne

PO-53 Yusei Kioka (Department of Electrical Engineering, Tokyo University of Science, Tokyo, 125-8585)
Ab Initio Calculations of Electrical Structures of Water Adsorbed on Graphene

PO-54 Eunjung Ko (KIST)
First-Principles Electronic Transport Properties of Ge/amorphous Al_2O_3/Au Structures

PO-55 Takao Kosaka (ISIR-SANKEN, Osaka University, Japan)
DFT-based engineering of Dirac surface states in topological insulator multilayers

PO-56 Taichi Kosugi (University of Tokyo)
Can exact KS potential reproduce HOMO-LUMO gap? : analytically solvable two-electron system

PO-57 Lin Kuan Bo (Academia Sinica, RCAS)
Electronic transport through Ni/ZrO_2 interface: First-principles calculation

PO-58 Artem Kuklin (Kyungpook National University)
Topological Stability of Two-Dimensional Penta-Structures: a case of $PdSe_2$

PO-59 Rameshbabu Kunchala (National Taiwan Univ.)
Electron-Phonon Coupling Superconductivity and nontrivial Band Topology in NbN Polytypes

PO-60 Fumiaki Kuroda (Osaka University)
Carrier doping effect on all-Heusler giant-magnetoresistance junctions with semimetallic Fe_2VAl studied by first-principles calculations

PO-61 Viet-Duc Le (KAIST)
First-principles Study of Band Gap Tunability in Hydrogenated Graphene

PO-62 Seunghyun Lee (KBSI, UNIST)
Chemical degradation of OLED host materials: the role of excited carriers in non-local interaction

PO-63 Chi-Cheng Lee (The University of Tokyo)
Revisiting Anomalous Hall Conductivity in BCC Iron via First-Principles Tight-Binding Calculations using Pseudo Atomic Orbitals

PO-64 Yea-Lee Lee (Korea Research Institute of Chemical Technology)
Topological Phases in One-dimensional Graphene Nanoribbons

PO-65 Hyunggeun Lee (KAIST)
Revisit to the molecular J_{eff} ground state of lacunar spinel compounds: A charge-density functional plus U study

PO-66 Weon-gyu Lee (SKKU)
New One-Dimensional Material Nb_2Se_9: Theoretical Prediction of Indirect to Direct Band Gap Transition Due to Dimensional Reduction

PO-67 Seungjun Lee (Kyung Hee University)
Versatile physical properties in new two-dimensional van der Waals materials composed of group IV-V elements

PO-68 Kyeongpung Lee (Seoul National University)
First-principles investigation on Al doping in $SrTiO_3$

PO-69 Jaichan Lee (Sungkyunkwan University)
withdrawn

PO-70 Juho Lee (KAIST)
Silicon Passivation of Zigzag Graphene Edge for Spintronic Nanosensor Applications

PO-71 Tianshu Li (Jilin University)
First-principles Calculations of Intrinsic Defect Properties in Halide Double Perovskites for Optoelectronic Applications

PO-72 Wei Liu (The University of Tokyo)
Voltage Dependence of Ni-Li Electrode on its Composition and Structure: A Density Functional Theory Study

PO-73 Gennevieve Macam (National Sun Yat-sen University)
Prediction of Quantum Anomalous Hall Effect in MBi and MSb (M:Ti Zr and Hf) Honeycombs

PO-74 Aniceto III Maghirang (National SUN YAT-SEN Univ.)
Two-dimensional topological insulators upon substitutional doping of monolayer VB-VIA transitional metal dichalcogenides

PO-75 Hong-guk Min (Sungkyunkwan University (skku))
Topological Dirac Insulator in a Nonsymmorphic Circuit Lattice

PO-76 Susumu Minami (Kanazawa University)
First-principles study of anomalous Nernst effect in Fe_3Al and related compounds

PO-77 Hiroyoshi Momida (Osaka University)
Guiding Principles for Enhancing Piezoelectricity in Wurtzite Materials: First-Principles Calculations

PO-78 Sutassana Na Phattalung (Walailak University)
Magnetic states and intervalence charge transfer of Ti and Fe defects in α-Al_2O_3: The origin of the blue in sapphire

PO-79 Masao Obata (Kanazawa University)
Magnetic Dipole-dipole Energy Evaluation on 1D 2D and 3D Periodicities using Density Functional Approach

PO-80 Yun-Tak Oh (Department of physics, Sungkyunkwan University)
Three-dimensional Dirac semimetal in a nonsymmorphic wallpaper multi-layer

PO-81 Taisuke Ozaki (Univ. of Tokyo)
Efficient O(N) divide-conquer method with localized natural orbitals

PO-82 Eun-Won Park (Sookmyung Women's University)
Simulated Scanning Tunneling Microscope Images of Intrinsic Defects in $MoTe_2$

PO-83 Hanjin Park (Kyung Hee University)
First Principle Study of Non-thermal Phase Transition Mechanism with Uniaxial Stress Applied Phase Transition Material : GeTe

PO-84 Jae-Hyeon Parq (Seoul National University)
Estimation of the Effective On-Site Coulomb Interaction Parameter U by Mapping Atomic Self-Interaction Correction onto GGA+U for Molecules

PO-85 Lien Pham Thi Thanh Tan (University of Ulsan)
Computational predictions of stable phase for antiperovskite Na_3OCl via rotation of ONa_6 octahedra

PO-86 Thantip Roongcharoen (Chiang Mai University)
Theoretical insight into methane oxidation to methanol on single Fe-embeded nitrogen-doped graphene

PO-87 Junga Ryou (KAIST)
Edge Effect of Graphene Adsorbed on the ZnO Surface : A First Principles Study

PO-88 Hirofumi Sakakibara (Tottori University)
Model mapped RPA: first-principles method to determine a Hubbard model Hamiltonian

PO-89 Rusrina Salaeh (Chiang Mai University)
Electronic and Photophysical Properties of Derivatives of 2-Phenylbenzothiazole and 2-(2´-Hydroxyphenyl) benzothiazole: Effect of Intramolecular Hydrogen Bonding

PO-90 Abdus Samad (University of Ulsan)
Ferroelectricity and Piezoelectricity in stable monolayers MoC WC WS and WSe

PO-91 Hikaru Sawahata (Kanazawa University)
First-principles study of Electric-field induced Z_2 topological phase transition in strained one-bilayer Bi(111)

PO-92 Smritijit sen (Department of Physics and Center for Theoretical Physics, National Taiwan University)
First Principles Investigations on a New 1111-type Fe-based Superconductor: ThFeAsN

PO-93 Insung Seo (Dept. Mater. Sci. Eng., Tokyo Institute of Technology, Japan)
First-Principles Study of Ir Desorption from Its Low-index Surfaces

PO-94 Aamir Shafique (University of Ulsan)
The effect of strain on the phonon thermal transport properties of the two-dimensional 2H-$MoTe_2$

PO-95 JaeHwan Shim (Seoul National University)
OpenMX interface for the Atomic Simulation Environment

PO-96 Koji Shimizu (The University of Tokyo)
Construction of Neural Network Potential to Study Li-Ion Distribution near Au(111)/Li_3PO_4 Interface

PO-97 Mahbubul Alam Shoaib (University of Ulsan)
Oxygen adsorption and oxygen dissociation on TiB2 monolayer.

PO-98 Jae-Hoon Sim (KAIST)
Open source code development for DFT + DMFT calculation: correlated subspace projection and analytic continuation

PO-99 Youngjoon Song (Korea University)
Searching for Antiferromagnetic Topological Phases

PO-100 Suhwan Song (Yonsei Univ.)
Correcting DFT problems for the spin-state of transition metal complexes

PO-101 Wan-Sheng Su (National Taiwan Science Education Center)
Structural and electronic properties of α-Te tubular nanostructures: a first-principles study

PO-102 Chattarika Sukpattanacharoen (Chiang Mai University)
Heteroatom effect on electronic and photophysical properties of 3-hydroxyquinolin-4(H)-one and its analogues enhancing in the excited-state intramolecular proton transfer processes: A TD-DFT study on substitution effect

PO-103 Terumasa Tadano (National Institute for Materials Science (NIMS))
First-Principles Study of Phonon Anharmonicity in $CsPbBr_3$

PO-104 Kengo Takashima (Tokyo University of Science)
Variance of GNR FET Characteristics Caused by Anderson localization phenomena

PO-105 Feng Tang (Nanjing University)
withdrawn

PO-106 Viet Dung Tran (University of Ulsan)
Surface effects in the (001) $BaTiO_3$ ferroelectric slab from first-principles calculations and phase field simulation

PO-107 Yoshihiro Ueda (Tokyo University of Science)
Secondary Electron Emission from Multi-layer Graphene by TDDFT Simulations

PO-108 Hamid Ullah (University of Ulsan)
Defective SnS monolayer as a candidate for long-range ferromagnetism

PO-109 Rovi Angelo Beloya Villaos (National Sun-yat Sen University)
Thickness Dependent Electronic Properties of Pt Dichalcogenides - PtX_2 (X = S Se and Te)

PO-110 Di Wang (Nanjing University)
withdrawn

PO-111 Yue Wang (Hanyang University)
Local work functions of clean tungsten surfaces under electric fields based on *ab initio* calculations

PO-112 Mei-Ling Xu (Department of Physics National Sun Yat-sen University)
Prediction of Large-Gap Topological Insulator in functionalized Ordered Double Transition Metal MXene

PO-113 Liangliang Xu (Hanyang University)
First principles study on electronic properties of magnetite for spin polarized electron emission

PO-114 Kunihiro Yananose (Seoul National University)
First principle Study on Surface States of Rocksalt SnSe

PO-115 Hyeonwoo Yeo (KAIST)
Electrochemical potential profiles of molecule junctions using constrained-search density functional study

PO-116 In Won Yeu (Seoul National University)
Vibrational effects on the surface energy of III-V compound semiconductors using *ab-initio* thermodynamics

PO-117 Hongkee Yoon (KAIST)
Analytic continuation via “domain-knowledge free” machine learning

PO-118 Daiki Yoshikawa (Kanazawa University)
First-Principles Density Functional Study in the Magnetically and Electrically polarized Pt/CoO/ZnO

PO-119 Kanako Yoshizawa (Research Organization for Information Science and Technology)
Performance information of first-principles codes in K computer

PO-120 Nan Zhao (Hanyang University)
First principles study on electronic properties of graphene nanostructures for high current density cathode

Abstracts

Oral Presentations

[Invited talk: 9:00 – 9:45, Oct.29, 2018]

Topological and Interaction Effects in Atomically Thin 1D & 2D Materials

Steven G. Louie[1,*]

[1] *Physics Department, University of California at Berkeley, and Lawrence Berkeley National Lab, Berkeley, California 94720 U.S.A.*

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Symmetry, interaction and topological effects, as well as environmental screening, dominate many of the quantum properties of reduced-dimensional systems and nanostructures. These effects often lead to manifestation of counter-intuitive concepts and phenomena that may not be so prominent or have not been seen in bulk materials. In this talk, I present some fascinating physical phenomena discovered in recent studies of atomically thin one-dimensional (1D) and two-dimensional (2D) materials. A number of highly interesting and unexpected behaviors have been found – e.g., strongly bound excitons (electron-hole pairs) with unusual energy level structures and new topology-dictated optical selection rules; tunable magnetism and plasmonic properties; novel topological phases; correlated multi-particle excitations; etc. – adding to the outstanding promise of 1D and 2D materials for exploration of new science and valuable applications.

This work was supported by the U. S. Department of Energy, National Science Foundation, and Office of Naval Research.

[Invited talk: 9:45 – 10:15, Oct.29, 2018]

Topics of Two-Dimensional Materials and Their Heterostructures

Chih-Piao Chuu,[1] Chi-Ruei Pan,[2] Kuan-Sen Lin,[3] and Mei-Yin Chou[1,2,3,*]

[1] *Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan*
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It has become possible in recent years to fabricate and manipulate two-dimensional nanomaterials in the laboratory that are as thin as one to few atomic layers. The reduced dimensionality gives rise to unique physical and chemical properties that differ from those of traditional bulk materials, and intriguing physical properties have been found in these few-layer systems. Computational studies have played a central role in understanding and predicting these novel properties. In this talk, I will focus on a few representative systems, including graphene systems and monolayers of transition metal dichalcogenides that exhibit properties ranging from charge density waves [1] to the quantum spin-Hall effect [2]. The hybrid system of boron nitride and graphene (h-BNC) at low BN doping serves as an ideal platform for band-gap engineering and valleytronic applications. The calculations find a linear dependence of the band gap on the BN concentration at low doping, arising from an induced effective on-site energy difference at the two C sublattices as they are substituted by B and N dopants alternately. In addition, our calculations show that the Moiré patterns in van der Waals heterostructures will modify the local band gap, interlayer interaction, and structural parameters [3-5]. I will also discuss one-dimensional topological insulators manifested in graphene nanoribbons, in which localized spin states may exist at the end or near the junctions. A symmetry protected Z_2 topological classification is formulated for any type of termination with a π-quantized Berry phase when summed over all occupied bands.

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[Invited talk: 10:45 – 11:15, Oct.29, 2018]

Electronic and Optical Properties of 2D-material-based Heterostructures

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The atomically thin nature of layered two-dimensional (2D) materials results in emerging properties that are different from their bulk counterparts. One often cited example is the reduced electronic screening resulting in stronger exciton binding energies in 2D materials. 2D materials are also interesting because of the potential for bottom-up design of various flexible heterostructures. In this regard, it is important to understand how the different components of the heterostructure affect the electronic and optical properties of the system. We will discuss 2D-material heterostructures based on the elemental material phosphorene, as well as hybrid organic-2D-material heterostructures. Using state-of-the-art GW+BSE methods, we show that bright interlayer excitons exist in the direct band gap phosphorene (BP)-based heterostructures (BP/GeS and BP/hBN), with a good compromise between binding energies, oscillator strength and radiative lifetimes.[1] Strong hybridization between GeS and BP increases the effective mass and room temperature exciton lifetimes, while the hBN spacer layer decouples the BP monolayers in BP/hBN/BP, resulting in the lowest energy exciton becoming dark. A single hBN layer reduces the exciton binding energy in monolayer BP by ~0.11 eV, while adding another hBN layer in hBN/BP/hBN further reduces the binding energy by ~0.03 eV. This brings us to our next topic, which is to investigate how a 2D material screens excitations *adjacent to* it, such as excitations in adsorbed molecules. We show that the extent to which a material screens the band gap of small adsorbed benzene molecules is given by the screening potential Vscr(r,r) at the position of the molecule. Interestingly, by computing Vscr(r,r) for a range of 2D materials and slabs of 3D materials, we find that Vscr(r,r) at a given distance away from the material scales approximately linearly with the quasiparticle gap in the same manner for all these materials. This is in contrast to the screening of excitations within materials, which differ significantly between 2D and 3D materials. Finally, if time permits, we will discuss Raman optical spectra for organics on 2D materials, where electron-phonon coupling leads to interesting chemical enhancement effects.

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[Invited talk: 11:15 – 11:45, Oct.29, 2018]

Engineering spin-valley physics in bilayers of $MoSe_2$

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Monolayers of transition metal dichalcogenides (MX_2, M=Mo,W) are found to have their valence band maximum at K point. In most instances when the second layer is added, the interaction between the two layers results in the valence band maximum shifting to Gamma. As the valence band maximum at K point is contributed primarily by d_{xy} and d_{x2-y2} orbitals of the transition metal atom, one finds that spin-orbit interactions lead to large spin splittings of the valence band maximum. This has interesting consequences as spin-orbit interactions alone cannot lead to magnetic order. This then implies that the spin splitting at the symmetry point -K is opposite in direction to that at K. In this talk I will present our recent results of how the spin splittings evolve for bilayers of $MoSe_2$.

This is work done in collaboration with Poonam Kumari and Joydeep Chatterjee.

[Invited talk: 11:45 – 12:15, Oct.29, 2018]

First-principles investigations of nonequilibrium states of periodically driven black phosphorous

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Recent advances in ultrafast spectroscopy open a route toward engineering new phase of solids with optical pumping. The nonequilibrium electronic states of solids driven by the electromagnetic field manifest novel topological states which don't exist at equilibrium conditions. Using first-principles calculations and Floquet theorem, we studied the dressed states of black phosphorous and graphene under periodic driving by laser. Intriguing photo-dressed electronic states including Floquet Dirac semimetals, Floquet topological insulators *etc* can be engineered in black phosphorous by changing the direction, intensity and frequency of incident laser [1]. The coexistence of type-I and type-II Floquet Dirac fermion (FDF) in graphene can be realized simultaneously, which can be monitored by simulating the pump-probe time and angular-resolved photoelectron spectroscopy. In the transition boundary between type-I and -II FDF, we found one critical type-III FDF, which could be utilized to achieve the highest Hawking temperature T_{H} hitherto reported [2]. Our works demonstrate examples of the nonequilibrium topological states of two-dimensional materials by first-principles calculations, and open an avenue towards the Floquet engineering of quantum materials.

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[Invited talk: 14:00 – 14:45, Oct.29, 2018]

2D, or not 2D?

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Quantum-mechanical simulations have become massively used tools for scientific discovery and technological advancement: thanks to their predictive power they can suggest, accelerate, support or even substitute actual physical experiments. This is a far-reaching paradigm shift, replacing the cost- and time-scales of brick-and-mortar facilities, equipment, and personnel with those, very different, of computing engines - aiming at understanding, predicting, or designing the properties and performance of novel or complex materials and devices.

I will briefly highlight the current accomplishments and challenges, outline the current roadmap for materials discovery driven by the convergence of high-performance and high-throughput computing, and I will illustrate its potential with the example of novel two-dimensional and layered materials, displaying promising electronic, optical, or topological properties [1]. In the process, I will discuss the software stack that we need to deploy to upscale materials simulations towards materials discovery, and the requirements for data curation, dissemination, and reproducibility [2].

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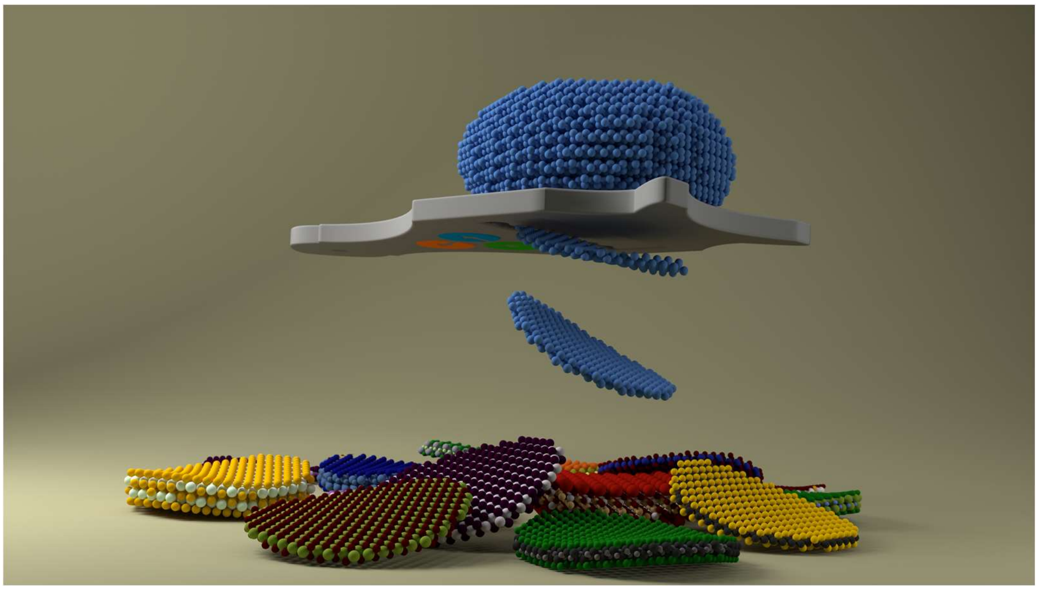

[Invited talk: 14:45 – 15:30, Oct.29, 2018]

All-electron electronic structure theory for new materials for light harvesting and light emission

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Materials for light harvesting and light emission are immensely fertile ground for electronic structure theory, for the simple reason that key physical phenomena behind a particular materials' function arise at the atomic scale. Key challenges for theory include: Structures can be complex; the computationally desired phase may compete for stability with an *a prio*ri unknown zoo of possible secondary phases; accurate predictions of excited-state phenomena in large structures remain a challenge for the field. In this talk, we describe our progress on these issues using the all-electron approach in the FHI-aims code [1], a high-accuracy, scalable and affordable general-purpose code for molecular and materials simulations. Examples include the nature of polymeric carbon-nitride materials for photocatalytic hydrogen evolution [2], new quaternary semiconductor materials I_2-II-IV-VI_4 (I=Cu, Ag; II=Sr,Ba; IV=Ge,Sn; VI=S,Se) for photovoltaics [3,4], and identifying the nature of carried levels in layered organic-inorganic perovskites with optically active organic components by large-scale hybrid density-functional theory[5]. We finally describe ongoing work on an open-source infrastructure "ELSI" to bridge between electronic structure user codes and massively parallel solver libraries for the large-scale (generalized) Kohn-Sham electronic structure problem, and we describe progress on distributed-parallel GPU architectures.

This overview talk covers joint work with many colleagues around the world, including the groups of Bettina Lotsch (Stuttgart/Munich), David Mitzi (Duke), Yosuke Kanai (UNC), Matthias Scheffler (FHI Berlin), Xinguo Ren (USTC Hefei), group members at Duke University, and the very large developer community of the FHI-aims code - all these and further interactions, as well as support from the National Science Foundation and the US Department of Energy, are gratefully acknowledged.

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[Invited talk: 16:30 – 17:00, Oct.29, 2018]

Novel Materials for Ferroelectric Photovoltaics

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Despite their potential to exceed the theoretical Shockley-Queisser limit, ferroelectric photovoltaics (FPVs) have performed inefficiently due to their extremely low photocurrents. In this talk, I will suggest novel ferroelectric materials that are likely to overcome the challenge, as a result of density functional theory calculations. These works indicate that the large band-gap and inefficient e-h separations of active layer materials are the most important issues to be addressed for FPVs to compete with conventional devices.

[Invited talk: 17:00 – 17:30, Oct.29, 2018]

First-principles theoretical study of catalytic reactions at surfaces and interfaces

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Chemical reactions at surfaces and interfaces play important roles in wide varieties of applications such as hegerogeneous catalysis, electrochemistry, fuel cells, batteries, etching processes of semiconductor materials, and so on. In this talk, we will present theoretical investigation and prediction of hydrogenation of CO_2 over Cu catalyst[1]. Adsorption and reaction of CO_2 on solid surfaces are attracting growing interest because of their importance in industrial, energy and environmental management. To clarify reaction mechanisms and to identify important factors governing the reactivity of CO_2 on solid surfaces are very important to develop more efficient catalysts or catalytic processes for utilization of CO_2. To this end, we investigated CO_2 adsorption and hydrogenation[1] on Cu surfaces using van der Waals density functionals as implemented in our home made STATE (Simulation tool for Atom TEchnology) program code [2]. We theoretically proposed a new reaction scheme to enhance the hydrogenation of CO_2 on Cu.

In the second topic, we will discuss enhancement of NO dissociation by hydrogen bonding. Nitric oxide (NO) emission from the exhaustive gas of combustion process has caused negative impacts on the environment, e.g, acid rain, photochemical smog, and ozone depletion. So far, catalytic activities for NO dissociation on the Cu surfaces have been recognized to be lower than that on Rh. Shiotari *et al*. experimentally found that the hydrogen bond between NO and water monomers promotes the NO dissociation to take place almost barrierlessly on the Cu(110) surface at a very low temperature (~12 K), which is a promising way to reduce the use of the precious Rh catalyst. would like to point out importance of the van der Waals density functional for describing . We present a DFT study to clarify the role of water molecules and the mechanism of the hydrogen bonding induced NO dissociation on the Cu(110) surface[3].

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[Invited talk: 17:30 – 18:00, Oct.29, 2018]

DFT Mechanistic Study of Carbon-Doped Boron Nitride Nanosheet as Highly Efficient Metal-Free Catalyst for NO Reduction

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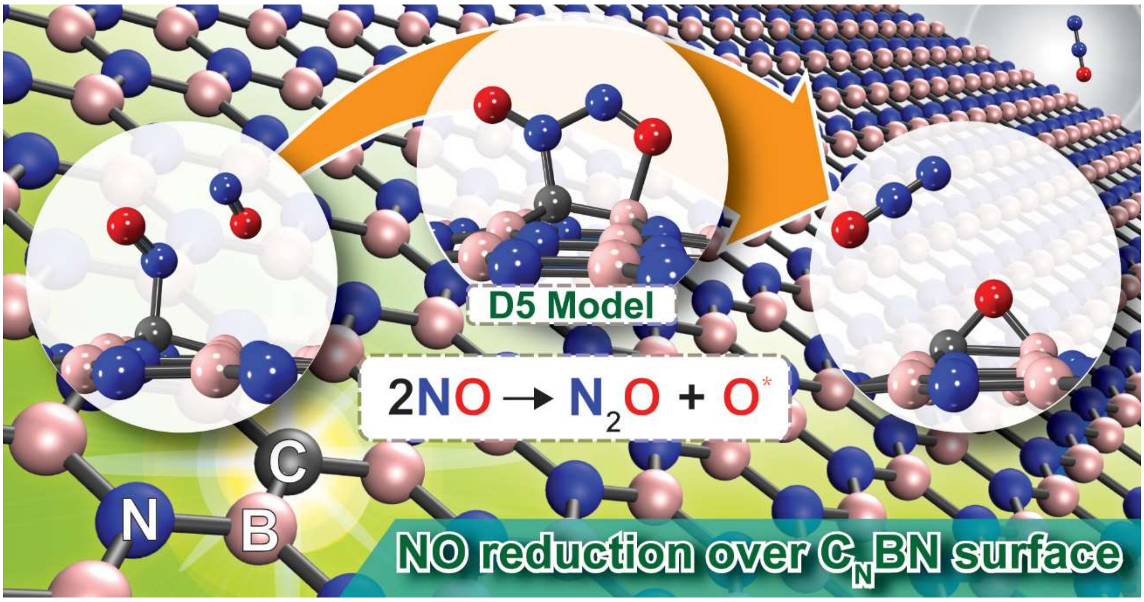
Many of their unique properties and applications of boron nitride nanosheets (h-BNs) have been much less recognized. This is the first time for the use of h-BNs as highly efficient metal-free catalyst for NO catalytic reduction to less-harmful products by density functional theory calculations. We found that the C_NBNs catalyst showed a comparable energy barrier compared to carbon-based and silicon-based catalysts. However, the higher thermal stability, intrinsically insulators and excellent impermeability of C_NBNs nanosheets make them superior to other metal-free catalysts in reusability aspect. The results showed that the trans-$(NO)_2$ dimer of C_NBNs (D5) is a potentially crucial intermediate with thermodynamically and kinetically favorable, in which the calculated barrier for the rate-determining step along the most energetically favorable pathway is 0.62 eV. Hence, we suggest that CNBNs can be used as highly active metal-free materials in NO removal, which will reduce NO into green products with kinetically, and thermodynamically favorable under ambient conditions.



Keywords: Metal-free catalyst, boron nitride nanosheets, nitrogen oxide reduction, DFT

[Invited talk: 9:45 – 10:15, Oct.30, 2018]

Vibrational effects in electronic structure: Temperature-dependence, zero-point motion, spectral functions

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Modifications of electronic eigenenergies due to vibrational effects and electron-phonon coupling are sizable in many materials with light atoms. While often neglected, they have been recently computed from first principles using different formalisms, including the perturbation-based Allen-Heine-Cardona (AHC) theory, in the adiabatic or non-adiabatic harmonic approximation.

I will provide an overview of the concepts and formalism, and discuss [1]: the DFT and GW corrections to the diamond bandgap, the latter (0.6 eV) being significantly higher than the former (0.4 eV); the breakdown of the adiabatic AHC theory for infrared-active materials, and fix of this problem in the non-adiabatic AHC theory. Then, focusing on the latter class of materials, I will establish the connection with a simple approach based on a generalized Frohlich Hamiltonian and discuss the near-cancellation between the first-principles Fan and Debye-Waller contributions [2].

Other consequences of interactions, visible in ARPES experiments, are broadening of quasi-particle peaks and appearance of sidebands in the electron spectral function. Migdal selfenergies and spectral functions will be presented for MgO and LiF. The spectral function obtained from the Dyson equation makes errors in the weight and energy of the quasi-particle (QP) peak and phonon-induced sidebands. Only one phonon satellite appears, with an unphysically large energy difference with respect to the QP peak. By contrast, the spectral function from a cumulant treatment is physically better, giving a quite accurate QP energy and several satellites approximately spaced by the LO phonon energy. I will provide a detailed comparison between the first-principles results and those of the Fröhlich Hamiltonian. Such an analysis applies widely to infra-red active materials.

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[Invited talk: 9:45 – 10:15, Oct.30, 2018]

High-throughput first-principles phonon calculation and phonon database

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First-principles phonon calculation has been popular in recent scientifc researches. In the harmonic appoximation, now we have enough computational hardware resource to achieve high-throughput phonon calculations for ~10,000 compounds [1-3]. However the high-throughput calculations are not a trivial task since we need a sophisticated workflow engine to systematically execute first-principles phonon calculations. Among workflow engines, `AiiDA` [4] and `atomate` [5] may be the most popular packages. A number of people are working to develop the workflow engines and a lot of efforts have been put into the development. These developlements are well organized on their github repositories that are open to everybody indeed. These workflow engines rely on many other software packages that are also expected to be robust. We have been contributing to them by providing crystal symmetry finder (`spglib` [6]) that is widely used in materials science. For the first-principles calculations to be run by the workflow engines, fortunately we have several realistic choices of DFT or DFPT plane-wave pseudopotential codes such as QUANTUM `ESPRESSO`, `ABINIT`, and `VASP` codes.
To achieve our phonon calculations [3], force constants were calculated in supercells with finite small atomic displacements (~0.03Å), where the initial crystal structures were obtained from the materials project [7]. This set of phonon calculations is performed under the approxmation valid at low temperatures. Thereofre non-negligile number of compounds exhibit imaginary modes that may be removed at elevated temperatures. To treat high temperature properties, several methods have been developted to obtain anharmonic force constants by large atomic displacements [8,9]. Our next challenge is high-throughput phonon calculation with anharmonicity for which we still have to develop robust software environment. We review current computing system to perform the high-throughtput harmonic phonon calculation and discuss what kinds of software packages will have to be developed for high-throughtput anharmonic phonon calculations.

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[Invited talk: 10:45 – 11:15, Oct.30, 2018]

Quasiparticule spectra based on wave function theory: Application of coupled-cluster theory and self-energy functional theory

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Coupled-cluster singles and doubles (CCSD) is one of wave-function theories and known as a highly accurate calculation scheme in the field of quantum chemistry. Recently, the relation between CCSD and GW approximation, which is known as a well sophisticated calculation method in condensed matter physics, was clarified [1] and CCSD has get growing attention also in condensed matter physics. However, the standard CCSD scheme cannot yield quasi-particle energy spectra directly. Recently, it has been reported that by employing the one-particle Green's function within the CCSD scheme (GFCCSD), one is capable of obtaining physical quantities including energy spectra [2]. Although the GFCCSD method has already been applied to uniform electron gases [3], there is no report of the application to realistic systems.

In this work, we have developed a code to calculate the quasi-particle energy spectra of isolated atoms and periodic systems through the GFCCSD method and applied it to several realistic materials for the first time [4-6]. We have also applied the self-energy functional theory to the systems for the first time and clarified the accuracy of the GFCCSD method. Consequently, we have found that the GFCCSD method is a powerful tool which enables us to calculate total energy and quasi-particle spectra self-consistently. In particular, the GFCCSD method successfully reproduces quasi-particle bands and satellite peaks at the same time as shown in Fig.1. Furthermore, we have also shown that the GFCCSD method can reproduce Mott gaps in finite systems.

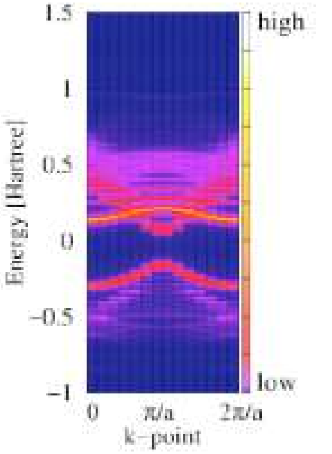

Fig. 1: Quasi-particle energy spectra of 1-dimensional Be chain calculated by the GFCCSD method. Fermi energy is ste to 0.

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[Invited talk: 11:15 – 11:45, Oct.30, 2018]

Toward the Better First-principles Description of Correlated Materials: Old Functionals and New Concepts

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In this talk, I will try to give a brief overview of recent progress in my research group for developing first-principle-based computation methods. In the first part, I will discuss LDA/GGA+U functionals. Although this method has become a standard tool ever since its first suggestion in 1991, the detailed understanding of the differences in between various functional recipes has not been reached yet which severely hampers the application to real material research. With this motivation, we recently performed the systematic and comparative analysis on this issue [1,2]. In the second part, I will discuss a new physical quantity temporally named as 'effective degeneracy' or 'effective entropy'. In understanding condensed matter systems, it is sometimes crucially important to develop or define a new physical concept which carries the key physical intuition. In order to understand multi-band Mott transitions, we suggest this quantity based on entropy-like term [3]. Its usefulness will be demonstrated with some materials examples. Finally (if time allows), I will also introduce our recent developments for the magnetic force linear response calculation techniques [4] as well as the new analytic continuation methods [5, 6].

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[Invited talk: 11:45 – 12:15, Oct.30, 2018]

Spin-orbital-entangled J_{eff} =1/2 state in 3*d* transition metal oxide $CuAl_2O_4$

Choong H. Kim,[1, 2] H. Cho,[1, 2] S. Baidya,[1, 2] V. V. Gapontsev,[3] S. V. Streltsov,[3, 4] Daniel I. Khomskii,[5] Je-Geun Park,[1, 2], Ara Go,[6], and Hosub Jin[7]

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The interplay of spin-orbit coupling (SOC) and Coulomb correlations have become one of the most active area in condensed matter physics. In particular, the spin-orbital-entangled Kramers pair known as the J_{eff}=1/2 state has been firstly shown in iridates from the intriguing role of large SOC assisted by small electron correlation. The newly found J_{eff}=1/2 state has brought about a variety of novel phenomena including the relativistic Mott phase, Kitaev quantum spin liquid, non-trivial topology, and so on. To date, however, most of studies have been limited to 4d and 5d transition metal compounds, where the correlation strength is relatively weak. It is mainly due to the existing consensus that large SOC strength is a prerequisite for this fully relativistic entity. During the long history of the 3d transition metal study, SOC has never been a dominating energy scale, rendering the spin-orbital-entangled state almost impractical. Thus, we are still far from understanding the behavior of the spin-orbital-entangled state under the strong correlation limit. Here we report on the $CuAl_2O_4$ spinel as the first example of a J_{eff}=1/2 Mott insulator in 3d transition metal compounds. Density functional theory combined with dynamical mean field theory calculations reveal that the J_{eff}=1/2 state survives the competition with the orbital-momentum-quenched S=1/2 state with the help of strong electron correlation. The fully relativistic entity found in $CuAl_2O_4$ provides insight into the untapped regime where the spin-orbital-entangled Kramers pair resides with strong electron correlation.

[Invited talk: 14:00 – 14:45, Oct.30, 2018]

First principle investigation of defect properties in energy materials

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First-principles study of semiconductor energy materials plays an important role in developing clean energy technologies because it can provide useful physical insights, fresh perspective and new design principles for developing innovative clean energy materials with high solar power conversion efficiency and reduced cost. Similar to other semiconductors, one of the most important issues in energy material is to control the defects, either for introducing charge carrier, improving charge transport, or reducing non-radiative carrier recombination. For example, a good solar cell material should have good defect properties so that it can be doped well such that charge carriers can be created easily to generate the required electric field and has less defect-induced recombination centers such that it has high carrier life time and minority carrier mobility, so photo-generated charge can be easily collected. In this talk, using thin-film solar cell absorber materials CdTe, CIGS and CZTS as examples, I will discuss how theoretical first-principles studies can be used to better understand and improve the solar cell performance. Control of doping in other optoelectronic energy materials such as TCOs will also be discussed.

[Invited talk: 14:45 – 15:15, Oct.30, 2018]

First-principles theory of defect-based qubits in heterogeneous semiconductors

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Recently, significant progress has been made toward full control of the quantum states of spins and charges in a variety of semiconductors and solid-state nanostructures for applications in quantum information processing, quantum optics, and quantum sensing. Such platforms include the NV center in diamond, dopants in silicon, single-photon emitters in 2-dimensional crystals, and solid-state quantum dots. Being in the solid-state, the listed platforms also have a significant potential for scalability. In the first part of the talk, we will outline the principles underlying the listed quantum defect systems in terms of its manipulation and operation schemes. In the second part of the talk, we will highlight some of our own research efforts [1-6] devoted to the point-defect-based qubits in heterogeneous semiconductors. First, we will discuss the Janus aspects of nuclear spin baths: the bad being the source of decoherence for electron spin qubits and the good being useful resources for quantum memory applications. We will show that it is possible to reconcile these conflicting aspects of nuclear spin baths by developing spin qubits either in heterogeneous crystals or low-dimensional crystals. Second, we will discuss computational defect designs to search for promising defect candidates in a variety of heterogeneous semiconductors toward scalable and coherent hybrid quantum systems.

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[Invited talk: 16:15 – 16:45, Oct.30, 2018]

Strain-Induced Half-Metallic States in Graphene: Application of Generalized Bloch Theorem

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Realization of half-metallicity in low dimensional materials is a fundamental challenge for nano spintronics, which is a critical component for next-generation information technology. Using the method of generalized Bloch theorem, we show that an in-plane bending can induce inhomogeneous strains, which in turn lead to spin-splitting in zigzag graphene nanoribbons and results in the highly desired half-metallic state. Unlike the previously proposed scheme that requires unrealistic strong external electric fields, the obtained halfmetallicity with sizeable half-metallic gap and high energetic stability of magnetic order of edge states requires only relatively low-level strain in the in-plane bending. Given the superior structural flexibility of graphene and the recent experimental advances in controllable synthesis of graphene nanoribbons, our design provides a hitherto more practical approach to the realization of half-metallicity in low dimensional systems.

[Invited talk: 16:45 – 17:15, Oct.30, 2018]

First-principles study of Berry-phase-mediated thermoelectric effects

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We are interested in how to achieve much higher thermoelectric conversion efficiency by effectively manipulating electron-spin degree of freedom. As one possibility, we have been studying *Berry-phase-mediated thermoelectric effects*, namely the contribution of the anomalous Hall conductivity (AHC) to thermoelectric power. What we target here is the anomalous Nernst effect (ANE), which is a heat-to-electricity conversion observed in magnetic materials and directly related to AHC. We discussed AHC mainly driven by an effective magnetic field, *Berry curvature,* induced by spin-orbit coupling and/or spin chirality.

In this presentation, we will present our recent first-principles computations [1] on topological magnet (skyrmion crystals) [2,3] and half-Heusler compounds [4]. We found that the effective magnetic field indeed generates large ANE. This behavior was clearly understood by the chemical potential dependence of AHC. Based on the gained knowledge, we will discuss how to enhance such Berry-phase-mediated thermoelectric effects.

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[Invited talk: 17:15 – 17:45, Oct.30, 2018]

Origin of high thermoelectric performance in n- and p-type SnSe crystals

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Tin selenide (SnSe) has emerged as a very promising thermoelectric material due to its record high figure of merit ZT for both n- and p-type crystals in mediate temperature range. In this talk, I will present our recent works regarding its electronic and thermal properties based on first-principles calculations, in combination with the Boltzman transport theory and experimental measurements. The origins of strongly anisotropic thermal and electrical behaviors in this layered lattice structure will be discussed, which give rise to the highest optimal ZT values along the a axis (out-of plane direction) in the n-type SnSe, whereas along b axis in p-type materials. In addition, I will discuss the effects of the intrinsic defects and dopants on its thermoelectric characteristics. Our calculations show reasonable agreements with the experimental observations and provide some guidance for optimizing the thermoelectric performance.

[Invited talk: 9:00 – 9:30, Oct.31, 2018]

Atom Dynamics in Solids Studied by Machine-Learning Techniques

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Development of novel information and energy devices demands deeper understanding on atom dynamics in solids, such as diffusion and vibration. First-principles calculations within the density functional theroy (DFT) is powerful to meet the demand. In practice, however, DFT often requires too heavy computations to tackle with atom dynamics in solids. In this context, interatomic potentials constructed with machine-learning technique and DFT calculation data have attracted much attention recently. In the prensent talk, we will describe our recent works on interatomic potentials constructed with one of machine-learning techniques, neural network (NN).

Our NN potentials are based on the method proposed by Behler and Parrinello [1]. We discuss NN potentials to examine diffusion behaviors of Cu in amorphous Ta_2O_5 [2] and Li in Li_3PO_4 [3]. The results agree well with DFT calculations, showing the high reliability of the constructed NN potentials. For Li in Li_3PO_4, the NN potential trained in a small supercell is successfully applied to calulations in much larger supercells, which suggests good transferability. We will also discuss (i) atom dynamics under electric fields, (ii) structures of metal/solid-electrolyte interfaces, and (iii) phonon bands and thermal transport, with describing our prelimienary results.

Our works presented in this talk were supported in part by “Materials research by Information Integration” Initiative (MI^{2}I) project of the Support Program for Starting Up Innovation Hub from Japan Science and Technology Agency (JST), CREST-JST, and JSPS KAKENHI, Japan.

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[Invited talk: 9:30 – 10:00, Oct.31, 2018]

TDDFT Study of Electron Scattering Processes

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Time-dependent density functional theory (TDDFT) is the most widely used first principles approach to study real-time many-electron dynamics. TDDFT with approximate exchange-correlation (XC) potentilas has been successfully applied to interpret and predict electron dynamics in a range of situations. Recently, it has been applied to the real-time nonperturbative calculations of electron wave packet scattering from atomic layer materials [1-5].

However, it is known that TDDFT with approximate XC potentials fails to even qualitatively reproduce the true dynamics in some applications to nonlinear time-resolved dynamics. In this study [6, 7], we address the question how accurate TDDFT with the currently available approximate XC potentials is for electron scattering. To this end, we have studied model systems of electron-H and electron-He^+ scattering that can be exactly solved numerically.

We have identified peak and valley structures in the exact XC potential that are crucial for accurately capturing time-resolved dynamics of electron scattering [6, 7]. Approximate functionals used today miss these structures and consequently underestimate the scattering probability. The dynamics can vary significantly depending on the choice of the initial Kohn-Sham state. A recently propsed nonadiabatic approximation is shown to correctly capture the approach of the electron to the target when the initial Kohn-Sham state is chosen judiciously, and it is more accurate than standard adiabatic functionals but ultimately fails to accurately capture reflection. These results may explain the underestimation of scattering probabilities in some recent studies on molecules and surfaces.

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[Invited talk: 10:00 – 10:30, Oct.31, 2018]

Band topologies and spin-phonon dynamics of spin-orbit coupled insulators: a study with the real-time TDDFT

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Topological phases of solid-state bands have been widely examined in these days condensed matter field, and global properties immune to local perturbations have been explored as topologically non-trivial observables. The computations of topological quantities of real materials are affordable only through the theories of linear responses over the static ground electronic structure. Here, we propose a conceptually novel and general method: we perform the time evolution of the solid state, $\psi_{\mathrm{n,k}}(\vec{r}, t)$, through the time-dependent Schrödinger equation, and calculate physical observables such as charge current or spin current as an expectation evaluated from the time-evolving states functions. We present exemplary cases of trivial insulator, a spin-frozen valley-Hall system, a spin-frozen Haldane-Chern insulator, and quantum spin-Hall insulators. The same real-time dynamics is also used for the phonon-coupled spin dynamics of semiconductors with strong spin-orbit coupling. We present that the spin precession dynamics of MoS_2 in which the spin is strongly coupled to a specific optical phonon. This dynamical spin state can be resolved into discrete Floquet-phononic spectra, and once the phonon is pumped so as to break time-reversal symmetry, the resulting spin-Floquet structures induce net out-of-plane magnetizations in the otherwise non-magnetic 2D material.

[Invited talk: 10:45 – 11:15, Oct.31, 2018]

Topological crystalline insulator: From symmetry indicators to material discovery

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Topological crystalline insulators (TCI) are insulating electronic phases of matter with nontrivial topology originating from crystalline symmetries. In the past decade, many materials have been demonstrated to be the topological insulators or the topological semimetals, however the exotic TCI states have remained elusive. Building upon recent theoretical works, we develop a feasible method to uniquely determine the novel rotational symmetry topological invariants based on first-principles calculations. In this talk, I will show how we predict new TCI materials and display their unusual electronic structures that entirely distinct from traditional topological materials [1].

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[Invited talk: 11:15 – 11:45, Oct.31, 2018]

Towards ideal topological materials: Comprehensive database searches using symmetry indicators

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Topological materials (TMs) showcase intriguing physical properties defying expectations based on conventional materials, and hold promise for the development of devices with new functionalities. While several theoretically proposed TMs have been experimentally confirmed, extensive experimental exploration of topological properties as well as applications in realistic devices have been held back due to the lack of excellent TMs in which interference from trivial Fermi surface states is minimized. We tackle this problem in the present work by applying our recently developed method of symmetry indicators to all non-magnetic compounds in the 230 space groups. An exhaustive database search reveals thousands of TM candidates. Of these, we highlight the excellent TMs, the 258 topological insulators and 165 topological crystalline insulators which have either noticeable full band gap or a considerable direct gap together with small trivial Fermi pockets. We also give a list of 489 topological semimetals with the band crossing points located near the Fermi level. All predictions obtained through standard generalized gradient approximation (GGA) calculations were cross-checked with the modified Becke-Johnson (MBJ) potential calculations, appropriate for narrow gap materials. With the electronic and optical behavior around the Fermi level dominated by the topologically non-trivial bands, these newly found TMs candidates open wide possibilities for realizing the promise of TMs in next-generation electronic devices.

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[Invited talk: 11:45 – 12:15, Oct.31, 2018]

Topological Materials

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Topological materials host various novel quantum phases of electrons which are characterized by band topology and topologically protected surface/edge states. [1] Despite recent progress, intense world-wide research activity in search of new classes of topological materials is continuing unabated. This interest is driven by the need for materials with greater structural flexibility and tunability to enable viable applications in spintronics and quantum computing. We have used first-principles band theory computations to successfully predict many new classes of 3D topologically interesting materials, including Bi_2Se_3 series, [2] the ternary half-Heusler compounds, [3] $TlBiSe_2$ family, [4] Li_2AgSb-class, and $GeBi_2Te_4$ family as well as topological crystalline insulator (TCI) SnTe family [5] and Weyl semimetals TaAs, [6,7] $SrSi_2$, [8] $(Mo,W)Te_2$, [9] Ta_3S_2, [10] and LaAlGe family. [11,12] I will also highlight our recent work on unconventional chiral fermions in RhSi, [13] cubic Dirac points in $LiOsO_3$, [14] and rotaional symmetry protected TCIs. [15]

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Abstracts

Poster Presentations

Density functional study of phonon-induced photocarrier capture in defective $MoSe_2$

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In recent years, optical electronic excitations and photocarrier dynamics in transition metal dichalcogenides (TMDCs) have been actively investigated in view of understanding photophysics in atomically thin materials and their optical device applications. According to recent studies on pristine TMDCs, acoustic phonons are involved in exciton generation and electron cooling processes [1,2]. In practical situations, TMDC samples usually contain a certain amount of defects and adsorbates, which act as ultrafast photocarrier trapping centers [3,4]. Meanwhile, although the exciton-phonon interaction in pristine TMDC is relatively well studied, defect-related photocarrier trappings remain vague.

Here, we present our theoretical study of defect-induced photocarrier capture in $MoSe_2$ by means of delta-self-consistent-field (ΔSCF) density functional theory calculations [5,6]. Starting from the ground-state $MoSe_2$ with various defects, we explicitly minimize the geometry of its excited states at defects, thus explicitly treating the nonradiative decay through multi-phonon emission processes. Comparing our computational results with pump-probe measurement data, we conclude that the exciton trapping at a Se vacancy adsorbed by an oxygen molecule is a dominant photocarrier capture mechanism.

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Poster-2

The Influence of Electron Correlation on the Electronic Structure of Transition Metal Phthalocyanines

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Transition metal phthalocyanines (TMPcs) are highly symmetric organic molecules with a transition metal atom at their centre. TMPcs have been in the focus of scientific research as possible candidates for applications in spintronics and molecular electronics, where the molecules are typically used when adsorbed on various surfaces [1].

The study of properties of molecules adsorbed on substrates requires the availability of theoretical methods that are accurate enough, but which also have a relatively low computational cost. From this point of view, the description of a TMPc adsorbed on a surface is not straightforward, especially due to the presence of the metal d electrons. A compromise between accuracy and computational cost is achieved by combining Density Functional Theory (DFT) with a Hubbard term exclusively acting on the correlated electrons. Many studies on TMPcs adsorbed on surfaces make use of this approach, but the choice of U is mainly based on previously reported values for similar systems. In this study [2], we provide a detailed analysis of the influence of U on the electronic structure of five TMPcs (Mn-, Fe-,Co-, Ni- and CuPc).

By comparing the calculated valence electronic structures of the single molecules to photoelectron spectroscopy experiments and by computing the Hubbard U term from linear response, we show that U is different for every phthalocyanine. For each TMPc, we provide a range of U values that show good agreement with the experiments. These values represent a safe starting point for DFT+U calculation of physisorbed TMPcs. By calculating a multiple-site linear response U, we also show that the atoms covalently bonded to the metal atom may influence the U value by as much as 1 eV. This point is especially important when estimating the Hubbard U value for chemisorbed molecules.

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Poster-4

Computational study of strain effect on the electronic properties of Cu-doped CdSe nanoplatelets

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Colloidal Copper-doped nanocrystals(NCs) such as CdSe and PbS NCs is appealing due to their unique luminescence properties which are kwon to broad and tunable photoluminescence(PL) via charge-transfer recombination of conduction band electrons with copper localized holes. [1] However, to the best of our knowledge, Cu-doped Nanoplatelets(NPLs) colloidal system have not been systemically studied yet. Herein, by means of density functional theory (DFT) calculation, we investigate the ground-states and excited-states geometry and electronic properties of Cu^{+}- and Cu^{2+}-doped CdSe NPLs at the atomic level. In particular, we focus on the strain effect on the electronic properties of Cu^{+}- and Cu^{2+}-doped CdSe NPL capped with oleic acid organic ligand because colloidal CdSe NPLs, experimentally, can be stressed by self-scrolled via crystal growth. Our results showed that strain affects excited-state nuclear reorganization, which is responsible for broad PL shape and large PL stokes shift. We also computationally examined singlet and triplet excited-states configuration. These calculations yield fundamental perspectives to understand strain effect on electronic structure and photophysical properties of Cu-doped NPLs.

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Energetics and optical properties of carbon impurities in rutile TiO_2

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Titanium dioxide (TiO_2) is one of the most promising materials for many applications such as solar-cell system and photocatalysis. Non-metal doping of TiO_2 is widely used to improve the photoconversion of the material by shifting the absorption edge from UV to visible-light region [1, 2]. Here, we employ hybrid density-functional calculations to investigate the energetics and electronic structures of carbon (C) impurities in rutile TiO_2. The predominant configurations of C impurities under the O-poor and O-rich growth conditions are identified through the calculated formation energies. Under the O-poor condition, we find the substitutional C occupying oxygen site (C_O), as shown in FIG. 1, is energetically favorable for Fermi-level values near the conduction band minimum (n-type TiO_2) where it acts as double acceptor. On the other hand, when Fermi-level positions decrease toward the valence band, C atoms favor to form the C_i-V_O complex, as shown in FIG. 2, acting as sextuple donor. Under the O-rich condition, the C_i-V_{Ti} complex is found to be energetically favorable in n-type TiO_2, and is exclusively stable in charge neutral. Our calculations based on the configuration coordinated diagram suggest that C_O is an origin of visible light absorbtion in n-type rutile TiO_2 fabricated under oxygen deflicient growth condition.

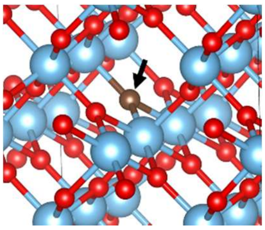

FIG. 1. (Color online) Local atomic configuration of the substitutional C occupying O site (C_O) in rutile TiO_2. The substitutional C is indicated by the arrow. [Ti: blue, O: red, C: dark brown].

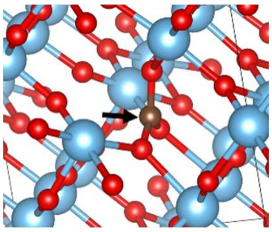

FIG. 2. (Color online) Local atomic configuration of the C_i-V_{Ti} complex. The interstitial C is indicated by the arrow.

[1] Asahi, R.; Morikawa, T.; Ohwaki, T.; Aoki, K.; Taga, Y. *Science* **2001**, *293*, 269.

[2] Khan, S. U. M.; Al-Shahry, M.; Ingler, W. B., Jr. *Science* **2002**, *297*, 2243.

Poster-7

Defect induced exciton states in transition metal dichalcogenide WSe2 monolayer from first principles

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Recent intriguing optical phenomena such as single photon emitters, defect-bound excitons, etc are observed in two dimensional transition metal dichalcogenide WSe2 monolayers. The nature of these exciton states are believed to be from either point defects or strain. However, a clear understanding of the exact origin and the light-matter interaction there is still lacking. The mostly abundant points defects in WSe_2 were believed to be Se vacancies. However, recent investigations from our group have shown that oxygen molecules can dissociate easily at Se vacancy sites at room temperature, largely passivating these vacancies with oxygen atoms and eliminating the in-gap defect bands. Furthermore, the oxygen atom can diffuse into the WSe_2 monolayer, forming an interstitial point defect. The simulated scanning tunnelling microscopy (STM) images for these defects agree well with recent experimental STM images at different bias voltages. The next most favourable point defects are predicted to be Se/W antisites, under typical Se-rich growth conditions. Here, using first principles density functional theory (DFT) method and many body perturbation theory based GW-BSE (Bethe-Salpeter equation) method, we investigate closely the implications of these three types of point defects (O/Se substitution, O interstitials, Se/W antisites) on the optical response of monolayer WSe_2. Based on our findings, we propose that oxygen interstitial defects are the most likely candidates for single photon emitters in WSe_2 monolayer, while O/Se substitution defect does not induce additional exciton states below the pristine WSe_2 A peak. Furthermore, spin-orbit splitting effects are considered to explain the experimentally observed multiple peaks of single photon emitters with energies ranging 40~80 meV below the pristine A peak. For Se/W antisites, a number of exciton states are found below the pristine A peak, with their emission properties determined by the relaxation dynamics. Overall, our first principles results here provide crucial insights and understandings about these defect induced exciton states in monolayer WSe_2, and paves the way for further optoelectronic and nanophotonic manipulation and device integration of these features in future studies.

Phonon-calculation validity of neural-network-potential

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We are planning to study the dynamical instability of the phase change material in the amorphous state by analyzing the characteristics of the vibrational frequencies. It is difficult to calculate with DFT because of large computational costs. Alternatively, Behler's neural network potential (NNP) can compute at much faster speeds with comparable accuracy to DFT calculations. [1] However, my current studies are showing that the force calculation using conventional NNP lacks the accuracy to calculate the vibrational frequencies of the amorphous solid. Therefore, it is essential to develop a new NNP descriptor prior to the following amorphous-solid-research. In this study, we have checked the validity of the existing Behler NNP for calculating various physical properties.

[1] J. Behler, M. Parrinello, Phys. Rev. Lett. **98**, 146401 (2007).

Emergence of Out-plane Ferroelectricity in Atomically Thin $A_{0.5}B_{0.5}X_2$ (A=W, Mo; B=Re, Tc; X=S, Se, Te) Monolayer

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Atomically thin out-plane ferroelectricity is rare phenomena because its depolarization field increases as thickness decreases. Using density functional theory, we found out-plane polarization in transition metal dichalcogenides (TMDCs) with 1:1 composition of VIB and VIIB transition metal. The magnitude of the polarization is ~ 0.08 μC/cm^2, which is comparable to the other reported atomically thin ferroelectric materials like distorted 1*T*-MoS_2 or $AgBiP_2Se_6$ [1]. Interestingly, the polarization is in the opposite direction of the point charge (ionic or Bader charge) approximation, implying unique distribution of electron density in these materials, like counterintuitive Born effective charge reported in other TMDCs [2].

[1] Bo Xu *et al.* Nanoscale **9**, 8427 (2017).
[2] Nicholas A. Pike *et al.* Phys. Rev. B **95**, 201106 (2017).

Excited electron dynamics in the 1T/2H heterophase of monolayer MoS_2: Real-time time dependent density functional theory study for photo-catalyst application

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Monolayer MoS_2, one of the two-dimensional transition metal dichalcogenide (TMD) materials, has two different phases, 2H and 1T phases. The 2H, the stable phase, is a semiconductor with direct band gap about 2.4 eV, and 1T, the meta-stable phase, has metallic phase. The 2H phase of MoS_2 has been studied and utilized as a hydrogen evolution reaction (HER) catalyst because of its photovoltaic and photo-catalytic features. On the other hand, the 1T phase of MoS_2 has been investigated in the perspective of nanoscale electronic device, such as ultrathin transistor and supercapacitor electrode component. Furthermore, the heterophase boundary of 2H and 1T phases was also synthesized and its microscopic dynamics was investigated in terms of phase boundary or phase transition.

In this study, we investigated geometric and electronic structure of the MoS_2 heterophase. We found that two different types of phase boundary lead to difference in the band alignments at MoS_2 phase boundaries. As a consequence, the excited electrons in the 2H phase region are transferred and accumulated in the 1T phase region, leading to the charging of the 1T phase region. We performed the real-time time dependent density functional theory (rt-TDDFT) calculation for this electron dynamics. We found that, as the 1T phase is charged, the activation barrier of dissociative adsorption of oxygen molecule on the planar surface of 1T phase is decreased. In the acidic condition, the oxygen reduction reaction (ORR) energy profile on the charged 1T phase region shows similar electrochemical properties with that on the platinum (100) surface. We suggest that the MoS_2 heterophase can serve as the novel low-dimensional ORR photo-catalyst.

Structural relaxation, electronic structure, and electron-phonon coupling in magic-angle twisted bilayer graphene

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Interplay between the interlayer coupling and the rotational mismatch between two graphene layers results in flattening of Dirac cones at certain special twist angles θ_M, called magic angles. Recently, correlated insulator behavior and superconductivity were experimentally observed near the first magic angle $\theta_M = 1.08°$, demonstrating rich physics induced by the presence of the flat bands. In this regard, more detailed characterizations for the magic-angle twisted bilayer graphene (MA-TBG) are being done. In this poster, we investigate structural relaxations, electronic structure, electron-phonon coupling in MA-TBG at the atomistic level. First, equilibrium atomic positions are determined by minimizing the total energy of the system, consisting of the in-plane strain energy and the interlayer binding energy. Then, we calculate the electronic structure and phonon spectrum using the tight-binding approach and the force constants, respectively. The electron-phonon matrix elements are then obtained from the modulation of hopping parameters due to atomic displacements of phonon modes. We present the electron-phonon coupling strength in MA-TBG with $\theta_M = 1.08°$ as a function of doping level, and discuss implications for superconductivity in this system.

This work was supported by NRF of Korea (Grant No. 2011-0018306) and KISTI supercomputing center (Project No. KSC-2017-C3-0079). Y.W.C. acknowledges support from NRF of Korea (Global Ph.D. Fellowship Program NRF-2017H1A2A1042152).

Poster-12

Poster-13

The structural and electronic properties of $Mo_6S_3I_6$ nanowires by theoretical compositional arrangement

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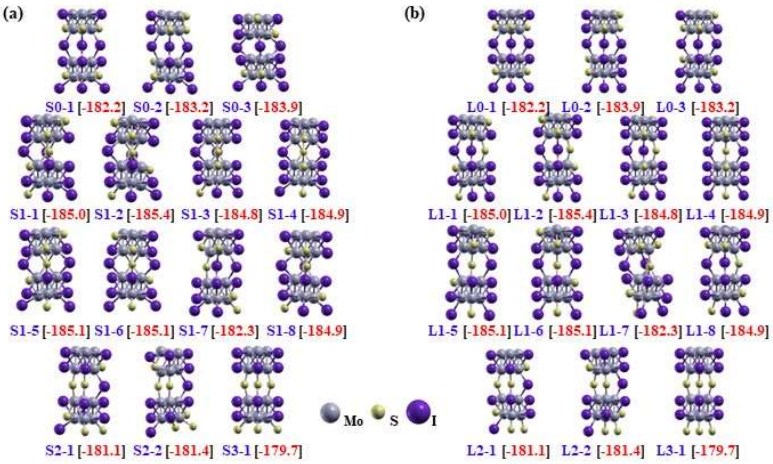
The structural, electronic, magnetic properties of molybdenum-based nanowires have been actively investigated for their potential applications as nanodevices; but further developments are retarded due to the lack of knowledge on the exact electronic and atomic structures of $Mo_6S_3I_6$. For further development of $Mo_6S_3I_6$ nanowire devices, we propose possible atomic structures and the corresponding electronic properties of $Mo_6S_3I_6$ nanowires based on our density functional theory calculations. We scanned various combinations of atomic structures by changing the decorative positions of sulfur and iodine linked to two Mo_6 octahedral. As a result, we found two stable local energy minimum structures characterized by elongation of S_3 linkage; and propose, based on the two stable structures, possible structures of twenty-eight atomic models according to the sulfur saturation in bridging plane. We calculated band structures of the newly proposed atomic models and finally found three atomic models of conductors. According to our compositional ordering structural analysis, we concluded (i) periodic distortion of the bond lengths influences the behavior of the electrons in a system, (ii) role of sulfur atoms in bridging plane is important for intramolecular charge transport by the delocalized charge differences, and (iii) electronic band gap energy is proportional to the integrated Mo-S bonding orbital energy.



Poster-14

First-principles Calculations of Stacking Stability of C_2N Bilayer Nanosheet

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In recent years, a 2D graphene-like sheet: monolayer C_2N was synthesized via a simple wetchemical reaction [1]. Here, we study the stability and electronic properties of bilayer C_2N. According to previous a study, a bilayer may exist in one of three highly symmetric stacking configurations, namely as AA, AB and AB'-stacking [2]. For the AA-stacking, the top layer is directly stacked on the bottom layer. Furthermore, AB- and AB'-stacking can be obtained by shifting the top layer of AA-stacking by **a**/3-**b**/3 along zigzag direction and by **a**/2 along armchair direction, respectively, where **a** and **b** are translation vectors of the unit cell. By using first-principles calculations, we calculated the stability of AA, AB and AB'-stacking C_2N and their electronic band structure. In previous result, the most favourable structure is AB-stacking. In present work, we furthermore examined the energy landscape and translation sliding barriers between stacking layers. From energy profiles, we interestingly found that the most stable positions are shifted from the high symmetry AB-stacking. In electronic band structure details, band characteristic can be modified according to the shift.

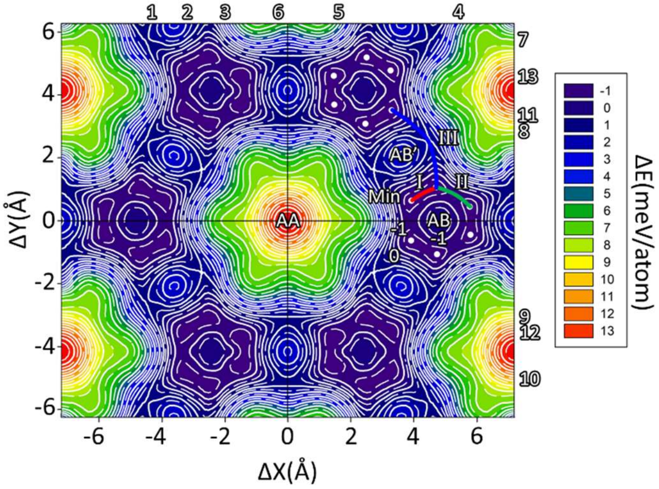

Fig 1. 2D-energy profile surface of bilayer C_2N depending on the inter-layer relative slide distance (ΔX, ΔY).

[1] J. Mahmood, E. K. Lee, M. Jung, D. Shin, I.-Y. Jeon, S.-M. Jung, H.-J. Choi, J.-M. Seo, S.-Y. Bae and S.-D. Sohn, Nature communications **6**, 6486 (2015).

[2] R. Zhang, B. Li and J. Yang, Nanoscale **7** (33), 14062-14070 (2015).

Standard model of the Rare-Earths analyzed from the Hubbard I approximation

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In this poster we examine critically the electronic structure of the rare-earth elements by use of the so-called Hubbard I approximation [1]. From the theoretical side all measured features of both occupied and unoccupied states are reproduced, without significant deviations between observations and theory. We also examine cohesive properties like the equilibrium volume and bulk modulus, where we find, in general, a good agreement between theory and measurements. In addition, we have reproduced the spin and orbital moments of these elements as they are reflected from measurements of the saturation moment. We have also employed the Hubbard I approximation to extract the interatomic exchange parameters of an effective spin Hamiltonian for the heavy rare earths. We show that the Hubbard I approximation gives results which are consistent with calculations where 4f electrons are treated as core states for Gd. The latter approach was also used to address the series of the heavy/late rare earths. Via Monte Carlo simulations we obtained ordering temperatures which reproduce measurements within about 20%. We have further illustrated the accuracy of these exchange parameters by comparing measured and calculated magnetic configurations for the heavy rare earths and the magnon dispersion for Gd.

[1] I. Locht *et al.* Phys. Rev. B **94**, 085137 (2016).

DFT+DMFT study of phase transitions with a large volume collapse in MnSe under pressure

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Manganese selenide is known to undergo the phase transition from cubic NaCl-type to orthorhombic MnP-type B31 (*Pnma*) with the large volume collapse of about 22% in the region of 20-30 GPa with an unknown tetrahedral phase in between and a metallization at 25 GPa [1]. We present a DFT+DMFT study of spectral, magnetic, and structural properties of the manganese selenide under pressure [2]. Our calculations reveal that a high-spin to low-spin transition occurs upon compression at volumes below 33 Å^3. The spin-state transition is accompanied by a metal-insulator transition and a structural phase transition with the large volume collapse of ~20% from the cubic B1 structure to the high-pressure MnP-type B31 structure at about 27 Å^3. We find that the spin-state transition is the main driving force for the structural transition in MnSe under pressure.

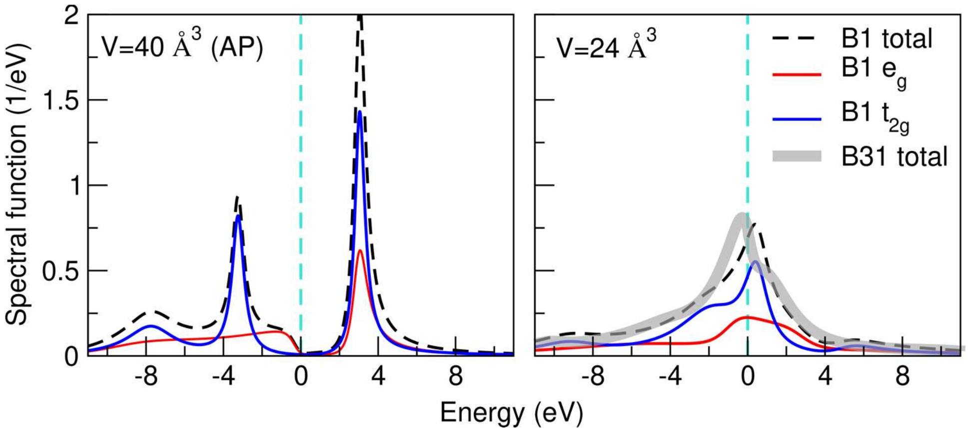

Figure 1: Calculated within the DFT+DMFT method Mn-3d spectral functions at 1000 K of the manganese selenide MnSe at ambient pressure (left) and after the volume collapse under pressure (right).

[1] Y. Wang *et al.* Angew. Chem. Int. Ed. **55**, 10350 (2016).
[2] A. A. Dyachenko *et al.* Phys. Rev. B **98**, 085139 (2018).

First-Principles Study on Electron Transport Properties of Halogenated Graphene

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Recently, an electronic device constructed from a graphene has been investigated extensively and has been expected to be a candidate for replacing silicon-based devices owing to several unique properties of the graphene (rapid electron transfer, good thermal conductivity, and splendid flexibility). A lot of experimental and theoretical studies on physical functionalizations and chemical modifications of graphene for tuning these properties have been performed. A chemical adsorption of atoms and molecules on the graphene surface is one of important modifications. In particular, a halogen adatom X (X=F, Cl, Br, and I) can change the atomic and electronic structures of the grapehen drastically, where the formation of C-X covalent bonds is accompanied by sp^2 to sp^3 structural transition of C-C bonds (Fig. 1).

In this work, the electron transport properties of the halogenated graphene are investigated. Here, we performed the molecular dynamics calculations to determine a fully-relaxed atomic geometry of halogenated graphene using the RSPACE code[1], which is based on the real-space finite difference approach within a framework of the density functional theory. Moreover, we curried out the electron transport simulations[2] to estimate the dependence of the electric conductivity and the spatial path of current flow on the coordinates and species of adsorbed halogen atoms. The details of this work are presented at the workshop.

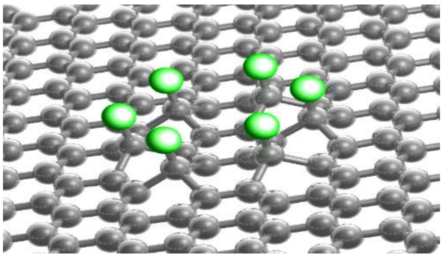

Fig. 1: Schematic view of a halogenated graphene. There are six halogen atoms (green spheres) and each atom form a covalent bond with a carbon atom (grey spheres).

[1] K. Hirose, T. Ono and Y. Fujimoto, and S. Tsukamoto, *First-Principles Calculations in Real-Space Formalism*, (Imperial College Press, London, 2005).

[2] Y. Egami, K. Hirose, T. Ono, Phys. Rev. E **82**, 056706 (2010); Y. Egami, S. Iwase, S. Tsukamoto, T. Ono, K. Hirose, Phys. Rev. E **92**, 033301 (2015).

Predicting topological insulators in hydrogenated transition metal dichalcogenide monolayers: A first-principles study

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Two dimensional (2D) transition metal dichalcogenides (TMD) monolayers have currently been of immense interest in materials research because of their versatility and tunable electronic properties. In this study, we perform systematically the first-principles calculations of possible topological insulator phases on 1T and 2H MX_2 monolayers, as well as the effects of hydrogenation on one or both sides of the films. With regards to structural stability, we find that Group IV(Ti, Zr, Hf)-, VI(Cr, Mo, W)-, and X(Ni, Pd, Pt)-based TMDs, respectively, adopted 1T, 2H, and 1T as their stable structures for unhydrogenated cases. However, upon hydrogenation, we observe structural phase transition from 1T to 2H for Group IV, and from 2H to 1T for Group VI, and no transition was observed for Group X. We find that for 2H $TiTe_2$ and 1T $CrTe_2$ with 1 hydrogen, as well as 2H $PdSe_2$ without hydrogenation, are identified to be topological insulators with large band gaps of 0.07eV, 0.21eV and 0.23eV, respectively. These findings show that these TMDs in quantum spin Hall phase have a great potential for spintronics applications.

Structure exploration for AB_2 type monolayers by high-throughput DFT calculations

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Two-dimensional (2D) monolayers have attracted incredible interest because of their peculiarities and novel properties. For example, graphene and silicene are well known as atomically thin monolayers. Boron nitride and silicon carbide are known as AB type monolayers. In addition, various kinds of monolayers of transion metal (A=Mo, W, etc.) dichalcogenides (B=S, Se or Te) with a formula AB_2, which are arranged in triatomic layers, have been recently synthesized experimentally for producing a AB_2 type 2D transition metal chalcogenide library [1]. These kinds of investigations have revealed interesting phenomena such as two-demensional superconductivity and quantum spin Hall effect. However, it can be considered that several kinds of 2D structures which can exist stably may have not been synthesized experimentally yet since the combination of the elements is diverse even only for the AB_2 composition. Therefore, there is a room for exploring unknown monolayers.

In this study, we performed high-throughput calculations based on the density functional theory by using OpenMX[2] to create a structure map for AB_2 type monolayers. At first, we categorized the AB_2 structures into planar, 1T (trigonal) phase (ex. ZrS_2 [1]), 2H (hexagonal) phase (ex. MoS_2 [1]), memory structure and the others. Here, the group of "planar" means B atoms form almost honeycomb structures and A atoms are on the center of the honeycombs. The group of "memory structure" means that the structure is similar to the planar, but A atoms are shifted from the plane formed by B atoms. Since the positions (up or down) of A atoms can represent binary digits, we **call** the backled structures "memory structure" here. This structure can be a candidate for a data strage application with an extremely high areal density. Next, we prepared 2×2 supercell AB_2 initial structures (1T, 2H and planar) for selected compounds (62 elements × 62 elements=3844 compounds), where compounds of noble gases, lanthanides and actinides are excluded. After geometry relaxations and variable cell optimizations were carried out, the most stable converged structures were summarized on the structure map for AB_2 type monolayers.

From the structure map, we predicted that some of the structures can be the memory structure. Some NEB calculations for these memory structures indicate that it may be possible to control them as binary digits strage applications. In this presentation, we report the details of the high-throughput calculations and show some obtained interesting structures.

[1] J. Zhou *et al.* Nature **556**, 355 (2018).

[2] OpenMX, http://www.openmx-square.org/.

Poster-20

Intermediate-phase Method for Computing the Natural Band Offset between Two Materials with Dissimilar Structures

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[2]*Collaborative Innovation Center of Advanced Microstructures, Nanjing, 210093, China*

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The band offset between different semiconductors is an important physical quantity determining carrier transport properties near the interface in heterostructure devices. Computation of the natural band offset is a longstanding challenge. We propose an intermediate-phase method to predict the natural band offset between two structures with different symmetry, for which the superlattice model cannot be directly constructed. With this method, and the intermediate phases obtained by our searching algorithm, we successfully calculate the natural band offsets for two representative systems, (i) zinc-blende CdTe and wurtzite CdS and (ii) diamond and graphite. The calculation shows that the valence band maximum (VBM) of zinc-blende CdTe lies 0.71 eV above that of wurtzite CdS, close to the result 0.76 eV obtained by the three-step method. For the natural band offset between diamond and graphite which could not be computed reliably with any superlattice methods, our calculation shows that the Fermi level of graphite lies 1.51 eV above the VBM of diamond using a newly identified intermediate phase. This method, under the assumption that the transitivity rule is valid, can be used to calculate the band offsets between any semiconductors with different symmetry on condition that the intermediate phase is reasonably designed.[1]

[1] H. J. Gu, Y. Y. Zhang, S. Y. Chen, H. J. Xiang, and X. G. Gong, Phys. Rev. B **97**, 235308 (2018)

Theoretical study on positronium formation at metal surfaces based on two-component density functonal theory

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When positrons are slowly incident onto the material surfaces, a portion of the positrons diffuse back to the surface. Then, positronium (Ps), which is a bound state between an electron and a positron, is formed and spontaneously emitted into the vacuum, when its work function is negative [1]. Since normally Ps is not formed in the bulk due to the strong electron screening effect to positrons, the Ps formation spectroscopy has been expected to be a sensitive probe for the surface electronic structures. In this respect, Ps formation processes at various surfaces have been studied both theoretically [2] and experimentally [3].

Recently, an experiment using spin-dependent Ps formation and annihilation, has been carried out to investigate the surface spin-polarization of ferromagnetic surfaces covered with graphene and boron-nitride white graphene (BNWG) [4]. This study demonstrated that the Ps is formed at the first surface layer (i.e., graphene or BNWG), and the surface spin-polarization is caused by orbital hybridization between the ferromagnets and graphene or BNWG. This finding implies the potential of Ps formation spectroscopy in determining the surface electronic structure at the first atomic layer.

However, the details of the Ps formation at surface have not yet been fully understood because of the lack of theoretical study on the Ps formation using *real material surfaces.* Previous theoretical studies on the Ps formation were carried out within a jellium model or by assuming bulk electronic band structures [2]. In order to understand the Ps formation mechanism precisely, we are conducting the calculation of two-component density functional theory (TCDFT) for the Ps formation energy spectrum (PsFES) at metal surfaces. TCDFT is the one of the most flexible and powerful tool to study electronic and positronic states in real materials [5].

We found that the calculated PsFES qualitatively reproduce the experimental data. We also examined the projections of PsFES to the surface electronic band structures. Consequently, we found that the PsFES significantly depends on surface electronic states. In the presentation, we will report further details of the Ps formation processes.

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A hybrid approach combining artificial neural network potentials with first-principles calculations

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Constructing accurate potential-energy surfaces (PES) as a function of atomic position is an important subject in both condensed matter physics and materials science to perform reliable atomic simulations. Recently, artificial neural networks (ANN) have been suggested to be a promising technique for constructing the PES of complicated systems. Reliable ANN potentials have several advantages in terms of efficiency and accuracy compared with other interatomic potentials and can replace first-principles calculations for crystal structure serach in which a vast number of configurations should be optimized to find the global mininum. However, for successful application of ANN potentials to crystal structure serach, improving its accuaracy and choosing proper training sets remain a challenging issue to overcome.

In this work, we propose a hybrid approach combining ANN atomic potentials with first-principles calculations, which improves the efficiency of crystal structure search. We generate high-dimensional ANN potentials for Si using the Behler-Parrinello approach. The weight parameters for the ANN potentials are optimized by using the machine learning technique. For applications to crystal structure search, these ANN potentials are combined with the conformational space annealing algorithm for global optimization. In each generation, we employ the so-called self-learning training in which configurations generated by the conformational space annealing algorithm are used as training sets. Although the self-learning ANN potentials cover a varierty of structures, the accuracy of these potentials is still not sufficient to perform the local energy minimization. To remove the residual forces and stresses, first-principles calcualtions are additionally performed for low-energy configurations prior to sorting configurations for the next generation. Our results show that ANN potentials can be used as an efficient local minizer with the help of first-principles calculations, greatly improving the crystal structure search for the stable as well as diverse metastable phases with reduced computational costs.

Phase Diagram of Ga(As,Sb) and (In,Ga)As by Cluster Expansion and DFT Calculations

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A solid solution is a chemical mixture of several components and forms a single phase in a certain range of composition. For a given composition of a solid solution, tremendous number of atomic cofigurations are possible and properties of a solid solution depend on the configuration [1][2]. Therefore, it is practically impossible to calculate the all possible configurations by DFT calculations. On the other hand, materials properties come from the interaction between atoms, and the properties of materials can be interpreted as the sum of the contribution of interactions of some atomic groups, which are called clusters. Cluster expansion method predicts the properties of any atomic configuration by calculating the contribution of each interaction on properties [3]. Predicted properties of each configuration are combined into properties of materials by the grand canonical ensemble.

In this study, the phase diagrams of Ga(As,Sb) and (In,Ga)As are calculated by the combined methods using ab-initio calculation, cluster expansion, canonical ensemble and grand canonical ensemble. Although Ga(As,Sb) and (In,Ga)As systems have been studied as one of the promising next-generation semiconductor channel materials, experimental studies on the phase diagram of (In,Ga)As have been rare [4] and the those on Ga(As,Sb) show ambiguous results [5][6]. we provide the phase diagrams of Ga(As,Sb) and (In,Ga)As phase and compare them with the previous experimental and theoretical results.

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Water droplet affects charge distribution of carbon nanotube

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Water can be found on varius material surfaces in nanometer scale layer in ambient air. This water layer often affect material surface propertes such as friction and adhension force, chemical reactivity or electrical conductivity onsurface.

With it's large surface area, carbon nanotube (CNT) is good material to resurch surface. CNT films are highly responsive, so they expected as promising materials for high sensitivity gas sensors. When CNT film gas sensors are used for NO_2 or formaldehyde, the response to water vapor is obstacle. Therefore, understanding the mechanism and magnitude of influence of water vapor on CNT films is needed to develop high accuracy CNT sensors. Although it is believed that the conductance change is primally caused by the charge transfer from water to CNTs, there is no carrier doping with simple physisorption of H_2O molecule in first-principles calculations [1]. The key is electrostatic interaction between water and CNT which was recently reported [2].

We consider that water molecules adsorbed on CNT do not donate holes or electrons, but they induce charge fluctuation in a CNT due to the electrostatic interaction between them. In this work, we investigated the charge fluctuation in a CNT with water droplet (Fig.1) using the first-principles simulation combined with the molecular dynamics simulation. We found the hole concentration in carbon atoms close to water droplet and the electron concentration in carbon atoms on the side of the droplet. This indicates a water droplet induces charge and opposite carriers electrostatically shield around the droplet. We also investigated the electronic transport in a water droplet absorbed CNT. We show that the water droplet significantly reduces the electronic conductance of a CNT and influences on the performance of CNT gas sensors.

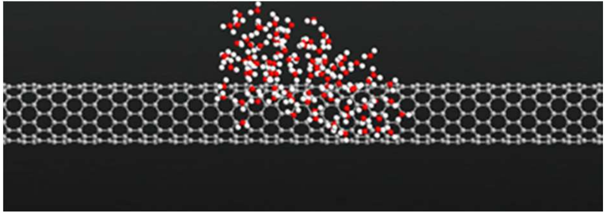

Fig. 1. Snap shot of a water-droplet-absorbed CNT in molecular dynamics simulation

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Poster-26

Swarm-Intelligence Guided Computational Design of Novel Silicon Allotropes

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Silicon (Si) in diamond structure is the most important material in current electronic and optoelectronic technology. There has been considerable interest to find other Si allotropes in different structures that have new properties for alternative applications. The discovered allotropes include graphene-like hexagonal puckered silicene, and limited metastable phases at high pressures. Besides the elementary phase, one can explore the idea of “Zintl-phase” compound and seek for Si allotropes in the compounds formed by silicon and active metals (alkali or alkali earth ones). The large electronegativity difference between Si and metals in Zintl-phase compounds leads to a nearly complete electron transfer and to the formation of strong covalent bonds stabilizing the ‘polyanionic motifs of Si’. Along this direction, the novel Si phases (for instance Si_{24})[1] has been discovered by involving alkali metals, and silicene has been synthesized by using the Zintl phase $CaSi_2$.[2,3] In this work, we reported via swarm-intelligence guided global structures search two never-before-reported novel silicon allotropes in the Zintl-phase Ba-Si systems.

They are Ba_2Si_3 and Ba_4Si_5. The silicon structure in Ba_2Si_3 is composed of the exotic hexagonal Si rings (resemblying the ‘planar’ Cyclopentasilane) that connect along one direction to form one-dimensional chain-like structure. Ba_4Si_5 shows also a one-dimensional silicon sublattice where three Si atoms assemble in triangle clusters accompanying with a two-Si tail. The stability of the two Si allotropes was evidenced by the energetic convex hull and phonon stability calculations. Their electronic structure, properties, and potential applications were discussed.[4]

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A first-principles study on the magnetism of Fe/Bi/MgO multilayers

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The magnetic tunnel junction (MTJ) has a structure consisting of two ferromagnetic layers separated by a thin insulating layer. MTJ is used for the magnetoresistive random access memory (MRAM) cell with giant magneto resistance ratio. MRAM is a nonvolatile memory without requiring standby power to keep information and has attracted much attention as a new generation of low power consumption memory. Strong perpendicular magnetic anisotropy to realize high density memory devices is highy desired for preventing thermal magnetic fluctuation in the ferromagnetic layer of MTJ. Perpendicular magnetic anisotropy originates from magnetocrystalline anisotropy (MCA) caused by spin-orbit coupling. In this study, we investigate the influence of a Bi layer insertion at Fe/MgO interface by first-principles density-functional calculations. We first propose models of Fe/Bi/MgO by considering lattice matching for the calculations and then study the magnetism of Fe/Bi/MgO as well as Fe monolayer and Fe/MgO films. It is found that enhancement in perpendicular magnetic anisotropy can be obtained by inserting the Bi layer at the Fe/MgO interface. The electronic origin of MCA in the systems is discussed from the viewpoint of Bruno's formula [1] and band structure within the second-order purturbation theory [2].

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Poster-28

Tunable Thermoelectric Effects of Bilayer Graphene by Vertical Electric Field

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Thermoelectric (TE) generation is a potential key technology for recovering energy from waste heat. Among the various potential candidates for TE materials, nanocarbon materials have attracted attention as flexible and high-performance TE materials. Most recently, Yamamoto and Fukuyama reported that the semiconducting carbon nanotubes (CNTs) exhibit high TE performance when the chemical potential μ locates near a band edge with sharp density of states (DOS) originating from its one dimensionality [1,2]. On the other hand, the graphene, which is a two-dimensional honeycomb lattice consisting of carbon atoms, cannot be expected to be high-TE performance because it has no band gap at the charge neutral point.

In this study, we focus on the bilayer graphene (BLG) since the bandgap can be opened by applying the electric field perpendicular to the BLG, as shown in Fig. 1 [3]. We have calculated the Seebeck coefficient S and the power factor PF of the BLG in the presence of vertical electric field $\boldsymbol{E}_\perp$ using the Kubo's linear response theory combined with thermal Green's function method which was recently developed [1,2]. We adopt the constant-τ approximation for self-energy due to carrier scattering [2].

We found that the values of S and PF can be controlled by changing the magnitude of $\boldsymbol{E}_\perp$. For example, we obtained $S \sim 200$ μV/K and $PF \sim 40$ mW/mK^2 when μ lies close to a band edge and the vertical electric field is $E_\perp = 4.8$ MV/cm. This is because the DOS of BLG under $\boldsymbol{E}_\perp$ has a sharp peak near the band edge, which is similar to carbon nanotubes. On the other hand, in the high-energy regimes where μ is much larger than the band gap, S is inversely proportional to the chemical potential, *i.e.*, $S \propto \mu^{-1}$. The μ^{-1} behavior of BLG is similar to the case of CNTs. In contrast to S, the thermoelectric conductivity L_{12}, which is defined as the electric current density in response to the temperature gradient, shows the different μ dependence between the *two-dimensional* BLG and *one-dimensional* CNTs.

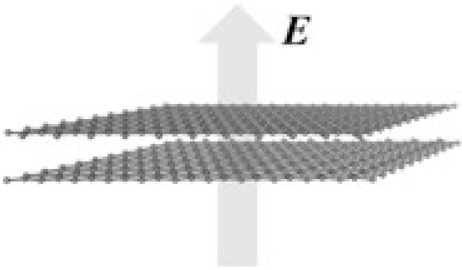

Fig. 1: Bilayer graphene under vertical electric field

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Poster-28

Noncollinear Spin Torque Effect in Magnetic Heterojunctions: Combined First-Principles Calculation and TB-NEGF Method

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Our theoretical researches focus on searching for novel nm-scale ferromagnetic/barrier/ferromagnetic (FM/B/FM) magnetic tunnel junctions (MTJs) with superior spin transport properties by choosing oxides [1] and organic molecules [2] as the central barriers. The relative orientation of two FM electrodes can be controlled by a spin-polarized current via the noncollinear spin torque effect. Recently, we have successfully employed the single-band tight-binding (SBTB) model to predict the noncollinear spin torque effect in FM/I/FM and FM/I/SF/I/FM [1] magnetic tunnel junctions, where I and SF represent insulting and spin-filter barriers, respectively. However, for real complex heterojunctions, the injected spin-polarized electrons from FM electrode can be strongly influenced by the complicated interfacial spin-polarized charge transfer, which is ignored in our previous SBTB model.

In this study, our newly developed "JunPy" [3] package successfully combined the self-consistent Hamiltonian by using the first-principles calculation, including multi-band dispersion relation and complicated interfacial coupling, with our newly derived TB model and non-equilibrium Green's function (NEGF) method to investigate the noncollinear magnetotransport properties in nm-scale magnetic heterojunctions. This program is first testified for the spin-polarized currents and the noncollinear spin torque effect in conventional Fe/MgO/Fe MTJ. We further employed it to predict the giant field-like spin torque (FLST) effect in the amine-ended single-molecule magnetic junction [5], which may open a new avenue for multifunctional manipulation in next-generation organic FLST-MRAMs with lower power consumption. We believe that this newly developed calculation process not only can efficiently resolve current self-consistent difficulties in first-principles calculation for non-collinear case, but also may inspire future experimental explorations in novel magnetic heterojunctions for future spintronics applications. This work is supported by the Ministry of Science and Technology (MOST 106-2112-M-008-011- and 106-2633-M-008-002-) and the National Center for Theoretical Sciences, Republic of China.

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Polarization dependent optical response and layer-controlled band gap of group IV monochalcogenides

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Sharing with the same bulk-like flake crystal structure of black phosphorus and phosphorene, group IV monochalcogenides exhibits unique many-electron effects in its electronic and optical properties. Few-layer group IV monochalcogenides absorbs light polarized along the structures' armchair direction and is transparent to light polarized along the zigzag direction, making them potentially viable linear polarized for applications [1]. In this work, we employ first-principles excitation calculations based on the combined GW+BSE approach to explore the electronic structure and optical response with respect to different polarizations of few-layer layered group IV monochalcogenides. In addition to the strong polarization dependence of the optical absorption spectra, the band gap, excitation binding energies, and optical absorption spectrum of group IV monochalcogenides can also be broadly tuned by changing the number of stacked layers. This scenario serves as a convenient and efficient method for engineering the layered material's excited-state properties.

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Electronic transport simulation in nitrogen-doped carbon nanotubes focusing on disappearance of Anderson localization due to phonon scattering

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Impurity-doped semiconducting carbon nanotubes (CNTs) are expected to be used as materials of next-generation field effect transistors or thermoelectric devices owing to their remarkable electrical properties. As electrical resistance of a doped CNT are characterized mainly by impurity and phonon scatterings, previous theoretical studies individually investigated their effects. When impurity concentration is high and the impurity scattering dominates at low temperature, conduction electrons localize in CNT and the resistance increases exponentially with tube length (non-ohmic transport). On the other hand, it is expected that, as temperature increases, the phonon scattering suppresses such a localization phenomenon and the transport property becomes ohmic transport. In order to know whether the localization occurs or not and estimate accurate the resistance at a certain temperature and impurity concentration, both scatterings must be simultaneously taken into account in electronic transport simulation.

In the present study, we investigated electronic transport properties in a nitrogen-doped (10,0)-CNT at finite temperatures using the Open-TDSE with MD simulation method developed in a previous study [1], which can simultaneously treat both effects of localization phenomena due to impurity scattering and quantum decoherence due to phonon scattering. We confirmed that electrical resistance of a long CNT increases exponentially with the tube length at 0 K (strong localization) while the resistance increases linearly at 300 K. This means that phonon scattering reduces phase coherence of electrons. This work is the first theoretical report to investigate electronic transport in a nitrogen-doped CNT focusing on disappearance of localization phenomena due to phonon scattering.

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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-33

Type-I and Type-II nodal lines in a magnetic hexagonal InC sheet

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Based on first-principles calculations, we design a novel two-dimensional magnetic material exhibiting symmetry-protected nodal lines in momentum space. We first show that indium carbide crystallizes in a single layered form of a hexagonal honeycomb lattice. Then, we show that hexagonal InC energetically favors ferromagnetic ordering of spins. An interesting feature unique to this magnetic two-dimensional material is the Fermi surface geometry. We find that both type-I and type-II nodal lines occur near the Fermi level in momentum space. While an alternating chain of electron and hole pockets appears in the Fermi sufrace for both type-I and type-II cases, it is shown that the Fermi surfaces exhibit characterisitc geometries distinctive between the type-I and type-II due to different signs of their band velocities. Our findings suggest that *h*-InC may provide a new venue for 2D magnetism and the Fermi surface topology.

DFT+DMFT study of Pressure dependent Insulator-to-Metal transition in molecular $J_{\mathrm{eff}} = 3/2$ Mott insulator, $GaTa_4Se_8$

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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 spin-orbit coupling (SOC) induce the $J_{\mathrm{eff}} = 3/2$ 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 $J_{\mathrm{eff}} = 3/2$ electronic structure [5]. 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. Using the realistic Hubbard U parameter from constrained RPA [7], we found that the formation of the $J_{\mathrm{eff}} = 3/2$ states with reasonable SOC is essential to reproduce IMT under the high pressure.

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Topological Phase Transition in $NaZnBi_xSb_{1-x}$

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Using first-principles calculations, we study the topological phase transition in $NaZnBi_xSb_{1-x}$ that happens as the doping concentration x is varied. We show that NaZnBi realizes Z_2 topological insulator phase in a tetragonal ABC-type lattice, while isostructural NaZnSb is a normal insulator. By employing virtual crystal approximation, we also show that a topological phase transition occurs by substituting Bi with Sb via the appearance of Dirac semimetal phase at $x = 0.45$, which defines a topological critical point. We elucidate the electronic structure responsible for the topological phase transition. The evolution of topological surface states is studied as a function of the doping concentration. Our results suggest that $NaZnBi_xSb_{1-x}$ should provide a new venue for the study of topological phenomena.

Poster-36

Weyl and Triple Nodal Points in half-metallic ferrimagnets

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For last decade years, many topological phases have been proposed and experimentally observed. Among them, recently, topological matters with various dimensional nodal points have been gained a lot of interest. For example, Dirac and Weyl nodes are zero-dimensional, nodal lines are one-dimensional, and nodal links are three-dimensional. In particular, a novel 0D triple nodal point is of interest, since it has no high energy counterpart.

In this presentation, we will address topological properties in the Cr-based inverse Heusler compounds, showing magnetic Weyl points, triple nodal points, and nodal links in the absence of spin-orbit coupling. Our surface state calculations, based on the Green function approach, show several Fermi arcs connecting each Weyl point and each triple nodal point. Furthermore, the triple nodal points are connected with the nodal links, leading to the so called nexus fermionic state near the Fermi level. Using first principles calculations, we will analyze the origin of these topological characters. Our results are expected to provide a platform of a novel topological phase.

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Dominant in-plane cleavage direction of CrPS4 monolayer

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In-plane cleavage directions of 2D crystals are displayed and often well-defined in their flakes exfoliated by the widely-used scotch-tape method. Here, we investigate the correlation between dominant in-plane cleavage direction and elastic properties in different directions. CrPS4 flakes show a preferential in-plane cleavage direction of 67.5˚, corresponding to <110> direction. To explain it, we calculated directional dependence of Young's modulus and fracture energy using first-principles density functional theory calculations. We found that fracture energy is directly relevant to the in-plane cleavage direction of CrPS4. Our study can provide a facile approach to figure out the direction of 2D crystals without complex characterization process, which is valuable for material processing of 2D materials.

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Poster-39

A Simple Method to Calculate the Exfoliation Energies of Layered Materials

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The exfoliation energy, the energy required to peel off an atomic layer from the surface of a bulk material, is of fundamental importance in the science and engineering of layered materials. Traditionally, the exfoliation energy has been obtained from first-principles by calculating the difference in the energy between (i) a slab of N layers ($N \gg 1$) and (ii) a slab of $N - 1$ layers plus a layer separated from the slab. Here, we prove that the exfoliation energy can be obtained *exactly* as the difference between the energy of a bulk material (per atomic layer) and that of an isolated single layer [1]. The proposed method is (i) tremendously lower in computational cost than the traditional approach because it does not require calculations on thick slabs, and (ii) still valid even if there is a surface reconstruction of any kind. Moreover, the method is (iii) capable of taking into account the relaxation of the exfoliated single layer, and (iv) easily combined with many-body computational methods. As a proof of principles, we calculate the exfoliation energies of graphene, hexagonal boron nitride, MoS_2, and phosphorene using density-functional theory.

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First-Principles Study of Alkali Metal Intercalated MoS_2

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MoS_2 is a compound in transition metal dichalcogenide (TMDC) family that is semiconductor with layered honeycomb structure having strong in-plane bonding and weak out-of-plane van der Waals interactions. In the bulk form, MoS_2 has an indirect band gap, whereas monolayer form has direct band gap which is more suitable for device applications. It has been proposed that the electronic characteristic of the monolayer can be reproduced experimentally in MoS_2 by K intercalation [1]. In this work, the effects of different alkali metal (such as Li, Na, K, and Rb) intercalation are investigated by using first-principles calculations within the 2×2×1 supercell. In order to provide guidance for measurement, the electronic structures from supercell calculations are unfolded onto the high symmetry paths [2] as defined in the first Brillouin zone of the primitive cell. The results show significant expansion of interlayer spacing and contribution of electron donation from alkali metal to the conduction band of MoS_2. The expansion obviously depends on atomic radii of the intercalated metals. Moreover, the conduction band minimum is changed to the same location of the valence band maximum in *k*-space because the expansion of the interlayer spacing reduces the electronic interactions between adjacent layers creating a quasi-monolayer character. It has been found that the interlayer spacing of $MoS_2K_{0.25}$ and $MoS_2Rb_{0.25}$ are large enough to exhibit quasi-monolayer character. Furthermore, the effects of concentration of alkali metal have been investigated by varying concentration of K within the given supercell. We found that in-plane lattice constant increases proportional to the concentration. Our results suggest that different atomic radii and concentration of intercalated alkali metals could provide an opportunity to tune electronic structures of TMDC materials.

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Quantum Anomalous Hall Effect with Higher Chern Numbers in Electron-Doped $CrSiTe_3$: A First-Principles Prediction

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The nontrivial topology of electronic band structure can give rise to many novel phenomena like the quantum spin Hall effect (QSHE) or the quantum anomalous Hall effect (QAHE). A Chern insulator is such a topological state of matter exhibiting a nonzero quantized Hall conductivity without an external magnetic field. There have been several experimental efforts to realize QAHE by doping magnetic impurities into topological-insulator thin films. Here we report that the Chern insulator can be realized in a single layer of electron-doped $CrSiTe_3$. We have performed first-principles density-functional-theory calculations to find the minimum energy configuration for both atomic and magnetic structures and determined that the ground state of pristine $CrSiTe_3$ is a ferromagnetic insulator. We use the Wannier function to calculate the Berry curvatures and prove the nontrivial Chern numbers for the conduction bands consisting of mostly Cr e_g orbitals hybridized with neighboring Te p orbitals in the honeycomb-lattice network of $CrTe_6$ octahedrons. Further, we demonstrate that the electron-doping can raise the Fermi level to the middle of the eg manifold, which opens up a band-gap of about 20 meV. Consequently, the electron-doped $CrSiTe_3$ becomes a QAHE insulator with higher Chern numbers. The origin of higher Chern numbers is attributed to the presence of multiple Dirac cones in the e_g-manifold band structures without spin-orbit coupling, together with the broken time-reversal symmetry of the ferromagnetic $CrSiTe_3$. We confirm that the nontrivial topology of the electron-doped $CrSiTe_3$ remains robust in its bulk structure by showing the chiral edge states by carrying out the edge state calculation. Our result suggests that there is a new family of Chern insulator materials in the form of MAX_2- or MX_3-type two-dimensional materials.

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Path Integral Molecular Dynamics Simulations for Muoniated Thioformaldehyde Radicals

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A considerable amount of knowledge for muonium (Mu; complex of a positive muon (μ^+) atom and an electron) chemistry has been accumulated for over 30 years [1]. A muon has a smaller mass and larger magnetic moment than those of proton. Because of these unique features, Mu atom is used as the muon spin resonance/rotation/relaxation (μSR), where hyperfine coupling constant (HFCC) is a good index for the magnetic interaction between electron and muon spins. In this study, we investigated the structures and "reduced" HFCC values for muoniated and hydrogenated thioformaldehyde radicals, a Mu or H atom is added to carbon atom (C-adduct) or sulfur atom (S-adduct) of the thioformaldehyde compound ($H_2C=S$) using the *on-the-fly ab initio* path integral molecular dynamics (PIMD) method [2, 3], which can include both nuclear quantum and thermal effects. The single point energy of C adduct structure with CCSD/aug-cc-pVDZ (optimized with MP2/6-311++G(d,p)) level is 13.48 lower than that of S-adduct structure, corresponding the previous study [4]. The HFCC values from a simple geometry optimization calculation of C adduct and S adduct are 22.42 and -7.39 MHz, respectively, at the BHandHLYP/6-31+G(d,p) level. In case of C-adduct, the reduce HFCC values of the muoniated thioformaldehyde radical by our PIMD simulation is slightly larger than that of hydrogenated radical with the same calculation level. We found that the local molecular structures affect the HFCC values, particularly, the Mu—C bondlength in the muoniated thioformaldehyde radical is lengthen due to the large nuclear quantum effect of moun.

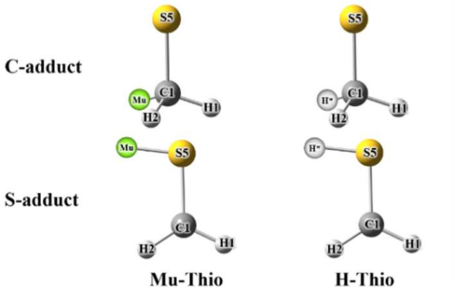

Figure 1. The optimized structure of muoniated and hydrogenated thioformaldehyde radicals (Mu-Thio and H-Thio).

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Benchmark of density functional theory for superconductors in elemental materials

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The first-principle calculation of the superconducting properties such as the transition temperature and the gap function is of great interest to explore new materials as well as to understand the mechanism of known superconductor. Density functional theory for superconductors (SCDFT) [1] is one of the framework for such calculations; this method enables us to perform fully non-empirical simulation in the superconducting phase within reasonable computational cost. In this method, we can treat the electron-phonon interaction, the electron-electron repulsion, and the spin-fluctuation mediated interaction [2] in the first-principles manner. However, the accuracy of the current approximated functional of SCDFT and the effects of the spin-orbit interaction (SOI), spin-fluctuation, and the phononic anharmonicity has not been verified systematically although such a verification is highly desirable before we apply this method to the wide range of materials. Such a benchmark is also useful to find the guideline for improving the superconducting density functional. For this purpose, we started the benchmark calculation of SCDFT with our newly developed first-principles program package Superconducting-Toolkit (SCTK) [3]. In this presentation, we show benchmark results of superconducting properties calculated by SCDFT for 32 elemental materials together with computational details, and discuss accuracy of predicted transition temperature T_C and the effect of the spin-orbit interaction up on T_C (see Fig. 1).

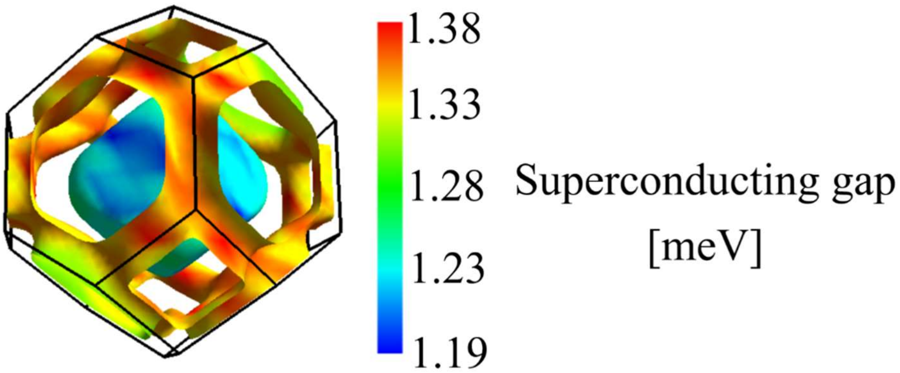

Figure 2: (color online) Superconducting gap of Pb computed by taking account of the spin-orbit interaction. If we ignore this interaction, the maximum- and the minimum- value of the gap function are reduced to 0.89 meV and 0.63 meV, respectively.

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Semimetallicity and Negative Differential Resistance from Hybrid Halide Perovskite Nanowires

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In the rapidly progressing research on organometal halide perovskites, the dimensional reduction could open up new venues to improve material properties and introduce additional functionalities. Herein, carrying out first-principles calculations, we consider the nanostructuring and device applications of the recently synthesized trimethylsulfonium lead triiodide $(CH_3)_3SPbI_3$ perovskite. We find that the one-dimensional (1D) $(CH_3)_3SPbI_3$ structure is energetically and dynamically stable, and the electronic structures of higher-dimensional forms are robustly determined at the 1D level. Upon removing organic ligands, the 1D PbI_3 column consisting of face-sharing $[PbI_6]$ octahedra is also found to be structurally stable and, more interestingly, have a semi-metallic character, contradicting the conventional assumption of semiconducting metal-halogen inorganic frameworks. Adopting the bundled nanowire junctions consisting of semiconducting $(CH_3)_3SPbI_3$ channels sandwiched between semi-metallic PbI_3 electrodes, we finally obtain a high negative differential resistance (NDR) characteristics. We show that the NDR results from a novel mechanism that involves the quantum-mechanical delocalization of channel electronic states and its disruption with increasing bias voltages. Our work demonstrates the great potential of low-dimensional hybrid perovskites toward advanced electronic devices beyond actively-pursued photonic applications.

Non-Covalent Interactions in Density Functional Calculations

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In this presentation, we introduce a practical method to correct various non-covalent interactions in density functional theory (DFT) using density-corrected DFT (DC-DFT)[1-2] and dispersion-corrected DFT (DFT-D). Various non-covalent interactions are considered an important role in the structure of materials and supramolecules. Despite DFT's good balance between accuracy and computational cost, there still remain some challenges in DFT. To solve one of these problems, S.Grimme's group developed the DFT-D3 method[3], an efficient silico-empirical method for non-covalent interactions with a predominance of dispersion. This correction can achieve better results in π-π interactions, hydrogen bonds, and some dispersion-dominant interactions using some standard benchmark sets. However, in the case of halogen bond, similar to hydrogen bonding in the aspect of dipole-dipole interaction, the result of DFT is worsened when dispersion correction is added. To classify the error in DFT, we employed the error classification of functional and density-driven errors. As a result, unlike other interactions, we found that halogen-bond is much more sensitive to density, which means density correction is necessary to cure the DFT error. By examining the B30 and the S22 datasets, we show that HF-DFT-D corrects the density and the dispersion simultaneously. The HF-DFT-D method provides more accurate results for non-covalent interactions, whether errors in standard DFT calculations are due to static or van der Waals forces.

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Odd-even phonon transport effects in strained carbon atomic chains bridging graphene nanoribbon electrodes

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Based on first-principles approaches, we study the ballistic phonon transport characteristics of finite monatomic carbon chains stretched between graphene nanoribbons, an sp^1-sp^2 hybrid carbon nanostructure that has recently seen significant experimental advances in its synthesis. We find that the lattice thermal conductance anomalously increases with tensile strain for the even-numbered carbon chains that adopt the alternating bond-length polyyne configuration. On the other hand, in the odd-numbered carbon chain cases, which assume the equal bondlength cumulene configuration, phonon conductance decreases with increasing strain. We show that the strong odd-even phonon transport effects originate from the characteristic longitudinal acoustic phonon modes of carbon wires and their unique strain-induced redshifts with respect to graphene nanoribbon phonon modes. The novel phonon transport properties and their atomistic mechanisms revealed in this work will provide valuable guidelines in designing hybrid carbon nanostructures for next-generation device applications such as nanobiosensors.

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Abnormalities in Density Functional Calculations on Ions and Radicals and its solution: Density-Corrected Density Functional Theory

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In this presentation, we introduce a systematic and practical way to correct various abnormalities in density functional theory(DFT) using density-corrected DFT (DC-DFT)[1-5]. DFT is a widely used electronic structure calculation method due to its good balance between accuracy and computational cost. One of the challenges in DFT is calculating equilibrium structures, electronic structures, and potential energy surfaces of anions and radicals, where it suffers greatly from the self-interaction error. This includes unphysical positive HOMO energies for anions, predicting incorrect ground state geometry for radical complexes, incorrect dissociative behavior for molecular species.

Here, we perform a very simple analysis on the source of error of DFT calculations and classify DFT calculations into two different groups: normal and abnormal calculation. We show that one can easily determine an abnormal calculation, and "cure" it using DC-DFT. We apply DC-DFT on problematic cases especially for ions and radicals and show it gives excellent results.

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

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A first-principles computation scheme to calculate ‘branching ratio’ in x-ray absorption spectroscopy has been applied to various 5*d*, 4*d*, and 3*d* transition-metal elements and compounds. This new method is based on an atomic theory which assumes the atomic core hole interacts 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 30 different materials and compare the calculation results with experimental data. 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 observed. The difference for 3*d* transition metal system is attributed to the neglect of core-valence interaction. We expect that our results shed light on the applicability of the method.

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Comparing two mapping formalisms for mixed quantum-classical simulations of complex systems

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Molecular dynamics simulations on multiple electronic states are important in understanding photochemical processes in complex systems. One of widely studied examples is the excited-state proton transfer in solvated pigment molecules. In this example, there are many degrees of freedom in pigment and solvent molecules which are intractable for full quantum mechanical descriptions. Instead, by combining quantum mechanical and classical mechanical treatments, one can carry out quantum dynamics simulations for important degrees of freedom and classical simulations for remaining ones. These hybrid methods are called as mixed quantum-classical (MQC) approaches. Several MQC algorithms were developed under mapping formalisms, which relate the dynamics in many electronic states to that of fictitious harmonic oscillators. These algorithms can be applied to all-atom molecular dynamics simulations of electronically excited systems. However, there is still a constant need for improving existing algorithms suitable for describing more complex systems in more efficient manner. To this end, I will present the analyses of two MQC approaches based on mapping formalisms, Poisson bracket mapping equation (PBME) and forward-backward trajectory solution (FBTS) of quantum-classical Liouville equation (QCLE). First of all, I will focus on the error of approximate PBME and FBTS of QCLE which should be accumulated in the long-time simulations. With our simulation results for two-state models, I will discuss how approximations made in deriving these approaches affect the population dynamics.

Poster-50

Poster-51

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 of the metal-TMDC interface remains a major obstacle to overcome. Recently, the phase engineering of TMDCs in the metal contact region has been demonstrated as a promising scheme to achieve low-resistance contacts for TMDC transistors, but its atomistic mechanisms remain 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 the phase-engineered TMDCs by considering different electrode metal species (In, Pd, Au) and the top and edge contact configurations. We will clarify the cooperative effects between the extrinsic metal|1T MoS_2 interface and the intrinsic 1T MoS_2|2H MoS_2 counterpart in improving the charge injection from the metal electrode into the 2H MoS_2 channel.

Z_2 monopole nodal lines in ABC graphdiyne

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A topological nodal line semimetal refers to a topological state of matter characterized by protected one-diemsional gapless excitations in momentum space. While a Z_2 Berry phase nodal line semiemtal is one of the most widely studied topological nodal line semimetals with many material realizations, there is yet another class of nodal line semimetal, referred to as Z_2 monopole nodal line semimetals, which has remained widely unexplored without a suggested material realization yet. Using first-principles calculations, we show that a three-dimensional carbon allotrope, ABC graphdiyene, realizes the Z_2 monopole nodal line semimetal [1]. We calculate a Z_2 Stiefel-Whitney number and a linking number that dictate the Z_2 monopole nodal line semimetal phase in ABC graphdiyene. We also show that ABC graphdiyne hosts two-dimensional Stiefel-Whitney insulating phase in two-dimensional subsystems of the Brillouin zone, which can be considered as a fragile topological insulator phase. Our findings suggest that ABC graphdiyene should serve as a new venue for the study of topological semimetals.

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Ab Initio Calculations of Electrical Structures of Water Adsorbed on Graphene

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A graphene, which consists of carbon atoms arranged in hexagonal lattice, is well suited for exploring an interaction between a material surface and a molecule. This is because it is an atomically flat and non-polar material. It had long been considered that graphene cannot be adsorbed by water molecules because it is a hydrophobic material. However, the previous molecular dynamics (MD) simulations confirmed that there are single or double water layers on a graphene surface, depending on the number of water molecules [1,2]. Similar layer structures have already been reported for a carbon nanotube by Homma *et.al.*, and they found such layer structures formed around the carbon nanotube by both photoluminescence measurements and classical MD simulations [3]. Although the layer structure perpendicular to a graphene surface has been rigorously researched, the microscopic structure parallel to the surface has not yet been fully characterized, meaning that the hydrogen bonding network in the water layers on graphene is not understood enough. Moreover, the influence of surface water on the electronic states of a graphene remains to be elucidated yet although this is essential for developing of graphene-based devices, such as a graphene field-effect transistor.

In this work, we constructed microscopic structures of surface water adsorbed on a free-standing graphene and a graphene attached on a hexagonal boron nitride substrate using classical molecular dynamics simulations. For the obtained structures, we investigated the influence of surface water on electronic states of a graphene using *ab initio* calculations based on the density functional theory. From the above methods, we clarified that the characteristic polygonal structures appear in the two-dimensional hydrogen-bond network [4]. We present that the structure of surface water and the electronic states of water adsorbed on a graphene.

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Poster-54

First-Principles Electronic Transport Properties of Ge/amorphous Al_2O_3/Au Structure

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The Ge-based metal-oxide-semiconductor devices have Ge/high-k dielectric oxide/metal gate structures. Although many experimental studies on the gate leakage current of these structures have been performed in terms of the scaling down issues, first-principles theoretical works on the tunneling current density and, even, electronic structures have been rarely reported. Therefore, we investigate the first-principles electronic structures and the tunneling effect through the potential barrier of high-k oxide. The Ge/a-Al_2O_3/Au structure was chosen as a model system and three different nanometer scale thicknesses of a-Al_2O_3 are considered. The electronic transport properties of the Ge/a-Al_2O_3/Au structure are compared with those of the Ge/a-Al_2O_3/Ge structure. The tunneling effect under a positive and negative bias in Ge/a-Al_2O_3/Au structures is also presented thus the current vs. bias voltage characteristic curve is shown.

Poster-55

DFT-based engineering of Dirac surface states in topological insulator multilayers

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Topological insulators exhibit the non-trivial quantum states which can be characterized by the insulating bulk states and spin-polarized metallic surface states, such as surface states with Dirac cone, being expected for spintronics device applications. The highly insulating bulk state and the tunable Dirac cone are required for the future device applications. Nevertheless, many of topological insulators have been found to be metallic due to the existence of impurities and disorder. It has been reported that the ternary tetradymite topological insulator materials such as Bi$_2$Te$_2$Se [1], which forms the ordered Te-Bi-Se-Bi-Te quintuple layers, and Bi$_{2-x}$Sb$_x$Te$_{3-y}$Se$_y$ solid solution [2,3] have highly bulk insulating states, because the defect formation is suppressed in these materials. In additoin to such defect control, one can obtain spin-polarized Dirac carries with the Dirac point in the band gap. In this study, we control the Dirac surface states by engineering topological multilayer structures using first-principles calculations based on density functional theory. The computational results show that the Dirac point can be modulated in energy by differentiating work functions between the surface layers and the inner layers to realize the desired band strcuture as shown in Fig. 1.

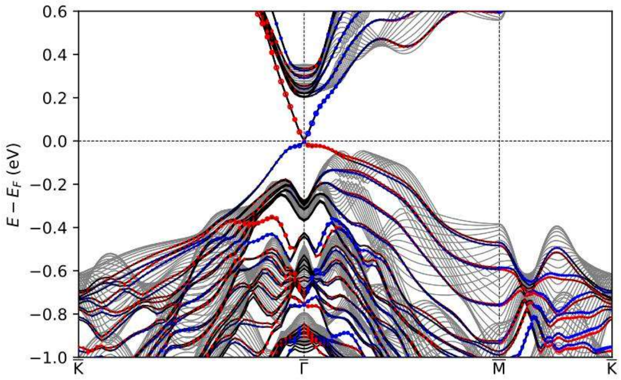

Fig. 1: Band sturcture of topological insulator multilayers: bulk band in black and

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Can exact KS potential reproduce HOMO-LUMO gap?: analytically solvable two-electron system

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Clear understanding of one-particle Green's function (GFs) for interacting electronic systems is important for material science since photoemission spectra are the GFs under some assumptions[1-3]. To capture the essential physics encoded in GFs, we study the one-particle GF of an interacting two-electron model system confined to a harmonic potential[4]. Since the calculation of GF requires the energy eigenstates of the corresponding three-electron system, we solve the Schroedinger equation analytically to obtain the exact solutions, from which we construct explicitly the simultaneous eigenstates of the energy and total spin for the first time. The solutions for the three-electron system allow us to derive analytic expressions for the exact one-particle GF for the two-electron system. We calculate the GF in frequency domain to examine systematically its behavior depending on the electronic interactions. We also compare the pole structure of non-interacting GF using the exact Kohn-Sham (KS) potential with that of the exact GF to find that the discrepancy of the energy gap between the KS system and the original system is larger for a stronger interaction. We perform numerical examination on the behavior of GFs in real space to demonstrate that the exact and KS GFs can have shapes quite different from each other. Our simple model will help to understand generic characteristics of interacting GFs.

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Electronic transport through the Ni/ZrO_2 interface: First-principles calculations

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Solid oxide fuel cells (SOFC) have advantages of higher energy density, higher conversion efficiency and non-pollution than other types of fuel cells. Although Ni/ZrO_2 is a conventional anode material of them and influences their conversion efficiency, the effect of interface orientations on junction conductance has been rarely addressed. In this work, we study the geometric and electronic properties of the Ni/ZrO_2 heterostructures from first-principle, based on density functional theory and non-equilibrium Green's function formalism, focusing on the effect of six interface orientations on conduction features. Whereas hydrogen and methane are the common fuels in the usage of SOFC and their open circuit voltages are respectively 1.05 V and 1.15 V, our results suggest that SOFC with the 90° heterostructure would offer better performance among the studied orientations.

Topological Stability of Two-Dimensional Penta-Structures: a case of $PdSe_2$

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Here, we report a new approach to analize stability and apply them to several recently proposed penta-structures including experimentally observed penta-$PdSe_2$ monolayer. Despite the fact that various 2D penta- structures have been predicted before, $PdSe_2$ is the only one observed experimentally. It is found that stabilization of 2D $PdSe_2$ is resulted from lowering of the symmetry during bulk-monolayer transition and structural-induced force compensation. The absence of internal flexural stresses in the single layer $PdSe_2$ is validated by finite cluster approach as well as calculations of different diameter and chirality nanotubes. Electronic properties of (n,0) nanotubes reveal the direct dependence of indirect bandgap width on dimeter of the nanotube while (n,n) tubes with a diameter of (12,12) and higher possess transition to the direct band semiconductor that can be suitable for optoelectronic applications. Applying the same metods to other recently-proposed penta-structures, large instability was found in penta-graphene, penta-SiC_2, penta-AlN_2, penta-B_2C, penta-CN_2, petna-SnS_2 and so on, that demonstrate the power of these methods.

Electron-Phonon Coupling, Superconductivity and nontrivial Band Topology in NbN Polytypes

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Materials that show both topological properties and superconductivity received considerable interest because of the realization of Majorana Fermions i.e., particles with their own anti-particles in such condensed matter systems [1]. Therefore, it is highly demanding to investigate for the materials that has topological properties and superconductivity. Niobium Nitride, NbN, a well-known transition metal nitride is a good superconducting material in its cubic structure (δ-NbN) with transition temperature Tc of 17.3 K [2]. Recent experiments on hexagonal NbN (ε-NbN) reveal the existence of superconductivity with a Tc of 11.6 K [3]. On the other hand tungsten carbide (WC) type NbN possesses topological properties with band crossing that has three fold degeneracy along a particular k-vector path in the Brillouin zone [4]. Therefore, NbN is a good candidate that show topological properties as well as superconductivity.

Here we study the electronic structure, lattice dynamics and electron-phonon interactions in δ-NbN, ε-NbN and WC-NbN by performing ab initio density functional calculations. The calculated electronic band structures indicate that the Nb *d*-states are dominant near Fermi level (E_F). Interestingly, they also reveal that all three NbN polytypes are topological metals. Specifically, δ-NbN and ε -NbN are, respectively, type-II and type-I Dirac metals, while WC-NbN is an emergent topological metal with exotic triply degenerate nodes. The calculated phonon dispersion relations of δ-NbN are in good agreement with neutron scatterring experiments. The phonon density of states and Eliashberg functions show that the electron-phonon coupling in δ-NbN (λ= 0.98) is much stronger than in ε-NbN (λ= 0.16) and WC-NbN (λ = 0.11). This results in a much higher superconducting transition temperature (T_c = 18 K) than in ε-NbN and WC-NbN (T_c ≤ 1.0 K). Our findings thus suggest that the three NbN polytypes would provide valuable opportunities for studying exotic phenomena arising from the interplay between superconductivity and band topology.

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Poster-60

Carrier doping effect on all-Heusler giant-magnetoresistance junctions with semimetallic Fe_2VAl studied by first-principles calculations

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For read sensors of ultrahigh-density hard disk drives (HDD) and Gbit-class spin transfer torque magnetoresistive random access memories (STT-MRAMs), magnetoresistive (MR) devices satisfying high MR ratio and small resistance–area (RA) have been required. Current-perpendicular-to-plane giant magnetoresistive (CPP-GMR) junctions are expected to be one of the good candidates that have much smaller RA than tunneling magnetoresistive junctions. However, small RA values are not suitable for read sensors, because high voltage output can not be obtained. Therefore, new junctions with a semiconducting spacer has drawn much attention [1,2]. In this work, we investigate interfacial magnetic couplings and spin-dependent transport property in all-Heusler based CPP-GMR junctions with a semimetallic Fe_2VAl spacer on the basis of first-principles calculations. A half-metallic ferrimagnet Mn_2VAl is used for a spin injector and is thought to be highly promising for spintronics devices at room temperature because the expected current to flip the spin would be rather low. The Korringha-Kohn-Rostoker (KKR) Green's function method with the AkaiKKR code is utilized to compute the magnetic coupling constants between the magnetic atoms. For calculating the ballistic conductance, we use the PWCOND code which is part of Quantum-Espresso package. It is found from our calculations that, in MnMn-VAl termination, the interfacial Mn atoms are antiferromagnetically coupled with V atoms of Fe_2VAl. In addition, half-metallic states are also preserved in the interfacial reigion. The transport property is governed by an electron pocket in the band structure, originating from the V *d* states. Electron-carrier doping in Fe_2VAl enhances the conductivity, while hole-carrier doping hardly affects it. This carrier doping effect from band matching leads to a new function in CPP-GMR junctions. When carriers are introduced in the spacer by a gate voltage, magnetoresistance might be changed significantly. Moreover, from comparison with spin injectors with other half-metallic Heusler alloys, controlling mechanisms in this type of CPP-GMR junctions is discussed.

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Poster-61

First-principles Study of Band Gap Tunability in Hydrogenated Graphene

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There have been on-going efforts to tune the electronic structure of graphene through chemical modifications. Notable examples include *graphane*, a two dimensional analogue of diamond, obtained through complete hydrogenation of graphene. The hydrogen coverage undoubtly presents a experimentally accessible way to open the band gap of graphene. In this study, we present a systematic approach to instill hydrocarbon motifs in single-side hydrogenated graphene (SSHG) presumably in contact with substrate. Here, we employed electron counting rules, a well-established formalism for dangling bonds at semiconductor surfaces, in combination with first-principles calculations to identify the most probably SSHG structures and their corresponding electronic properties. Here, the bandgap opening can be atributed to quantum confinement of isolated aromatic hydrocarbon motifs based on benzene embedded in graphene through hydrogenation. In contrast, conducting polymer motif based on polyacetylene gives rise to robust metallic properties against Peierls distortion. Our results suggest an efficient way to prepare graphene-based devices with suitable band gap through controllable hydrogenation.

Poster-62

Chemical degradation of OLED host materials: The role of excited carriers in non-local interaction

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Despite the conspicuous advances in organic light-emitting devices (OLEDs) and even their successful implementation in commercial displays, device degradation still remains as the most important issues. Because degradation occurs mostly in working conditions, the underlying mechanism is thought be linked to excited state of carriers. While several theoretical and experimental studies have focused on the mechanisms of OLED degradation, the microscopic role of the excited carrier remains elusive. In this work, using occupation-constrained density functional theory calculations, we study how chemical degradation is driven by the excited carrier in OLED host materials. We show that the C-N bond is a weak link of the OLED molecules both in the electronic ground and excited states, and the rupture of the bond is the main cause for chemical degradation. While the excited carrier generally weakens the bond, the effect can be mitigated by the non-local interaction with the other bonding and anti-bonding states. We suggest that the presence of such a non-local interaction can contribute to an enhancement of the chemical stability in the excited state.

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Revisiting Anomalous Hall Conductivity in BCC Iron via First-Principles Tight-Binding Calculations using Pseudo Atomic Orbitals

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The frequency-dependent Hall conductivity in ferromagnetic bcc Fe serves as a standard example for benchmarking the first-principles calculations based on a variety of different approaches. So far the first-principles calculations obtained via the generalized gradient approximation have been found to well describe the available experimental data [1,2]. In the poster presentation, we will show that better agreement with the magnetic circular dichroism experiments can be reached once the effect of the bandwidth renormalization [3] is taken into account. We will also present how to calculate the frequency-dependent optical conductivity based on the first-principles tight-binding Hamiltonian that is straightforwardly obtained after finishing a self-consistent calculation using the bases of pseudo atomic orbitals implemented in the OpenMX code [4]. In particular, a general formula without assuming the orthonormal relation between orbitals for calculating the momentum matrix elements needed for obtaining the conductivity based on the Kubo-Greenwood formula will be given. The position matrix elements will be demonstrated to be important for delivering the exact momentum matrix elements. We note that the only needed information in the derived formula is the position matrix element and the ingredients that have already contained in the tight-binding representation, evidencing the usefulness of the derived formula.

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Topological Phases in One-dimensional Graphene Nanoribbons

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Topology of electronic band structures has been of great interest to unusual physical phenomena derived from topologically nontrivial Bloch band systems. Recently, atomically thin one-dimensional graphene nanoribbons (GNRs) have been shown to possess distinct topological phases in general, characterized by a Z_2 invariant. [1] In this work, we extend the study of GNR topological phases to various GNR geometries such as cove-edged and chevron GNRs. [2] We then explore the consequences of having topological phase differences at heterojunctions or ends of finite segments of such GNRs, resulting in emergence of topologically-driven metallic states at interfaces or ends, respectively. The topological physics in GNR systems can be developed for valuable applications, including e.g., quantum topological band engineering and quantum information

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Revisit to the molecular J_{eff} ground state of lacunar spinel compounds: A charge-density functional plus U study

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After the discovery of the $J_{\mathrm{eff}} = 1/2$ ground state in Sr_2IrO_4 [1], spin-orbit entangled J_{eff} state has attracted a great deal of attention. This intriguing ground state can exhibit exotic phases of matter such as unconventional superconductivity [2] and quantum spin liquid [3]. The previous theoretical study predicted the molecular J_{eff} ground state in the lacunar spinel compounds, GaM_4X_8 (M = Nb, Mo, Ta and W; X = S, Se and Te) [4]. Furthermore, RIXS (resonant inelastic X-ray scattering) experiment together with the first-principles calculations reported the $J_{\mathrm{eff}} = 3/2$ ground state in $GaTa_4Se_8$ [5]. Recently, it was reported that widely-used DFT+U functional based on the spin-density could easily lead to unphysical results due to the competition between the spin-density energy and the double counting term [6]. In order to avoid such an artifact, charge-density based DFT+U functional was suggested to be the desirable choice. Since all the previous studies of lacunar spinel compounds were performed within spin-density framework, it is strongly requested to re-investigate the previous results. In this study, by introducing a new parameter, J_{eff}-ness, we analyzed the J_{eff} electronic structure with respect to Hubbard U and Hund J within charge-densty framework. As a result, we confirmed the robustness of the molecule J_{eff} ground states in the lacunar spinel compounds.

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New One-Dimensional Material Nb_2Se_9: Theoretical Prediction of Indirect to Direct Band Gap Transition Due to Dimensional Reduction

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Dimensionality reduction of some two-dimensional transition metal chalcogenides can produce direct band gap where three-dimensional structure shows indirect band gap. Recently, Nb_2Se_9 is made as 1-dimensional structure by solid state reaction. This is composed of periodically stacked single-chain atomic crystals (SCAC) where the SCACs form inorganic bulk crystals due to strong bonds within the chain but weak inter-chain interactions. To find whether the band gap transition is occurred in this SCAC materials, the band structures of Nb_2Se_9 SCACs composed of 1-7 single chains is calculated using density functional theory. Unlike the bulk structure of Nb_2Se_9, that chain bundles composed of up to 21 single SCACs would have a direct band gap. Band gap increase as the number of chains in the bundle decreased. Accordingly, Nb_2Se_9 bundle SCAC with a diameter of 3.6 nm is expected that it can cause the electronic transition without being disturbed by the phononic environment due to the direct band gap, and can be used in photoluminescence applications.

Poster-67

Versatile physical properties in new two-dimensional van der Waals materials composed of group IV-V elements

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Using first-principles calculations, we introduce layered IV-V compounds as novel 2D vdW material group with versatile physical properties. Our predicted IV-V compounds are in the form of A_2B_2, where A and B are elements in group IV (C, Si, Ge, Sn) and group V (N, P, As, Sb, Bi), forming the similar crystal structure as those of layered III-VI compounds, such as GaSe or InSe. We revealed that these newly proposed IV-V compounds have two stable distinct phases, one with the mirror symmetry and the other with the inversion symmetry. To explore their physical properties, we evaluate their phonon dispersion relations; electronic band structure; electrical and thermal transport properties; and estimate activation barrier of the phase transitions. Furthermore, we discovered the local Rashba spin splitting and topological non-trivial properties found in some of our structures containing heavy elements.

First-principles Investigation on Al Doping in $SrTiO_3$

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$SrTiO_3$ (STO) is regarded as a representative high-k material in oxide electronics, owing to its high mobility and dielectric constant (~300). However, because of its n-type nature and relatively small band gap (3.3 eV), Schottky barrier between the metal-STO interface is under 1 eV, which leads to large leakage current.

It has been repeatedly reported that the intrinsic n-type nature of STO originates from thermodynamically stable oxygen vacancy. The most straight forward approach to control the Fermi level of STO is the acceptor doping, which reduces the n-type carrier concentration and hence increases the Schottky barrier.

There have been many studies about the effect of extrinsic dopant on STO, and it was found that the doping of Fe or Cr ions at Ti sites reduces the leakage current significantly. Even though it is expected that Al doping on STO should give similar behavior, the detailed analysis with regard to the doping effect has been hardly carried out.

In this study, first-principles calculation on Al dopant in STO is carried out. The defect formation energies including intrinsic defects are calculated with hybrid density functional method. The concentration of each defect configuration and the position of the Fermi level is found. This study will give a meaningful insight into the designing of oxide electronic devices.

Poster-69

Silicon Passivation of Zigzag Graphene Edge for Spintronic Nanosensor Applications

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Zigzag graphene edges can ideally host spinpolarized edge states, providing significant potential for spintronics applications. However, because the high chemical reactivity of a pure sp^2 termination easily destabilizes zigzag edges, preparing well-defined zigzag graphene edges at ambient conditions remains a formidable practical challenge. Based on first-principles calculations, we herein demonstrate that the silicon passivation of zigzag graphene edges is a robust method to preserve the spin-polarized edge states and furthermore to improve their electronic connectivity with neighboring nanostructures. We find that finite-length silicon chains are the preferable edge configurations, and they allow the sp^2-type carbon edge structure and associated spinpolarized edge states to be well preserved. Calculating the quantum tunneling across a DNA nucleobase located in a nanogap between two Si-passivated zigzag graphene edges, we finally demonstrate that the Si passivation expands the graphene edge transport channels and result in significantly enhance spin-polarized transmissions. Pointing out that the synthetic feasibility is well supported by several recent experiments, we propose that the Si passivation of zigzag graphene edges will open up new avenues to develop graphene-based spintronic devices including nanosensors.

First-principles Calculations of Intrinsic Defect Properties in Halide Double Perovskites for Optoelectronic Applications

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Lead-free halide double perovskites (HDPs) with the formula of quaternary $A_2^+B^+B'^{3+}X_6^-$ have recently attracted intense interest as alternatives to lead-halide-perovskite-based optoelectronic materials for their non-toxicity and enhanced chemical and thermodynamic stability. In particular, a series of materials represented by $Cs_2AgInCl_6$ and Cs_2AgBiX_6 (X=Cl, Br) have been successfully synthesized in experiment. With the measured physical properties, including band gaps (2.0-3.0 eV), ultra-long carrier lifetime (6μs for $Cs_2AgInCl_6$) and low trap density (towards 10^8 cm^{-3}), these HDPs have shown desirable potential as useful optoelectronic materials. Controlling defect properties is of vital importance for intrinsic carrier density and transport. Therefore, a comprehensive understanding of carrier trapping at defects and carrier compensation is crucial for the development of HDPs. In this paper, using advanced first-principle energetics calculations, we identify deep-level defects that are detrimental to carrier transport in $Cs_2AgInCl_6$, $Cs_2AgBiCl_6$ and $Cs_2AgBiBr_6$. By evaluating defect formation energies of intrinsic defects using different chemical potentials of composed elements, our calculations reveal the ideal growth conditions to grow *p*-type $Cs_2AgInCl_6$ and $Cs_2AgBiCl_6$. So they can be potentially used as *p*-type solar absorbers and photon detectors. In contrast, semi-insulating $Cs_2AgBiBr_6$ with low carrier density, which is consistent with high observed resistivity in experiment, is a promising semiconductor radiation detection material. Our work provides valuable guidelines for further exploration of Pb-free perovskites for diverse applications.[1]

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Poster-72

Voltage Dependence of Ni-Li Electrode on its Composition and Structure: A Density Functional Theory Study

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Recently a new prototype all-solid-state memory device has been fabricated, which consists of Li electrode, Li_3PO_4, and another electrode such as Au and Ni [1]. The device has a few states with different open-circuit voltages, which can switch using an external applied bias. Though the switching has been demonstrated, its mechanism and the atomic structures of different states have not been well understood yet except that the movement of Li atoms near the electrode-Li_3PO_4 interface must play a crucial role. In the present study, using the density functional theory calculations, we examine the dependence of electrode open-circuit voltage on its composition and structure to understand the switching mechanism of this novel device.

In this presentation, we focus on the Ni electrode, because Ni does not form alloy with Li, which is expected to make the interface structure simpler. As the first step, we consider models without Li_3PO_4, more specifically, the Ni(111) slab and Ni $\Sigma5(210)$ grain boundary structure. The open-circuit voltage of Ni electrode is estimated by the method which has been widely adopted in previous studies on lithium ion batteries [2]. Our calculation results show that sites inside the Ni electrode and at the grain boundary are energetically unfavorable for a Li atom. On the other hand, Li atoms are energetically stable in some cases when they are on the surface of Ni electrode. The open-circuit voltage of Ni electrode decreases as the surface coverage of Li atoms increases. These results suggest that the atomic structures of Ni electrode with different Li surface coverage are likely to correspond to the states with different open-circuit voltages.

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Prediction of Quantum Anomalous Hall Effect in MBi and MSb (M:Ti, Zr, and Hf) Honeycombs

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The abounding possibilities of discovering novel materials has driven enhanced research effort in the field of materials physics. Only recently, the quantum anomalous hall effect (QAHE) was realized in magnetic topological insulators (TIs) albeit existing at extremely low temperatures. Here, we predict that MPn (M=Ti, Zr, and Hf; Pn=Sb and Bi) honeycombs are capable of possessing QAH insulating phases based on first-principles electronic structure calculations. The application of strain shows that HfBi, HfSb, TiBi, and TiSb honeycomb systems possess QAHE with the largest band gap of 15 meV. In low-buckled HfBi honeycomb, we observed decreasing Chern number with increasing lattice constant. The band crossings occurred at low symmetry points. We found that by varying the buckling distance we can induce a phase transition such that the band crossing between two Hf d-orbitals occurs along high-symmetry point K2. Moreover, edge states are demonstrated in buckled HfBi zigzag nanoribbons. This study contributes additional novel materials to the current pool of predicted QAH insulators which have promising applications in spintronics.

Keywords: Quantum anomalous Hall effect, Topological phase transition, TM-Bi honeycomb, Electronic structures, First-principles calculations

Two-dimensional topological insulators upon substitutional doping of monolayer VB-VIA transitional metal dichalcogenides

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Substitutional doping of two-dimensional transition metal dichalcogenides (TMDs) is of importance in tuning and possible enhancement of its electronic, physical and chemical properties for vast industrial applications. Here we report a systematic first-principles study of possible 2D topological insulator phases, also known as quantum spin Hall (QSH) insulator, upon halogen (Cl, Br, I) or pnictogen (P, As, Sb, Bi) substitution of monolayer group VB (V, Nb, Ta) - VIA (S, Se, Te) TMDs, including the effects of one-sided hydrogen adsorption, for both 1T and 2H crystal structures. A structural phase transition, from 2H to 1T, was observed for all the pnictogen substituted TMDs while no structural phase transition upon halogen substitution or hydrogen adsorption. Nontrivial phases were obtained upon pnictogen substitution and trivial phases upon halogen substitution and hydrogen adsorption. The topology of some transition metal dichalcogenides (TMDs) becomes nontrivial upon pnictogen substitution, demonstrating its suitability for synthesis on various substrates.

Topological Dirac Insulator in a Nonsymmorphic Circuit Lattice

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Recent development of topological band theory has allowed the exciting discoveries of a variety of topological phases beyond condensed matter systems, including phononic, photonic, and magnetic systems. More recently, it has been shown that the energy-momentum relationship of electromagnetic waves in an electronic circuit features varius topologically protected gapless modes, eabling the electronic circuit realization of Weyl nodes [1], topological nodal lines [?], and Zak phase [2]. In the present study, we introduce our efforts to realize a novel topological crystalline phase reffered to as the topological Dirac insulator [3] in an nonsymmorphic circuit lattice. We construct a minimal curcuit lattice that hosts required nonsymmorphic space group and show their topological phase using Wilson band calculations.

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First-principles study of anomalous Nernst effect in Fe_3Al and related compounds

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The anomalous Nernst effect (ANE) has expected as a new mechanism of thermoelectric generation systems[1].The ANE magnitude can be enhanced either by two components as follows: (i) strong asymmetry of the anomalous Hall conductivity (AHC) along the energy axis; (ii) large product of Seebeck coefficient and Hall angle ratio[2]. The intrinsic contribution of AHC is induced by spontaneous magnetization[3]. It implies that large ANE could be found in magnetic materials with large anomalous Hall effect and/or large Seebeck effect.

Heusler compounds are one candidate materials to realize large ANE according to the two terms (i) and (ii)[4]. $D0_3$-type Heusler alloys Fe_3Al is known as the ferromagnetic materials with Curie temperature of 760 K[5]. Furthermore, Fe_2VAl in which one Fe atom of Fe_3Al is substituted by V atom, which is correspond to 2 hole-doped per formula unit shows semiconductorlike behavior and large Seebeck coefficient ($S=-180$ μV/K) at room temperature[6].

In this work, we investigated carrier concentration dpendence of thermoelectric properties on Fe_3Al and related compounds Fe_2MnAl, and Fe_2CrAl. We have performed first-principles calculations on Heusler compounds with OpenMX code[7]. The transport properties has been calculated based on the semiclassical Boltzmann transport theory with Wannier90 code[8]. We have found that a large ANE in hole-doped Fe_3Al by using the rigid band apprximation. In the presentation, we discuss the origin of large ANE based on the systematic computations of thermoelectric properties.

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Guiding Principles for Enhancing Piezoelectricity in Wurtzite Materials: First-Principles Calculations

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Recently, piezoelectric wurtzite materials such as ZnO and GaN have received a lot of attention as piezotronics device materials. The wurtzite materials, especially AlN, have another advantage of applicability in high-temperatures such as sensors in automobile engines, because of the good thermodynamic stability of their noncentrosymmetric crystal structures even at high temperatures. However, the piezoelectric constants of wurtzite-type materials are generally much smaller than those of the perovskite-type materials such as $Pb(Zr_xTi_{1-x})O_3$ by a few orders. It remains a challenge to explore better piezoelectric wurtzite materials. Among the wurtzite materials, the highest piezoelectricity has been experimentally discovered for $Sc_xAl_{1-x}N$ (about 25 pC/N for $x \sim 0.5$). Novel low-cost materials, which are superior to $Sc_xAl_{1-x}N$, have not been synthesized yet as there are no clear and general materials-design criteria practically usable for enhancing the piezoelectricity of wurtzite materials.

In this study, we calculate longitudinal piezoelectric constants (e_{33}) of more than a dozen binary wurtzite materials, which are listed in the crystal structure databases, by the first-principles methods, and we study relations between the piezoelectric constants and several material parameters using the statistical-learning methods [1]. The results show that the wurtzite materials with high e_{33} generally have small lattice constant ratios (c/a) almost independent of constituent elements, and approximately expressed as $e_{33} \propto c/a - (c/a)_0$ with the ideal lattice constant ratio $(c/a)_0$. We find that this simple relation also holds for highly-piezoelectric ternary materials such as the calculated e_{33} values of $Sc_xAl_{1-x}N$ [2]. Therefore, this material-design criterion can be applicable to the case in doped ternary materials. Based on the insight above, we have conducted a computational search for highly-piezoelectric wurtzite materials by identifying materials with smaller c/a. Effects of in-plane strain on piezoelectricity of AlN, element-combination effects in LiX (X = halogen elements), and element-doping effects into ZnO are examined. The result shows that the piezoelectricity of ZnO can be significantly enhanced by partial substitutions of Zn with Ca. Though the calculated value of e_{33} of $Ca_xZn_{1-x}O$ is still smaller than that of $Sc_xAl_{1-x}N$, we expect that $Ca_xZn_{1-x}O$ is at a definite advantage in materials cost and natural resource in abundance of constituent elements.

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Poster-78

Magnetic States and Intervalence Charge Transfer of Ti and Fe Defects in α-Al_2O_3: The Origin of the Blue in Sapphire

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Aiming to identify the spin configuration and its alignment of Ti and Fe of ground-state configuration in blue sapphire, we investigate various spin configurations of Ti and Fe in Al_2O_3 in search of the spin configuration which give the lowest energy. To examine the electronic, energetic, and structural properties, we perform first-principles density-functional-theory calculations within the PBEsol generalised gradient functional with adding Hubbard U potential. From the total energy results, we show that the high-spin state of Ti^{IV}-Fe^{II} with an anti-ferromangetic alignment between Ti and Fe is the ground state for both edge- and face-sharing orientations. Among several meta-stable states, the high-spin state of Ti^{III}-Fe^{III} with an anti-ferromagnetic alignment is connected to the Ti^{IV}-Fe^{II} ground state. An optical transition from the highest occupied Fe defect level to the lowest unoccupied Ti leads to an excited state of the high-spin Ti^{III}-Fe^{III} configuration together with a donation of electron from Fe^{II} to Ti^{IV}. It explains that the Ti^{IV}-Fe^{II} is the ground state and the intervalence charge transfer of Ti^{IV}-Fe^{II} to Ti^{III}-Fe^{III} would be responsible for the color of blue in sapphire. We find that both edge- and face-sharing alignments can be found in nature since their ground state energies are different by only 0.02 eV. However, only the edge-sharing alignment would be expected to be the origin of the blue in sapphire. The corresponding optical excitation energies of this transfer of edge- and face-sharing alignments are 1.99 and 1.36 eV, respectively.

Magnetic Dipole-dipole Energy Evaluation on 1D, 2D, and 3D Periodicities using Density Functional Approach

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Magnetic dipole-dipole interaction is one important factor for determining the magnetization direction of magnets as well as the spin-orbit interaction. Furthermore, it may also contribute to emergences of peculiar non-collinear magnetism, such as magnetic skyrmions, multi-ferroic polarization, etc. In general, the magnetic dipole-dipole interaction is estimated by the arrangement of atomic magnetic moments so far. However, in the case where there is a large spatial anisotropy in the electron spin density, reliability of that treatment remains uncertain. Therefore, we have investigated the way of estimating magnetic dipole-dipole energy through the spin density obtained from density functional theory [1,2,3].

Since the magnetic dipole-dipole interaction proportional to the minus third power of the distance between the dipoles, the effect from long distances cannot be ignored. Moreover, its long-range feature requires some special treatment for numerical evaluation, based on the dimension of periodicity and boundary condition in the target system. One can estimate the magnetic dipole-dipole energy on each dimension with a high efficiency, using the Coulomb Green function of the respective dimension (one-, two-, or three-dimension).

As a demonstration of our implementation, we calculated the magnetic anisotropy energy of simple 1D, 2D, and 3D magnetic structures. The result provided the same value as in the calculation with a localized spin moment model, assuming a spherical local spin density on each atom. Apart from this, we investigated several extreme cases for checking the implementation and reproduced the previous results successfully. In addition, we investigated magnetic anisotropy of the solid oxygen which is known as antiferromagnetic molecular crystal. In the oxygen molecule, the spin density distribution much deviates from a spherical one because of electron orbital anisotropy. We found that the spin density distribution also plays an important role for the magnetic dipole-dipole interaction aside from those of atomic spin alignment. Our results are in a good agreement with the experimental data, indicating a reliability of our method. For example, in the α-phase of solid oxygen, both the spin density distribution and spin-orbit interaction on molecule favor a direction perpendicular to the molecular axis and the crystal field originating from the magnetic dipole-dipole interaction limits the stable direction to the b-axis which has the mirror planes of the crystal structure.

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Poster-80

Three-dimensional Dirac semimetal in a nonsymmorphic wallpaper multi-layer

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Using an explicit tight-binding model and first-principles calculations, we show that a three-dimensional stack of two-dimensional layers in the *p4g* or *pgg* wallpaper group hosts fourfold-degenerate Dirac points at time-reversal invariant momenta of the Brillouin zone, realizing the three-dimensional Dirac semimetal phase. Our Chern number calculations support that the system hosts Dirac` points in momentum space. In addition, we show that Doubly-degenerate doubly-degenerate Weyl nodal lines coexist with the Dirac points in momentum space, giving rise to topological surface states. We establish topological phase diagrams accessible from the Dirac semimetal phase via symmetry-breaking strains. Our first-principles calculations show that the proposed 3D Dirac semimetal phase is realized in an existing set of materials, including $BaLaCuBO_5$ and $BaLaAuBO_5$.

Poster-81

Efficient O(*N*) divide-conquer method with localized natural orbitals

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An efficient O(*N*) divide-conquer (DC) method based on localized natural orbitals (LNOs) is presented for large-scale density functional theories (DFT) calculations of gapped and metallic systems [1]. The LNOs are non-iteratively calculated by a low-rank approximation via a local eigendecomposition of a projection operator for the occupied space. Introducing LNOs to represent the long range region of a truncated cluster reduces the computational cost of the DC method while keeping computational accuracy. The novel O(N) method has been implementd into OpenMX DFT code which is based on optimized localized numerical orbitals and norm-conserving pseudopotentials [2], and a series of benchmark calculations and high parallel efficiency in a multilevel parallelization clearly demonstrate that the O(*N*) method enables us to perform large-scale simulations for a wide variety of materials including metals with sufficient accuracy in accordance with development of massively parallel computers.

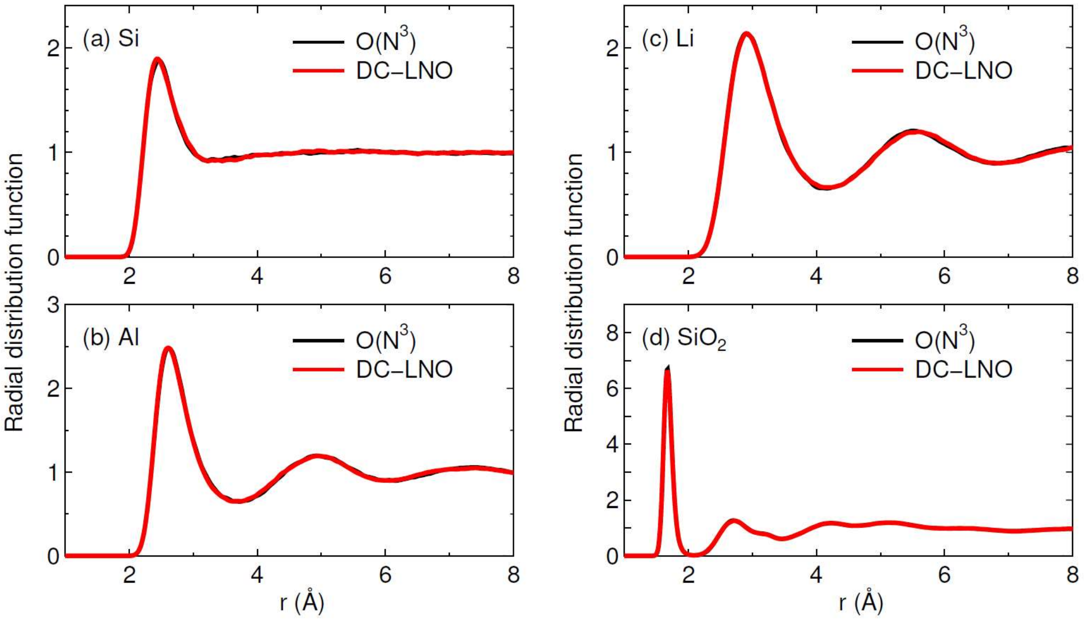

Fig. Radial distribution functions of liquids for (a) Si at 3500 K, (b) Al at 2500 K, (c) Li at 800 K, and (d) SiO2 at 3000 K calculated by the O(N^3) and DC-LNO methods.

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Simulated Scanning Tunneling Microscope Images of Intrinsic Defects in $MoTe_2$

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Transition metal dichalcogenides (TMDCs) are layered compounds made up of X-TM-X trilayers, where TM and X refer to transition metal and chalcogen atoms, respectively. $MoTe_2$ is one of the representative TMDCs and has been studied extensively due to its high current-on/off ratio implying potential applicability in field-effect transistors [1-5]. In a previous study, intrinsic defects in the single $MoTe_2$ trilayer were investigated systematically and the Te adatom on top of a Te atom was found to be the most stable defect [6]. In this work, we studied intrinsic defects in $MoTe_2$ three trilayers. We performed density functional theory (DFT) calculations by using Vienna *ab-initio* simulation package. We used the PBE exchange-correlation functional in conjunction with the DFT-D3 method to describe the van der Waals (vdW) interaction between the trilayers. We used the 5×5 surface supercell to simulate isolated intrinsic defects. We investigated vacancies, adatoms, interstitials, and vdW gap intercalations for Mo and Te. The most stable structure is found to be the Te adatom on top of a Te atom in both Te-rich and Mo-rich conditions (the corresponding defect formation energies are 1.06 and 1.35 eV) in agreement with the previous study. In addition, we simulated the constant-current STM images for pristine $MoTe_2$ and intrinsic defects within the Tersoff-Hamann approximation. The simulated STM images exhibit strong bias-dependence, which can be used as fingerprints in identifying intrinsic defects.

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Poster-83

First-principles Study of Non-thermal Phase Transition Mechanism with Uniaxial Stress Applied Phase Transition Material: GeTe

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Recently, phase change materials (PCM) have attracted attention as candidate for next generation memory device elements. But it has several problems in power consumption, information storage capacity, energy efficiency, and so on. We use *ab initio* density functional theory to investigate *non thermal* phase transition of a prototypical phase change material, GeTe, induced by uniaxial strain. We focus on the rhombohedral structure which can be interpreted as a layered strucuture, in which layers are seperated by long bonds. It is found that GeTe layered structure experiences a phase transition from one crytalline phase to the other crystalline one under external uniaxial tensile stress. We identify that the latter phase is essentially regarded as another layered structure rotated from the former phase through the exchange mechansm between short and long bonds. Our electronic transport calculation also shows that the conductance changes significantly during such phase transition, implying that uniaxial strain may induce non-thermal phase transition in GeTe.

Estimation of the Effective On-Site Coulomb Interaction Parameter U by Mapping Atomic Self-Interaction Correction onto GGA+U for Molecules

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It is known that the on-site Coulomb interaction parameter, also called as the Hubbard U parameter, can be obtained from a density functional theory (DFT) linear-response method [1], but this approach is not available to DFT calculation on atom-centered basis sets because density response to a localized potential shift cannot be described due to the unclear definition of the Hubbard U values for multiple-zeta orbitals and the limit of accuracy reinforcement by increasing the number of basis functions.
I propose a calculation method for effective on-site interaction U parameters by taking advantage of the relationship between GGA+U (or LDA+U) and atomic self-interaction correction (ASIC) [2]. Because molecular orbitals containing transition metal 3*d* orbitals are often close to atomic-like orbitals, the unitary matrix (transformation between Kohn-Sham orbitals and so-called ‘localized orbitals’) elements related with the 3*d* orbitals can be assumed to be square-roots of the Mulliken 3*d* orbital populations for molecular orbitals. From the specific unitary matrix elements, one can obtain the localized orbitals corresponding to the 3*d* orbitals, which can give effective U values.
Calculated effective U values were reasonable for simple molecules containing a transition metal atom when a numerical atomic orbital code package, OpenMX was used with dual projectors [3]. My results are comparable to the results of the linear-response method on plane-wave basis sets.

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Poster-85

Estimation computational predictions of stable phase for antiperovskite Na_3OCl via rotation of ONa_6 octahedra

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Antiperovskite Na_3OCl has been considered as a candidate material for solid electrolyte. Hippler et al. reported Na_3OCl in cubic phase $Pm\bar{3}m$ [1] but Zinenko et al. showed unstable phonon modes at the R and M points for cubic Na_3OCl [2]. In this work, we study the structural stability of Na_3OCl in terms of energy landscapes and phonon spectra with the rotation of ONa_6 octahedra. We prove that the cubic Na_3OCl can be energetically stabilized through octahedral tilts among 15 possible tilted systems consistent with Howard and Stokes' group-theoretical analysis of octahedral tilting in perovskites [3]. We find that all 14 tilted structures of Na_3OCl are more stable than the cubic $Pm\bar{3}m$ by 11-16 meV per five-atom unit cell. The tilt angles along the pseudocubic [100], [010], and [001] directions vary in the range of 2.6–9.3. While the Pnma and P21/m structures of Na_3OCl are found as the two most stable ones, only the P21/m phase has stable phonon vibrations with a direct band gap of 3.38 eV at the G point.

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Poster-86

Theoretical insight into methane oxidation to methanol on single Fe-embeded nitrogen-doped graphene

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Methane, a major component in natural gas and biogas, is an important chemical feedstock for synthesis of methanol as more valuable compound. Methanol is renewable source in many industries. To convert methane to methanol, there are several technologies such as supercritical water process, plasma technology, biological process, photo-catalysts, and catalytic process. Among them, catalytic process is popular approach because the methane goes through oxidation processes under mild condition with high yield. Different types of catalysts methane oxidation such as metal-exchanged zeolites, metal catalyst, and carbon-based catalyst have been widely investigated. Modified graphene as one of carbon-based materials has become attractive catalysts because its properties are suitable for example, high specific surface volume ratio, low energy consumption, low cost, and non-toxic materials. Among the modified graphene materials, Fe embedded on nitrogen-doped graphene (Fe-N_xG; x=1,2,3) is one of the most interesting catalysts because it has specific active sites and can modulate the Femi-level leading to enhancement of catalytic activity. These materials (Fe-N_xG) exhibit high chemical activity in various fields for example, Fe-N3G, and Fe-N4G for oxygen reduction reaction (ORR). However, the reactivity of Fe-N_xG catalysts in methane oxidation are not well understood. Therefore, in this work, the methane oxidation mechanism using Fe-N_xG catalysts will be systematically investigated. Finally, the reactivity of Fe-N_xG will be compared with other catalysts.

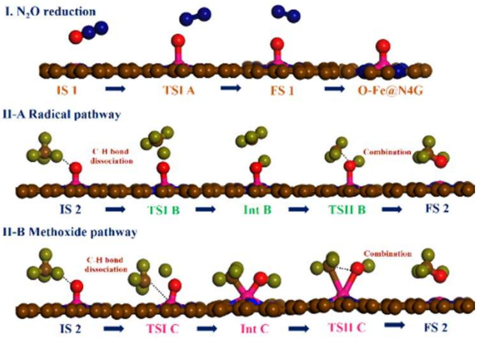

Fig.1 Proposed mechanism of methane oxidation present of N_2O reduction on Fe-embedded on functionalized graphene (Fe-N_xG).

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Poster-87

Graphene edge contacts to ZnO: A first-principles study

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In spite of the attractive material properties of graphene, there still exist numerous obstacles in employing it into the standard field-effect transistor archictecture for device applications. As an alternative route, Yang *et al.* [1] recently proposed a novel barristor device concept, a device operates based on the tunable Schottky barrier between graphene and semiconductors. In this work, having the graphene barristor based on ZnO in mind, we investigate several graphene/ZnO contact models using density functional theory calculations. By adopting graphene or graphene nanoribbon (GNR) in contact with several ZnO surface types, we systematically study the electronic structures of graphene/ZnO interfaces. We particularly comapre the top- and edge-contact models, and clarify the deerimental role of Fermi-level pinning effect amplified for the graphene edge contacts.

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Model mapped RPA: first-principles method to determine a Hubbard model Hamiltonian

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Curious physical phenomena such as superconductivity may often be driven by electron correlations. Such correlations are usually investigated by assuming Hubbard type models. The hopping integrals can be evaluated from first-principles calculations by calculating Maximally Localized Wannier Functions [1]. For the evaluations of Hubbard interactions U, the constrained random phase approximation (cRPA) is often adopted [2,3,4]. However, cRPA contains several problems [5]. For example, interaction parameters calculated in cRPA become finite between distant sites because cRPA removes the metallic screenings for Coulomb interactions.

To amend such problems, we have introduced a new method named model-mapped RPA (mRPA) [5]. The mRPA method requires the constraint $W = W_{\mathrm{M}}$ on U, where W and W_{M} are the screened interactions calculated in first-principles calculations and Hubbard model calculations, respectively. Owing to the constraint, we can obtain short-ranged model interactions. The method of mRPA may be technically simpler and theoretically clearer than that of cRPA.

The method of mRPA also includes the procedure to remove the double counting of one-body terms. The mean-field terms given by two-body Hamiltonians should be removed because one-body Hamiltonian derived from first-principles contains such effects [5]. This is crucial for multi-orbital models.

We will present the value of U assuming two-orbital model for the cuprate superconductors La_2CuO_4 and $HgBa_2CuO_4$. We analyze the material dependence of U given by the apical oxygen height [6]. Through the analysis, U obtained from mRPA results in different tendency with cRPA. This implies that the value of U may be ambiguous in principles.

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Electronic and Photophysical Properties of Derivatives of 2-Phenylbenzothiazole and 2-(2´-Hydroxyphenyl) benzothiazole: Effect of Intramolecular Hydrogen Bonding

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Photophysical properties of 2-phenylbenzothiazole (PBT) denoted as a No-PT type compound and 2-(2´-hydroxyphenyl)benzothiazole (HBT) denoted as a PT type compound as well as their derivatives have been investigated using six different DFT and TD-DFT methods. The B3LYP exchange-correlation functional with 20% HF exchange is found to be the most suitable method for reproducing experimentally photophysical data. Overall, the simulated absorption and emission spectra of all derivatives are red-shifted compared with their parent compounds, PBT and HBT, except emission spectrum of TPy-1 is blue-shifted. Especially, TPy-3 and HTP-2, of which the carbon atoms at 4,7-positions of the benzothiazole core are replaced by nitrogen atoms and hydrogen atoms in the 2,6-positions are substituted by dimethylamino phenyl groups, show more red-shifted absorption spectra than other compounds caused by lone pair electron of nitrogen atoms and electron donating group that has the effect on the π-conjugated system. In addition, TPy-4 and HTP-3 also have the similar effect on π-conjugated system. As expected, the calculated Stokes shifts of the PT type compounds are larger than that of the No-PT type compounds, because of the tautomer formation through the excited state intramolecular proton transfer (ESIPT) process. The potential energy curves (PECs) scanned along the proton transfer (PT) coordinate of the PT type compounds reveal that the ESIPT process is more likely to proceed in the S_1 state. The ESIPT process in HBT, HTP and HTP-1 occurs with a small barrier or barrierless, whereas that in HTP-2 and HTP-3 involves a higher barrier. The PT barriers were found to be in the order of HTP ~ HBT > HTP-1 > HTP-2 > HTP-3. The knowledge accumulated through these studies is expected to be useful for the rational design of fluorescent molecular probes.

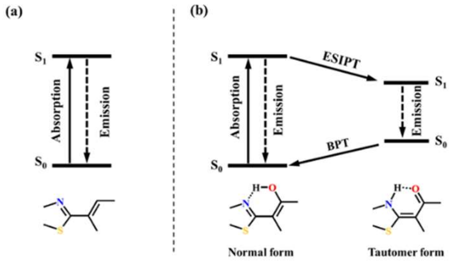

Figure 1. Photocycle of (a) molecules without proton transfer (No-PT type) and (b) molecules with intramolecular proton transfer (PT type)

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Ferroelectricity and piezoelectricity in stable monolayers MoC, WC, WS, and WSe

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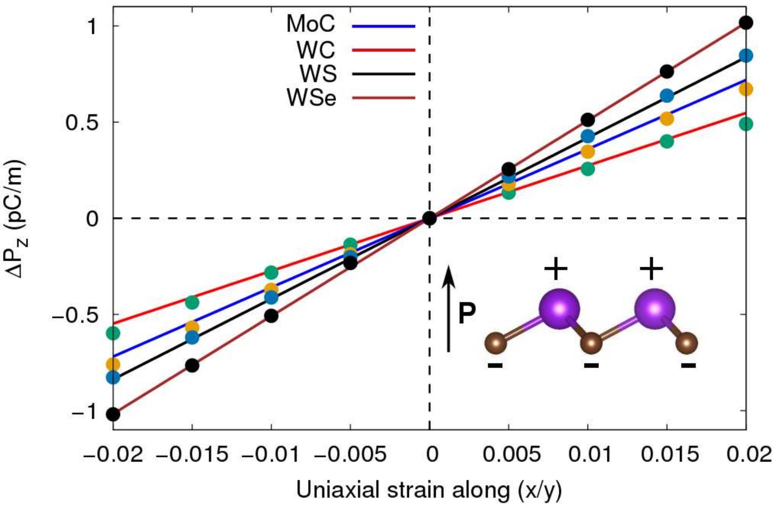
Ferroelectricity has been a rare phenomenon in the ultra-low thin films of the ferroelectric materials. With the aid of density functional theory calculations, we have designed buckled hexagonal monolayers MoC, WC, WS, and WSe. These monolayers are stable energetically and dynamically with high spontaneous out-of-plane polarization due to different electronegativities and their asymmetric buckled structures. e_{31}=50.9, 39.0, 45.0, 55.4 pC/m for monolayer MoC, WC, WS, and WSe respectively. While the in-plane piezoelectric stress coefficient along the zigzag direction does not exist due to the mirror plane along the armchair direction, a strain along the armchair direction causes high piezoelectric stress coefficients of 1.0×10^3 pC/m for monolayers MoC and WC and 0.47, 0.49×10^3 pC/m for WS and WSe respectively. The in-plane piezoelectric stress coefficient for monolayer MoS_2 is reported as 3.00×10^2 pC/m. Thus the in-plane piezoelectric stress coefficients of these monolayers are larger than the one reported for MoS_2 monolayer. The out-of-plane polarizations of these materials may be switchable with the relatively high switching energy barriers in the range from 0.55 to 2.7 eV per formula unit. Furthermore, we are studying the growth of these monolayers on the layered substrates, such as graphene or MoS_2 to enhance their stability and reduce the polarization switching barriers.



Poster-91

First-principles study of electric-field induced Z_2 topological phase transition in strained one-bilayer Bi(111)

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Electric-field induced Z_2 topological phase transition is important for applications of a Z_2 topological insulator. If we are able to switch from Z_2 topological insulating phase to trivial insulating phase or vice versa by the electric field, novel devices using edge spin currents could be realized. We predicted that one-bilayer Bi(111) shows electric-field induced Z_2 topological phase transition by first-principles calculations[1]. The bandgap is closed at the electric field E = 2.1 V/Å and one-bilayer Bi(111) shows Z_2 topological phase transition from Z_2 topological insulating phase ($E < 2.1$ V/Å) to trivial insulating phase ($E > 2.1$ V/Å). In order to realize device applications, the critical electric field should be reduced by tuning the bandgap.

In this study, we performed fully relativistic density functional calculations of the bandgap and Z_2 topological invariant in strained one-bilayer Bi(111) shown in Fig. (a). In order to compute Z_2 topological invariant using OpenMX code [2], we have implemented Fukui-Hatsugai method[3] which can be applied to the system without space inversion symmetry. Figure (b) shows the Z_2 topological phase diagram of one-bilayer Bi(111) in the space of the electric field and strain with the 3D plot of the band structure at the strain 0.5 %. The bandgap of one-bilayer Bi(111) is closed at the strain 0.5 %, and quadratic band touching[4] appears at Γ point. Near the strain 0.5 %, the critical electric field is reduced to $E < 1.0$ V/Å. In the poster session, we will present our detailed calculated results and how to implement Fukui-Hatsugai method in OpenMX code.

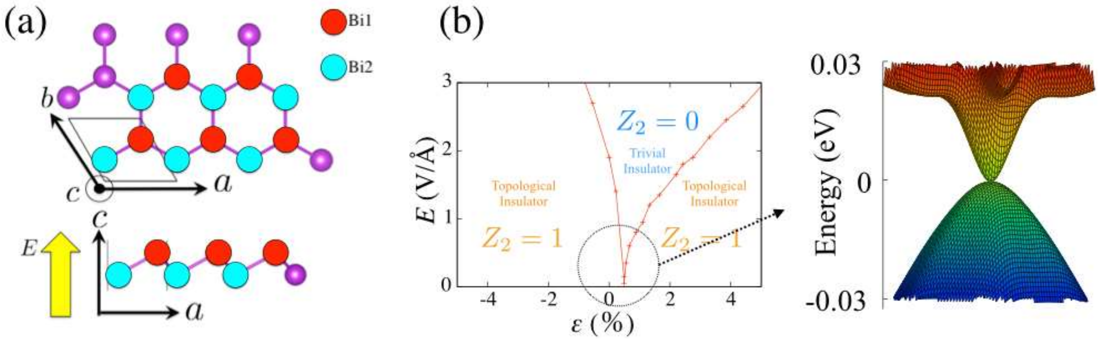

Figure: (a) The structure of one-bilayer Bi(111) (b) The Z_2 topological phase diagram with the 3D plot of quadratic band touching at the strain 0.5 %

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First Principles Investigations on a New 1111-type Fe-based Superconductor: ThFeAsN

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Recent discovery of superconductivity at 30K in stoichiometric ThFeAsN compound [1], in absence of spin density wave order [2] stipulate a possibility of non-magnetic origin of high temperature superconductivity. In contrary to the experimental results, first principles calculation within GGA predicts a stripe antiferromagnetic ground state in this system [3]. In order to explore the emergence of superconductivity in ThFeAsN, we perform electronic structure calculations within density functional theory (DFT). Our first principles electronic structure calculations reveal the semi metallic behavior of ThFeAsN, which resembles with that of the LaFeAsO and most of the other Fe-based superconductors. Fig. 1 depicts our calculated orbital projected band structure of ThFeAsN in non-magnetic state. The dominance of Fe d_{yz}, d_{xz} and d_{xy} orbitals at the Fermi level is in well agreement with that of the previous experimental as well as theoretical results [1,4].

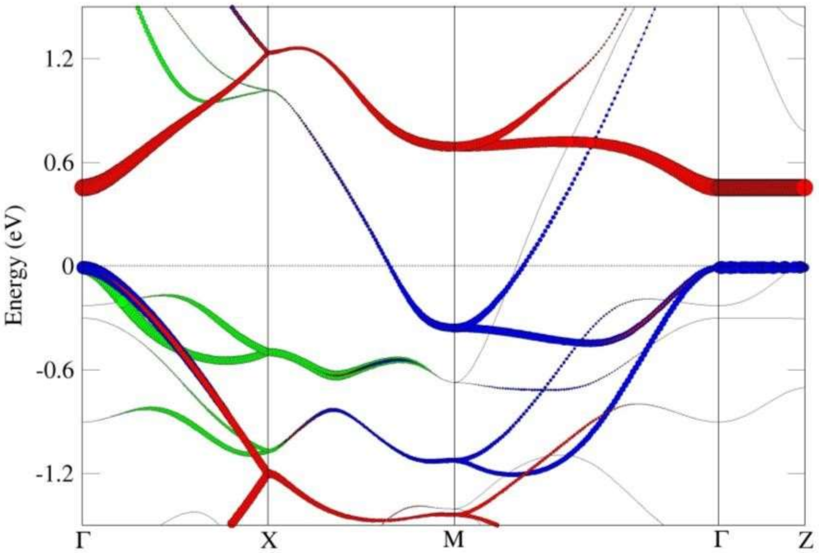

Fig. 1: *Calculated orbital projected [Fe- d_{yz} (green), d_{xz} (blue), d_{xy} (red)] band structure of ThFeAsN with GGA optimized structure in non-magnetic state.*

Moreover, the role of electron-phonon coupling to superconductivity in this system is still not known [5]. In this work we present the electronic structures of ThFeAsN and the role of phonon in the mechanism of superconductivity in this system.

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First-Principles Study of Ir Desorption from Its Low-index Surfaces

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Iridium is one of the metals in platinum group. Due to good mechanical properties and chemical inertness especially at high temperature, iridium is broadly used on industries, such as crucibles for single crystal growth, spark plugs in car engines, etc. However iridium has desorption problems[1]. Although iridium has the lowest oxygen permeability, iridium surfaces are oxidized above 1000K, and produce gaseous oxide molecules, such as IrO_3[2]. To solve this desorption problem, fundamental understanding of the desorption process is naturally necesarry.

In this study, we investigate oxidation of low index surfaces of iridium such as Ir(110) and Ir(111) to find energetically favorable surface oxides and its IrO_3 desorption energy, by using first-principles calculations based on density functional theory. We used OpenMX code, which is based on norm-conserdving pseudopotentials and pseudo-atomic localized basis functions[3]. The GGA-PBE exchange-correlation functional[4] is adopted. Since desorption process is only occurred at high temperture, we used a thermodynamical method, which gives temperature dependence of the free energy or chemical potential by combining DFT calculation with experimental thermodynamic data, particularly useful to gas molecules. This method give us insight of the IrO_3 desorption at high temperature, in terms of the temperature dependence of the desorption energy. We find that IrO_3 desorption is energetically favorable on some iridium surfaces.

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The effect of strain on the phonon thermal transport properties of the two-dimensional 2H-$MoTe_2$

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The strain is a handy and useful tool to enhance the performance of the semiconducting devices. It can tune electronic, optical, and thermoelectric properties. However, the effect of tensile strain on the phonon thermal transport of two-dimensional materials is unpredictable because the flexural acoustic (ZA) mode becomes harder and transverse acoustic (TA) and longitudinal acoustic (LA) modes become softened. Here, we study strain-dependent lattice thermal conductivity and other phonon properties such as phonon group velocity, phonon anharmonicity, phonon lifetime of the two-dimensional 2H-$MoTe_2$ using the Boltzmann transport theory for phonon coupled with the first principles calculations. We find that the lattice thermal conductivity is reduced approximately 2.5 times at 8% tensile strain for the two-dimensional 2H-$MoTe_2$ contrary to graphene, germanene, silicene, germanene, and Penta-SiC_2. The reduction in lattice thermal conductivity attributes to the reduction in the phonon group velocity, the phonon heat capacity, and the phonon scattering time. We have also evaluated the contribution of each mode to the lattice thermal conductivity. The ZA mode contribution decreases while the TA/LA modes contributions increase under tensile strain. These results highlight that tensile strain is a key parameter to tune the lattice thermal conductivity and other phonon thermal transport properties of the two-dimensional 2H-$MoTe_2$.

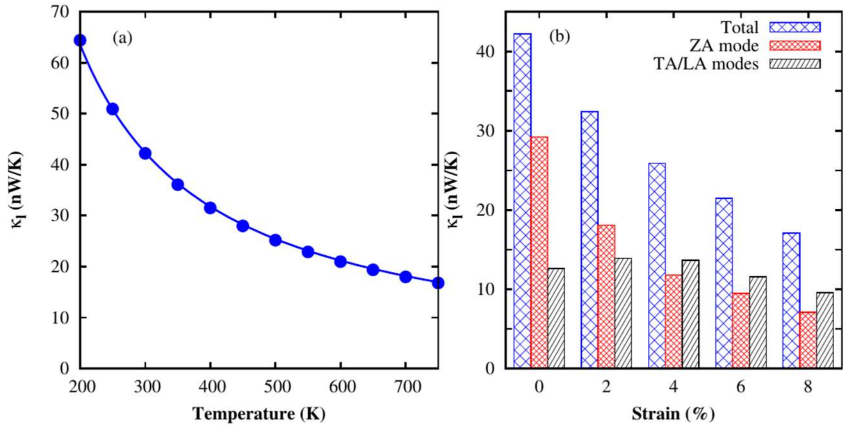

Figure 1: (a) Lattice thermal conductivity of monolayer 2H-$MoTe_2$ as a function of temperature at zero strain, and (b) total lattice thermal conductivity, showing the contribution of the ZA and TA/LA modes to the lattice thermal conductivity at 300 K as a function of tensile strain at 300K.

OpenMX interface for the Atomistic Simulation Environment

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The Atomic Simulation Environment (ASE) package written in Python is aimed at providing an easy, flexible and customizable environment for density-functional-theory (DFT) calculations. Currently, the ASE package supports interfaces over 30 Calculators including ABINIT, SIESTA, Quantum Espresso and VASP. While most of *ab initio* calculations require massive computational resources and opt for high efficiency, the Python language behind the ASE package provides a copious number of library modules which make swift code developments possible. Here, we like to take advantage of both the OpenMX code and the ASE/Python modules by implementing the OpenMX interface for the ASE. For example, combining the LAMMPS and OpenMX codes, we can seamlessly perform molecular dynamics simulations without compensating coding efficiencies. Even benchmarking the OpenMX results against VASP is a breeze. Since the modules in ASE are highly scalable, we can utilize some of the features of ASE modules, eg., the phonon module, for the OpenMX calculations. We hope that this platform can be used for combining DFT calculations. We hope that this platform can be used for combining DFT calculations with machine learning and big data, where the famous Python modules like Spark and TensorFlow can be employed to conduct deep learning research.

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Construction of Neural Network Potential to Study Li-Ion Distribution near Au(111)/Li_3PO_4 Interface

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Li_3PO_4 based materials are used for solid electrolytes in thin film Li-ion batteries. Recently, its application as non-volatile memory devices is also being explored: Au/Li_3PO_4/Li as well as Ni/Li_3PO_4/Li stacked structures were found to exhibit a few different voltage states, which can be controlled by applied voltages [1]. To develop novel memory devices using this phenomenon, understanding on Li-ion distribution near the metal/Li_3PO_4 interfaces is crucially important. We had investigated these issues using density functional theory (DFT) based molecular dynamics (MD) calculations. However, their high computational costs hinder analysis of interface systems including an amorphous solid electrolyte. Considering this situation, we constructed the interatomic potentials for the Au/Li_3PO_4 interface system with adopting the framework of the high-dimensional neural network potential (NNP) [2, 3], which is expected to acheive high reliability and low computational costs simultaneously.

We constructed the four-elements NNP using the dataset obtained by DFT calculations, which includes bulk and surface structures of Au and Li_3PO_4, Au surfaces with Li adatoms, and Au/Li_3PO_4 interface. We created 236,322 structures in total, and these structures were randomly divided into the training (80%) and test (20%) sets. The root-mean-square-errors of the predicted total energies were 41.3 meV/atom and 41.4 meV/atom for the training and test sets, respectively. Next, we constructed the NNP using a little different procedure to explore the possibility of acceralating the construction process. First, we constructed two separate NNPs optimized for Au and Li_3PO_4, respectively. We then constructed the NNP for the Au(111)/Li_3PO_4 system starting from the above two NNPs and adding the interactions of Au-Li, -P, and -O. We found that the NNPs obtained from the two procedures show comparable accuracy, while the second approach required less computational time for NNP optimization. This work was supported by CREST, JST.

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Oxygen adsorption and oxygen dissociation on TiB_2 monolayer

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Boron based two dimensional crystals have many excellent properties and received rapid developments recently. Being the neighboring atom of carbon in the periodic table, boron resemblances to carbon as it has similarities in electronic properties and prospective applications, such as, biological compounds and super hard materials. The open electron shell structure of Boron lacks one electron to be half filled. Therefore, it has paved the way for Boron to combined with various transition metals to discover new 2D metal borides. TiB_2 have been studied and revealed that it has high stability and fascinating properties. A perfect monolayer of TiB_2 is found over Boron since the movement of Ti is restricted due to it's bonding with Boron and thus they stabilizes each other. It has a possibility to be more reactive due to the metal surface in Ti whereas graphene or boro nitrite is very inert. Oxygen being the second most abundant gas existing in the earth's atmosphere might play an important role as a possible gas adsorbate by substantially altering the properties of 2D materials based devices through doping, resulting low performance in practical applications. A self-consistent periodic density functional theory (DFT) study is presented here on the adsorption of O and O_2 and the dissociation of O_2 over TiB_2 monolayer. It is observed that a barrierless O_2 dissociation is occurred due to the strong interaction between the TiB_2 surface and the O_2 molecules approaching towards it.

Open source code development for DFT + DMFT calculation: Correlated subspace projection and analytic continuation

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In the strongly correlated electron systems, it is crucial to provide an appropriate theoretical formalism that can handle many-body effects in a material-specific context. One of the successful approaches is the dynamical mean-field theory (DMFT) combined with the DFT [1]. We implemented DFT+DMFT based on OpenMX, a pseudo-atomic orbital basis DFT code [2]. The implementation is characterized as follows: i) the wide energy window on which the hybridization function is defined, including ligand orbitals, e.g., oxygen *p* orbitals. ii) projection method that defines correlated subspace based on the natural atomic orbitals (NAOs) [3]. With this NAOs-based projector, *d*-*p* hybridization can be reasonably described. We also discuss the newly developed methods for analytic continuation problem, the so-called maximum quantum entropy method (MQEM) [4]. We show that the results are stable for numerical parameter changes, applying our methods to the typical transition metal oxide systems.

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Searching for Antiferromagnetic Topological Phases

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After the suggestion by Haldane[1], a realization of quantum anomalous Hall insulator (QAHI), also called Chern insulator(CI), has been one of the challenging topics in condensed matter. A couple of years ago, at an extremely low temperature this phase has been realized. Without applying any external fields, CI has robust edge states that is energy dissipation-less and fully spin-polarized in direction of its magnetization. Due to these fascinating properties, industry and academy have thought this CI as a promising candidate for the next generation low power consumed electronic devices. Although this phase has been realized only in one compound a couple of years ago, this phase is observable at an extremely low temperature. So, realistic compounds have been required for applications.

Nowadays attempts to realize CIs in antiferromagnets (AFMs), which often are insulators with a high Neel temperature, have initiated in theoretical studies. Our goal is to find promising candidates of CI in AFMs, using theoretical studies based on the first-principles calculations. We have been focused on the buckled honeycomb lattices, consisting of (111)-oriented cubic perovskite on $SrTiO_3$ substrate. Our results show nonzero Chern numbers in one spin channel. It is expected a CI state to be emerged by tunable external electric fields in this AFM system.

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Correcting DFT problems for the spin-state of transition metal complexes

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We present calculations for small transition metal complexes using a recently proposed density-corrected density functional theory (DC-DFT) method[1]. Despite its efficiency and reasonable accuracy, density functional theory (DFT) is known to be inaccurate in problematic cases like spin-state changing system. In case of transition metal systems, DFT fails to give accurate spin states consistently and the energy difference between high spin and low spin states are inaccurate. Since controlling spin states in transition metal systems experimentally is extremely difficult, one needs to use computationally costly methods like coupled cluster and quantum Monte Carlo in order to predict preferred spin states. Here we show Hartree-Fock DFT (HF-DFT), one of the simplest ways to perform DC-DFT, gives prediction in spin states with accuracy comparable to coupled cluster results while its computation cost is similar to DFT. In HF-DFT, one evaluates DFT energy on HF densities which results in reducing density-driven error compared to conventional DFT calculation, and has shown promising results in open-shell systems. We believe such improvement in transition metal systems could be expanded to obtain correct spin-densities at no more cost than standard DFT approximations and ultimately to determine magnetization.

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Structural and electronic properties of α-Te tubular nanostructures: A first-principles study

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We employed density functional theory to investigate the structural and electronic properties of α-Te tubular nanostructures. These α-Te tube-like structures, similar to that of carbon nanotubes, in armchair and zigzag types are semiconductors with moderate band gaps. The nanotubes in armchair configurations have an indirect-to-direct band gap transition as tube diameter is decreased to a specific critical tube size, while those in zigzag configurations are always semiconductors with direct gap independent of the tube diameter. The calculated projected density of states reveal that such an indirect-to-direct band gap transition found in armchair nanotube can be attributed to the contributions of the different p-orbitals near the VBM edges. These findings are not only helpful for better understanding the physical characteristics of α-Te nanotubes, but also will open up the possibility of its use in device applications.

Heteroatom effect on electronic and photophysical properties of 3-hydroxyquinolin-4(H)-one and its analogues enhancing in the excited-state intramolecular proton transfer processes: A TD-DFT study on substitution effect

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The effect of hetero oxygen and nitrogen substituted of 3HX derivatives (3HQ, 3HF, 3HTF, and 3HSO where X=NH, O, S, and SO_2 respectively) on the electronic, photophysical properties, and excited-state intramolecular proton transfer (ESIPT) was investigated using density functional theory (DFT) and time-dependent DFT (TD-DFT). Geometries and absorption spectra as well as emission spectra of 3HX derivatives were carried out by using DFT and TD-DFT at the B3LYP/TZVP level. The important parameters for bond distances involving the intramolecular H-bond reveal that H-bonds of 3HX derivatives in excited-state are stronger than those in the ground state, supported by the red-shift of O–H vibrational modes in the excited-state. The heteroatom substitution of 3HX causes the red-shift emission spectra, implying that the lone pair of electron in the substituted heteroatom has the effect on the intramolecular charge transfer. In addition, results of frontier molecular orbitals show that vertical $S_0 \rightarrow S_1$ transition of these molecules corresponds essentially to the excitation from HOMO (π) to LUMO (π*). The potential energy curves (PECs) of intramolecular proton transfer (IntraPT) process of all derivatives were used to investigate the occurrence of ESIPT. The hetero sulfur on X positions of 3HX derivatives could easily facilitate the ESIPT process because sulfur makes O_1–H_1 bond of 3HTF weaker than those of other derivatives confirmed by its more red-shifted vibrational modes in the excited-state compared with other heteroatom substitutions, resulting in lower ESIntraPT barrier. The obtained information of the electronic structure, the photophysical property and the chance of ESIPT of heteroatom substituted 3HX molecules are useful for the molecular design of fluorescent molecular probes.

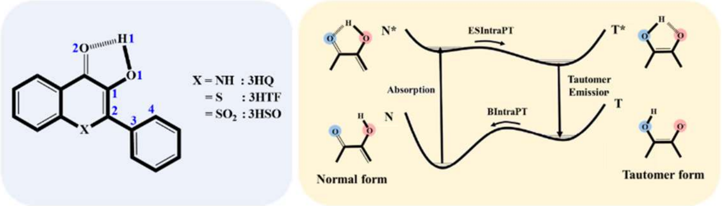

Figure. Schematic of 3HQ, 3HF, 3HTF, and 3HSO and Schematic diagram of the general ESIPT process, a proton donor and proton acceptor are circled with red and blue, respectively.

Keywords: Excited state proton transfer (ESPT), 3-Hydroxyquinolin-4(H)-one, Heteroatom effect, B3LYP

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First-Principles Study of Phonon Anharmonicity in $CsPbBr_3$

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Halide perovskites ABX_3 (A=CH_3NH_3,Cs; B=Pb,Sn; X=Cl,Br,I) have attracted significant attention in recent years for their excellent optoelectronic properties. Both organic-inorganic (A=CH_3NH_3) and all-inorganic (A=Cs) halides perovskites have been investigated for potential applications in light- and energy-harvesting devices such as photovoltaics and thermoelectrics. Recent experimental studies have shown that the lattice thermal conductivity κ_L of $CH_3NH_3PbI_3$ is unusually low (~ 0.5 W/mK), which was attributed to the rotational motion of the guest molecule. However, a similar value of κ_L has also been reported in $CsPbX_3$, which is free from the rotational degree of freedom of the guest molecule. While several theoretical studies on $CsBX_3$ have been reported so far, the origin of the ultralow κ_L is still an open question.

To elucidate the microscopic origin of the ultralow κ_L of halide perovskites, we have investigated phonon anharmonicity and thermal conductivity of $CsPbBr_3$ by using accurate first-principles methods. To see the effect of the structural phase transition on phonon anharmonicity, we have compared thermal conductivities of three different phases of $CsPbBr_3$: cubic, tetragonal, and orthorhombic (see Fig.). For the high-temperature phases, we have conducted the self-consistent phonon (SCP) calculations [1,2] to obtain the well-defined stable phonons at finite temperature. We will show the temperature dependence of phonon frequencies and lattice thermal conductivity of $CsPbBr_3$ and discuss the origin of the ultralow κ_L.

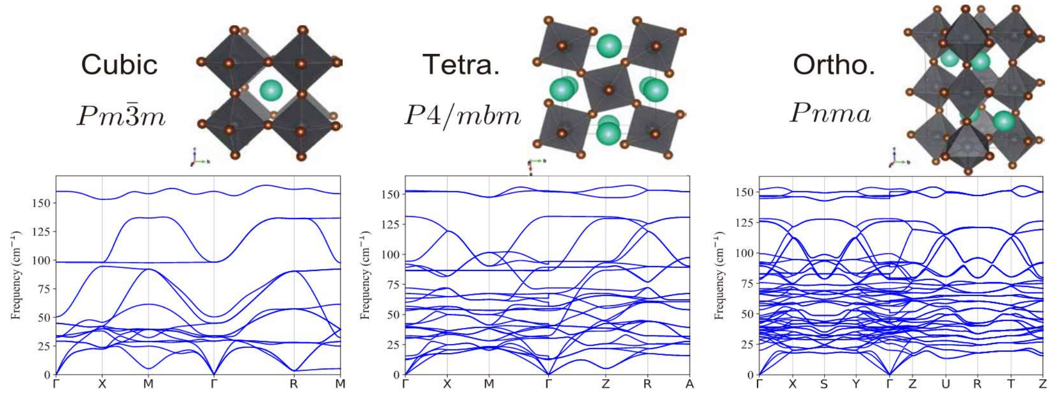

Figure: Calculated phonon dispersion curves of three phases of $CsPbBr_3$.

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Variance of GNR FET characteristics caused by Anderson localization phenomena

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Graphene is expected to be a channel material of field effect transistors (FETs) because of its high carrier mobility. However, no band gap of the graphene is a serious problem for its FET application. One possible way to overcome the gap-opening problem is to process it in the form of a nanometer width ribbon, referred as graphene nanoribbons (GNRs). They have been successfully applied to FETs with high on-off ratio. Although the resistance of GNR is known to increase dramatically with edge disorder[1][2], the effects of edge roughness on the FET characteristics (e.g., on-off ratio and subthreshold) have not been clarified yet.

In this study, we have investigated the coherent electronic transport in edge-disordered armchair GNR FETs (ED-AGNR-FETs) using the nonequilibrium Green's function method combined with a tight-binding model[3]. In our simulation model, the edge roghness is modeled by adding or removing pairs of carbon atoms at the edges (Fig. 1). We calculated drain current(I_d) versus gate voltage(V_g) characters of ED-AGNR-FETs by changing the roughness concentration P from 0% to 30% and the ribbon-width from 2.21nm (Fig. 2). We confirmed that average values of device characteristics deteriorated with increasing of P. However, even for P = 30%, some GNR-FETs show that sub-threshold slope values are smaller than 60mv/dec which is the limit value of planer FET as considered here. Furthermore, we investigate optimal position of edge roughness to improve FET characteristics.

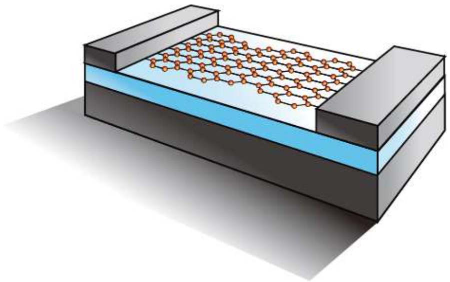

Fig. 1 Edge-disordered AGNR-FET

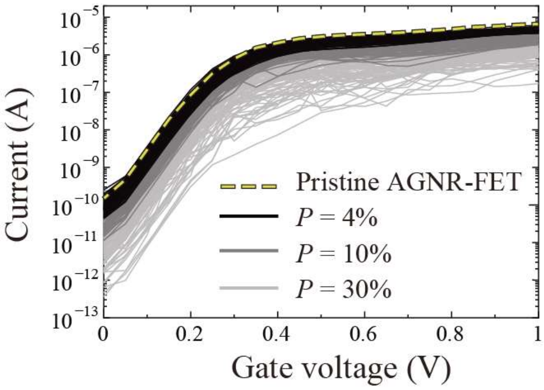

Fig. 2 I_d-V_g curves of edge-disordered AGNR-FETs

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Poster-105

Poster-106

Surface effects in the (001) $BaTiO_3$ ferroelectric slab from first-principles calculations and phase field simulation

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We have investigated out-of-plane polarization in the (001) ferroelectric $BaTiO_3$ slab using first-principles and phase-field calculations. In the phase-field simulation, the change of polarization near the surface by the surface relazation effect has been modeled using an extrapolation length. The effects of $BaTiO_3$ slab size, surface terminations (BaO and TiO_2 terminated surfaces) and value of extrapolation lengths have been obtained from ab initio calculations on the basis of density functional theory. By combining with phase field simulation based on Landau-Ginzburg theory[1], it was found that the polarization of ferroelectric thin films is dependent fully on the extrapolation length of films.

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Poster-107

Secondary Electron Emission from Multi-layer Graphene by TDDFT Simulations

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Scanning Electron Microscopy (SEM) that observes secondary electron emission (SEE) has great achievements in surface science. However, the physical interpretation of SEM images, especially, of atomic sheets such as graphene is not clear. Some experiments comparing the amount of SEs before and after coating graphene on the substrates have been reported, and it has been found that graphene coating decreases the amount of SEs[1-3]. However, the mechanism of SEE from graphene itself is totally unkown because it is difficult to distuinguish experimantaly SEE of the graphene from that of the substrates. Therefore, a theoretical study of SEE from graphene is worth doing for clarifying the underlying mechanism of SEE leading to the SEM images.

A time-dependent density functional theory (TDDFT) simulation in real time has been successfully applied to electron wave-packet scattering by graphene in our previous studies[4-7]. The present TDDFT study enables a fully dynamic description of both the target and incident electrons, which is necessary for modeling nanostructures. Compared with the conventional scattering theory, the TDDFT method has an advantage in that multiple and inelastic scatterings are *automatically* included in the simulations.

In this study, we investigated SEE of multi-layer graphene (MLG) by the TDDFT simulations, and determined the incident energy dependence and the layer-number dependence of SEs from MLG. The amount of SEs tends to converge to a certain value with the increase of the number of layers, especialy, upon low-energy (< 200 eV) electron impact. The convergence originates from attenuation of incident electron and relationship between the amount of bound excited electrons and total excited electrons[8]. Finally, we determined the SEE of bulk graphite that is comaparable to the experiment[9].

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Defective SnS monolayer as a candidate for long-range ferromagnetism

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We investigate the formation and migration of vacancies at both tin (Sn) and sulfur (S) sites in SnS monolayer using first principles calculations. Since the vacancy formation at the Sn site (4.75 eV/Sn) is more probable than that at the S site (6.03 eV/S), we expect that the Sn vacancies will be more likely to be observed in experiments. Due to the high vacancy migration energy barrier, we expect that the S vacancy will remain at the position where it is created, reducing the formation of vacancy clusters. SnS monolayer remains non-magnetic with the creation of both Sn and S vacancies. To induce magnetism in SnS, we replace Sn with transition metals (TMs = Mn, Fe, Co) and find a significant influence on the electronic and magnetic properties of monolayer SnS. The doping of TM alters the non-magnetic nature of SnS monolayer into magnetic one, but keeps it semiconducting. Additionally, long-range ferromagnetic behaviors are observed for all the doped systems. Hence, the addition of TM in monolayer SnS could be a promising process to realize two-dimensional diluted magnetic semiconductors. More interestingly, all the doped configurations show a high spin state, which can be used in nanoscale spintronic applications such as spin-filtering devices. [1,2]

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Thickness Dependent Electronic Properties of Pt Dichalcogenides – PtX_2 (X = S, Se, and Te)

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Using first-principles calculation, we explore the tunability of the electronic properties of PtX_2 (X = S, Se, and Te) with respect to the film thickness. We examine different known structures, including 1T, 2H, and 3R. For bulk and layered structures (1 to 10 layers), octahedral 1T is the most stable. Surprisingly, we also find that the 3R structure has comparable stability relative to the 1T, implying possible synthesis of 3R. For a bulk 1T structure, PtS_2 is semiconducting with an indirect band gap of 0.25eV, while $PtSe_2$ and $PtTe_2$ are both semi-metallic. Still, all their corresponding monolayers exhibit an indirect semiconducting phase with band gaps of 1.68eV, 1.18eV, and 0.40eV for PtS_2, $PtSe_2$, and $PtTe_2$, respectively. For the layer dependence of band properties, we observe that all PtX_2 transition metal dichalcogenides (TMDs) manifest decreasing/closing of indirect bandgap with increasing thickness, a consequence of quantum confinement and interlayer interaction. Moreover, we discover that applying strain can manipulate van Hove singularity resulting to high density of states at the maximum valence band. Our results show that the sensitivity and tunability of electronic properties of PtX_2 pave a new path for future potential applications.

Poster-110

Poster-111

Local work functions of clean tungsten surfaces under electric fields based on *ab initio* calculations

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Tungsten, the common choice for vacuum tube filaments, can survive under high temperatures and provide thermionic emission of electrons. However, the emission is largely limited due to its relatively high work function (approximately 4.5 eV). First principles or *ab initio* calculations are used to study the local work functions of tungsten (W) clean (100), (110), and (111) surfaces under external electric fields. The authors carefully and systematically tested the convergence of density-functional-theory (DFT) calculations in the local-density approximation (LDA) or generalized-gradient approximation (GGA) with a plane-wave basis set the projector-augmented wave method as implemented in the Vienna *ab-initio* simulation package (VASP). Several pseudopotentials have been tested for comparion. With the tungsten model under electric fields applied on both sides, we can investigate the dependence of the local work function and effective work function on field strength. In addition to thermionic emission, tungsten has been considered for use as a field emission (FE) electron source.

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Prediction of Large-Gap Topological Insulator in Functionalized Ordered Double Transition Metal MXene

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MXenes have become popular 2D materials in the recent years owing to their various composition and surface functional possibilities. Though numerous MXenes were predicted to possess topological properties [1-3], the exploration of topological phase in MXenes is still ongoing. Here, we conduct a rigorous search study on V_2TiC_2 with various surface terminations, X_2 (X = F, Cl, I, Br, O, H, and OH) using first-principles calculations. We find that $V_2TiC_2F_2$ is a topological insulator determined from the calculations of the topological invariant and the parities of wave functions at the time reversal invariant momentum (TRIM) points of the Brillouin zone below the fermi level. It has a non-trivial band gap of 40 meV and 251 meV using GGA and hybrid functionals, respectively. Further analysis shows that majority of the contribution of band inversion are from the *d*-orbitals of V atoms. We also find that $V_2TiC_2F_2$ remains a robust topological insulator against tensile strain up to 19%. The combined unique properties of topological insulators and MXenes makes it a valuable 2D material worth of further study with a potential to play an important role in the development of technology.

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First principles study on electronic properties of magnetite for spin polarized electron emission

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Magnetite is a mineral and one of the main iron ores. With the chemical formula Fe_3O_4, it is one of the oxides of iron. Magnetite is the earliest discovered magnet, around 1500 B.C. It crystallizes in the inverse cubic spinel structure (Fd3m) above the so-called Verwey transition temperature which is about 120 K. It has been found that a high temperature phase magnetite has a negative polarization of 100% at the Fermi surface, i.e., near the Fermi surface, only the spin down subband exists and the spin-up subband is far away from the Fermi surface. As a half-metallic material, Fe_3O_4 shows normal metallic behavior in the minority spin, while at the same time there is a gap of about 0.5 eV in the majority spin at the Fermi level. Although extensive studies of magnetite with considerable effort have been carried out over the past decades, the interesting electronic, magnetic, and transport properties as well as the potential industrial applications in magnetic multilayer devices, magnetite has still attracted much attention in recent years. In this work, we study the electronic properties of magnetite using first principles or *ab initio* calculations based on density functional theory in order to investigate a spin polarized electron emission. The work functions of magnetite Fe_3O_4 on different surfaces have been determined. In addition, local work functions have been analyzed and the correspondences with electron charge density distribution have been found. With this approach, one can investigate spin polarized properties of different materials such as ferrite accurately and efficiently. The magnetite as a half-metal can possibly be used as a field emitter for generating a spin polarized electron emission which may help in future analysis of noninvasive surface probes for biological systems or nanoelectronics.

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Poster-114

First-Principles Study on Surface States of Rocksalt SnSe

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The rocksalt SnSe compound is known as the topological crystalline insulator in which the gapless surface state is protected by the non-trivial mirror Chern number of (110) mirror plane. In the absence of the spin-orbit coupling, however, it becomes a topological nodal line semimetal. The nodal line is a line of degenerate points in the k-space between the conduction and the valence bands. In this study, we explore the nodal line structure in rocksalt SnSe. We calculate the Zak phase of SnSe and verify that the Zak phase is quantized and jumps by π at the nodal line, which is consistent with Ref. [2]. Zak phase is a Berry phase integrated along the straight line in Brillouin zone. Recently, the bulk boundary correspondence for nodal-line semi-metal using Zak phase was suggested that there is drum-head like flat surface band in the region of π-Zak phase. However, some exceptions was also reported. In that context, we calculate the surface states of SnSe with and without spin-orbit coupling and check the bulk-boundary correspondence. Further, we explore the condition such as passivation and relaxation that reproduces the experimentally observed Dirac cone at gamma-bar point of SnSe (111) surface. There is no surface state at gamma-bar point in the calculation of pristine SnSe.

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Electrochemical potential profiles within non-equilibrium nanoscale junctions from first principles

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Reliable first-principles simulations of nonequilibrium junction systems at finite bias voltages is highly desirable for the understanding of open quantum systems and development of next-generation nano-electronic/energy/bio devices. While the non-equilibrium Green's function (NEGF) formalism based on density functional theory (DFT) output has been established as the standard approach for this purpose in the past decade or so, it suffers from several intrinsic shortcomings. We have recently developed a multi-space constrained search density functional theory (MS-DFT) formulation for nonequilibrium quantum transport calculations and revealed the atomistic origins of negative differential resistance appearing in van der Waals heterojunction transistors based on graphene electrodes [1]. In this presentation, taking molecular junctions as test systems, we first systematically compare DFT-NEGF and MS-DFT and establish the practical equivalence between the two formalisms. An important feature of MS-DFT that differentiates it from DFT-NEGF is that it relies on the determination of electrochemical potentials or quasi-Fermi levels across the channel, which are not explicitly provided within DFT-NEGF unlike their electrostatic potential counterparts. Analyzing the spatial profiles of electrochemical potentials for different molecular channel cases, we extract important insights into the nature of nonequilibrium quantum transport in nanoscale devices. The integrated microscopic information will provide critical insights on the biased nanoelectrode interfaces, opening new avenues toward the study of nano-electronic/energy/bio devices.

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Poster-116

Vibrational effects on the surface energy of III-V compound semiconductors using ab-initio thermodynamics

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The surface energy is important in understanding the surface structure and crystal shape which are crucial to design materials for various applications. The conventional density functional theory (DFT) provided a method to obtain the surface energy, γ, as a function of chemical potential, μ. One of the main difficulties of using $\gamma(\mu)$ is that it cannot be directly compared with the experimental results because (i) $\gamma(\mu)$ is the electronic energy difference of the ground state; (ii) it is almost impossible to control μ through the experimental variables of temperature (T) and pressure (P); and (iii) the surface vibrational and configurational entropy effects which are calculated as a function of T cannot be consistently combined with $\gamma(\mu)$.

We reccently estabilished a thorough method to calculate the surface energy as a function of T and P by combining DFT and thermodynamics [1]. In addtion, the surface energy including the effects of surface vibration was obtained for the typical III-V compounds, such as GaAs and InAs by considereing various reconstructions with different stoichiometry and bonding geometry. As a result, we confirmed that some reconstructions which are unstable in terms of electronic surface energy become energetically stable at high T due to the surface vibrational effects. The calculation results were compared with the previous experimental works and showed good agreements. Such a correspondence of the calculations and experiments for a given T and P has not been available in the previous DFT calculations.

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Analytic continuation via “domain-knowledge free” machine learning

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We present a machine-learning (ML) approach to a long-standing issue in quantum many-body physics, namely, analytic continuation. This notorious ill-conditioned problem of obtaining spectral function from Matsubara Green's function has been a focus of new method developments for past decades. Therefore, many crafty approaches exist; such as maximum entropy method [1,2], stochastic method [3], Pade’s approximation [4]. These approaches require a deep understanding of the details of the problem. We call this detail as ‘domain-knowledge’; such as physical/mathematical approximations and assumptions. Here we show that the ML-based kernel can be realized without ‘domain-knowledge’, using modern ML techniques [5], e.g. convolutional neural network (CNN) and Adam optimizers [6]. Furthermore, the ML-based kernel is more robust to noise from Green’s function. We will also examine the possibility of extending the ML-based analytic continuation to the matrix-valued continuation problem, which recently been tackled by maximum quantum entropy method (MQEM) [7]. Our results illustrate that the ML approach can be a new direction to solved ill-posed physical problem.

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First-Principles Density Functional Study in the Magnetically and Electrically Polarized Pt/CoO/ZnO

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Non-volatile and low-energy-consumption memory, for examples, Magnetoresistive Random Access Memory (MRAM) or Ferroelectric RAM (FeRAM), has been investigated for over ten years. Recently the junction of CoPt/MgZnO was fabricated and investigated as an interesting hybrid [1]. Atomic layer stacking of CoPt has a large magnetic anisotropy energy (MAE) because of large spin-orbit interaction (SOI), and wurtzite-ZnO can provide a spontenious electric polarization depending on its surface edge. The CoPt magnetic metal with ZnO-based tunnel junction is a candidate of materials for the new device hybridizing MRAM and FeRAM. The electronic structure at the ferromagnetic/ferroelectric interface is so mysterious that the mechanism of interaction between ferromagnetics and ferroelectrics has still been veiled.

We investigated electronic structure of Pt(111)/CoO/ZnO(0001) slab system by using a first-principles calculation based on density functional theory. The method covers the effects of magnetic and electric polarizations for slabs [2,3]. To analyse modulation with respect to the electric polarization direction of ZnO, we considered that two ZnO structures; Zn adjacent to CoO plane as P+, and O adjacent to CoO as P−. The in-plane lattice constant was fixed a ZnO value extracted from the bulk and we induced out-of-plane structural relaxation for P+ and P−, respectivly. After a self-consistent computation, we confirmed both a spin polarization in PtCo layer and a spontenious electric polarization of ZnO, simultaneously. The direction of P+ is toward CoO, and the direction of P− is opposite. In each resulting slab, the electric polarization of ZnO is cancelled out by the electrostatic potential to fulfill a Poisson's equation. The result shows that in P+ electrons around CoO tend to sweep out to ZnO side (electron depletion state). On the other hand, electrons in P− is attracted to CoO side (electron accumulation state). This is consistent with the number of electrons in Co atomic sphere. We also analysed partial density of states (PDOS). There are large exchange splittings in the PDOSs of Co and adjacent Pt. There is a large component in d-orbital of Co and d($3z^2$-r^2)-orbital of Pt around the Fermi energy. These states have large difference between P+ and P−. In particular, the peak of d($3z^2$-r^2)-orbital in Pt gets down across the Fermi energy from P+ to P−. These changes in electronic structure might contribute to a favor of in-plane easy axis because of a large SOI of Pt. In the presentation, we will discuss electronic structures like a multi-ferroic material in terms of ferromagnetic and ferroelectric properties in the interface.

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Poster-119

Performance information of first-principles codes in K computer

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HPCI (High Performance Computing Infrastructure) System including "K computer" [1] provides high performance computing services for scientists and researchers around the world. User selection and support is conducted by RIST (Research Organization for Information Science and Technology) in HPCI. As part of the user support, RIST has installed application software most commonly used in HPCI research projects. The installation status and usage information of each software are introduced [2].
I have measured the performance of first-principles codes in K computer as port of usage information. The performance information of Quantum ESPRESSO (PWscf) [3] for Titanium dioxide (TiO_2) is shown in Figure. I show not only the performance information but also efficient execution methods (e.g. specifying the runtime options) in K computer.

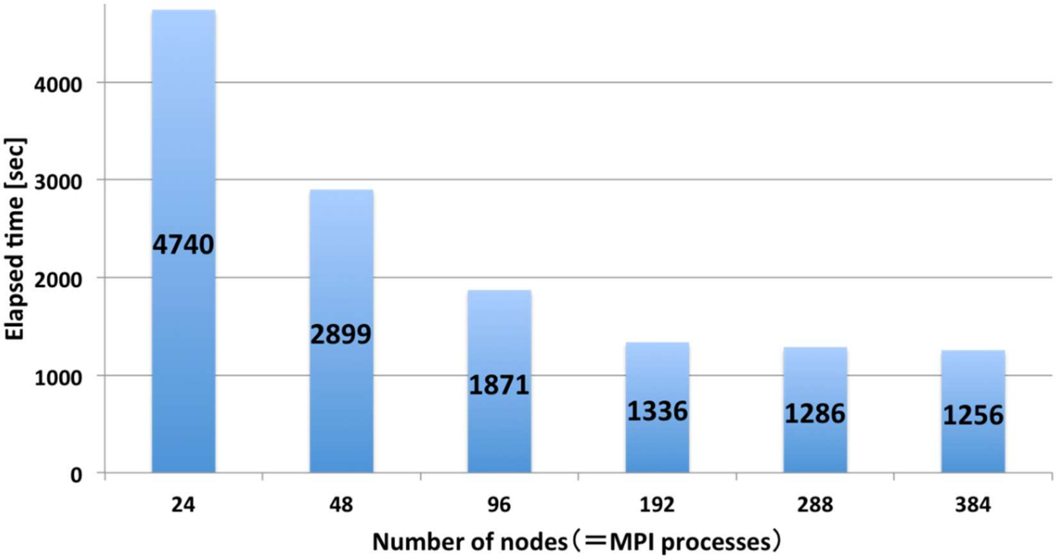

Figure: The performance information of PWscf v6.1 for addition of a hydrogen in rutile TiO_2 (217 atoms per unit cell). The hybrid parallel job running multiple processes and 8 threads.

[1] http://www.hpci-office.jp/folders/english.

[2] http://www.hpci-office.jp/pages/e_appli_software.

[3] http://www.quantum-espresso.org.

First principles study on electronic properties of graphene nanostructures for high current density cathode

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Graphene is a crystalline allotrope of carbon with two-dimensional properties. Its carbon atoms are densely packed in a nano-scale hexagonal pattern. Graphene has many unusual properties. It is about 200 times stronger than the strongest steel. It can efficiently conduct heat and electricity and is nearly transparent. In this work, we study the electronic properties of graphene using first principles or *ab initio* calculations based on density functional theory (DFT) in order to explore its applications in field emission devices. The electronic structure and density of states of graphene are calculated using both CPMD and VASP codes for comparison. The work function value is a key parameter and highly desirable for successful graphene applications in the field emisson research area. The change of work function due to the lattice deformation of graphene is investigated using a supercell including a vacuum layer which is thick enough so that the layer interaction is negligible. It is found that the work function is very sensitive to the lattice size. As the lattice site increases, the work function increases proportionally. However, the work function is reduced doubly while the lattice site is reduced. The local work function of graphene has also been determined and this can be used to predict field emission current from Fowler-Nordheim equation more accurately. For realistic applications, this approach has been used to calculate the work function of carbon nanoribbons with different widths and terminating edges with and without passivation.

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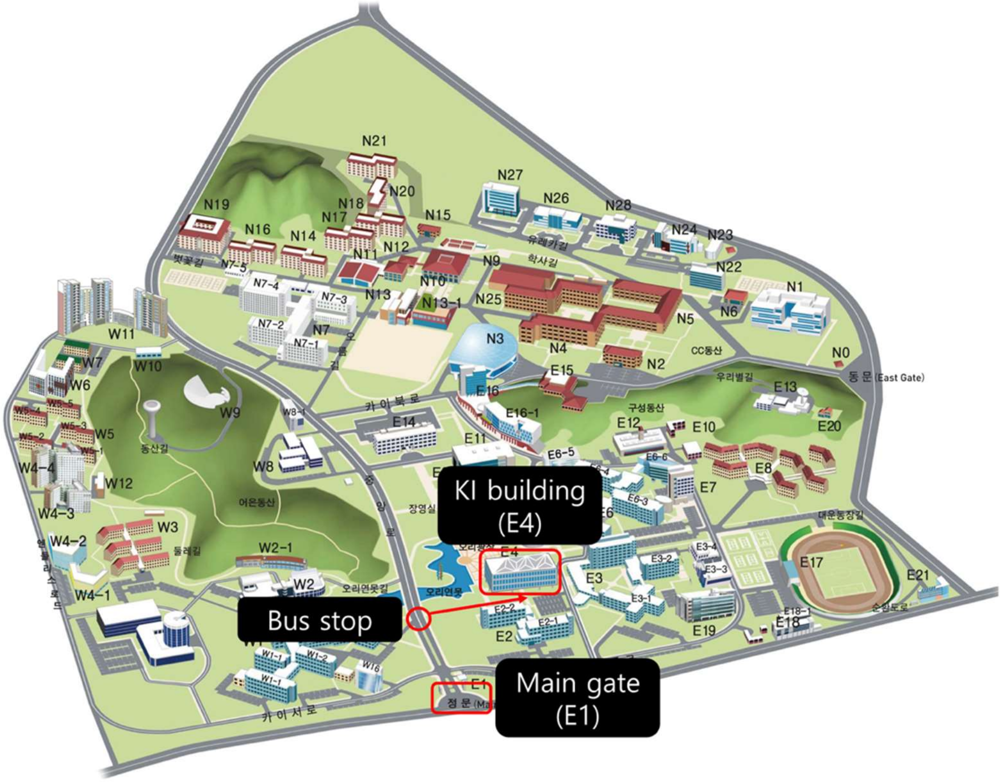
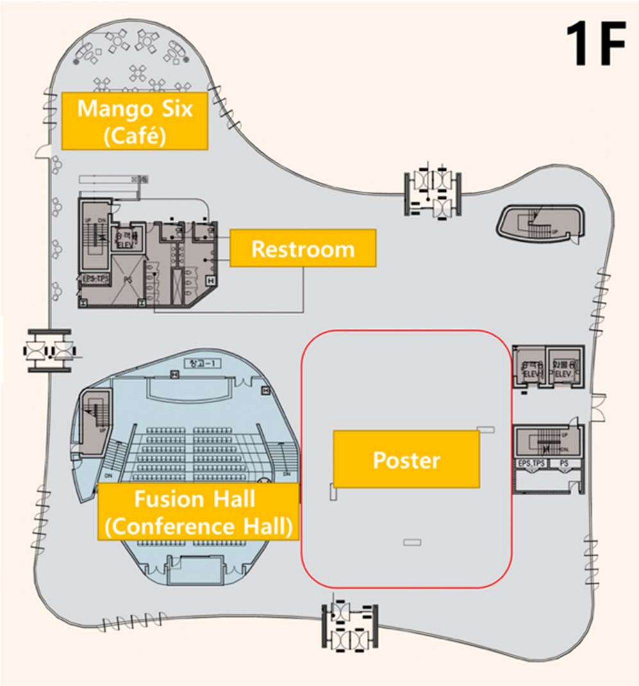
Information

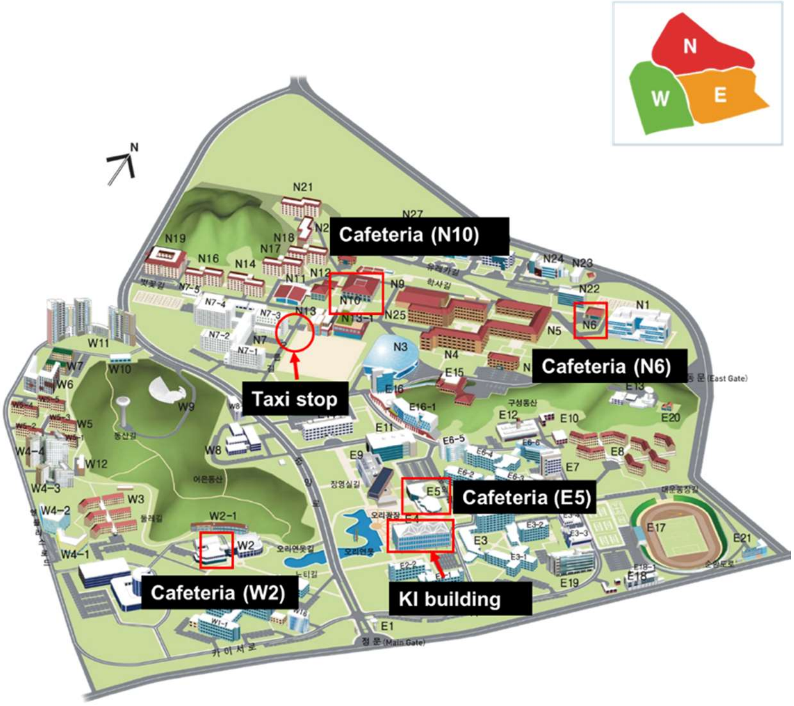
KAIST main campus map



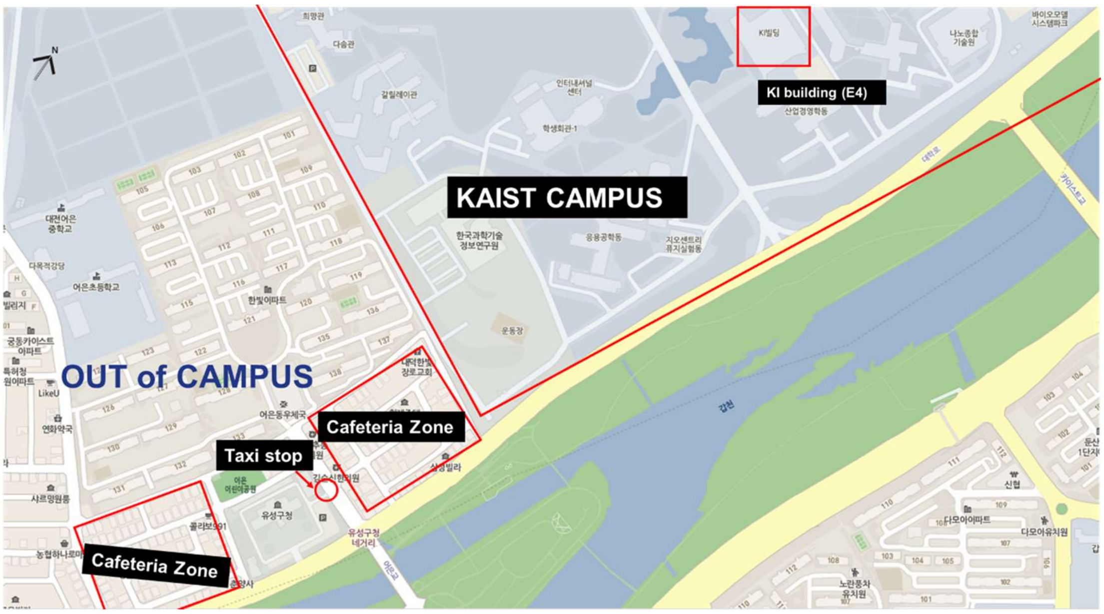
KAIST Institutes (KI) B/D map



On-campus cafeteria



Off-campus restaurants



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