Program

Oct. 28 (Monday)

(Registration@ Osaka University Hall) 8:30 – 17:00

(Welcome Session)

8:50 – 9:00 Opening Remarks

(Session 1) Chair: Kee Joo Chang (KAIST, Korea)

9:00 – 9:45 Stefan Blügel (Forschungszentrum Jülich, Germany)
Ab initio Spin-Orbitronics – From Spin-Orbit Interaction to Skyrmionics in real Materials

9:45 – 10:15 Ashis Kumar Nandy (National Institute of Science Education and Research, India)
Spin and Orbital Rashba-Edelstein Effect in Noncentrosymmetric Antiferromagnets

(Coffee Break) 10:15 – 10:45

(Session 2) Chair: Atsuto Seko (Kyoto University, Japan)

10:45 – 11:15 Chi-Hsuan Lee (National Center for Theoretical Sciences, Taiwan)
Topological surface states of thin films modulated with impurities

11:15 – 11:45 Chen Fang (Chinese Academy of Sciences, China)
Fast prediction of topological materials from first-principle calculations

11:45 – 12:15 Mikito Koshino (Osaka University, Japan)
Physics of twisted bilayer graphenes

(Lunch) 12:15 – 14:00

(Session 3) Chair: Mei-Yin Chou (Academia Sinica, Taiwan)

14:00 – 14:45 Feliciano Giustino (University of Texas at Austin, U.S.A.)
Polarons from First Principles

14:45 – 15:15 Osamu Sugino (University of Tokyo, Japan)
Density Functional Approach to Hydrogen on Electrode

(Poster Session) Chair: Kazunori Sato (Osaka University, Japan)

(Session 4) Chair: Ikutaro Hamada (Osaka University, Japan)

16:15 – 16:45 Chi-Cheng Lee (Tamkang University, Taiwan)
A Many-Body Approach for Calculating Absolute Values of Core-Level Binding Energies

16:45 – 17:15 Jian Sun (Nanjing University, China)
New materials and new states under extreme conditions

17:15 – 17:45 Seungwu Han (Seoul National University, Korea)
Atomic energy mapping of neural network potential

Oct. 29 (Tuesday)

(Registration@ Osaka University Hall) 8:30 – 17:00

(Session 1) Chair: Jaejun Yu (Seoul National University, Korea)

9:00 – 9:45 Silvia Picozzi (CNR-SPIN, Italy)
Spins meet electric dipoles: modelling, discoveries and perspectives

9:45 – 10:15 Heung-Sik Kim (Kangwon National University, Korea)
Dynamical magnetoelectric coupling and optical effect in Ni_3TeO_6: from ab-initio simulation of optical d-d excitation spectra

(Coffee Break) 10:15 – 10:45

(Session 2) Chair: Atsushi Togo (Kyoto University, Japan)

10:45 – 11:15 Tetsuya Fukushima (University of Tokyo, Japan)
Design of spintronics and magnetic materials by Korringa-Kohn-Rostoker Green's function method

11:15 – 11:45 Horng-Tay Jeng (National Tsing Hua University, Taiwan)
2 Dimensional Magnetic Semiconductors Based on Transition-Metal Dichalcogenides

11:45 – 12:15 Gil Young Cho (POSTECH, Korea)
Hidden Corner States in Quantum Spin Hall Flakes

(Lunch) 12:15 – 14:00

(Session 3) Chair: Isao Tanaka (Kyoto University, Japan)

14:00 – 14:45 Laurent Chaput (Lorraine University, France)
Ab initio calculations of the lattice thermal conductivity: the discovery of new materials and multi-scale modeling

14:45 – 15:15 Chee Kwan Gan (Institute of High Performance Computing, Singapore)
An efficient generalized Gruneisen method for a first-principles determination of thermal expansion coefficients for all crystal types

(Poster Session) Chair: Kazunori Sato (Osaka University, Japan)

(Session 4) Chair: Satoshi Watanabe (University of Tokyo, Japan)

16:15 – 16:45 Jin Zhao (University of Science and Technology of China, China)
Time Dependent Nonadiabatic Molecular Dynamics Investigations on the Excited Carrier Dynamics in Condensed Matter Systems

16:45 – 17:15 Yasushi Shinohara (University of Tokyo, Japan)
Real-time ab-initio simulations for crystalline solids driven by strong laser pulse

17:15 – 17:45 Sooran Kim (Kyungpook National University, Korea)
Apical Ion Dynamics-Modulated In-Plane Transport Properties of Cuprates

(Banquet @ Cafeteria in Campus)

Oct. 30 (Wednesday)

(Registration@ Osaka University Hall) 8:30 – 12:00

(Session 1) Chair: Atsushi Oshiyama (Nagoya University, Japan)

9:00 – 9:45 Bjørk Hammer (Aarhus University, Denmark)
Machine learning enabled structure optimization

9:45 – 10:15 Takahiro Ishikawa (NIMS, Japan)
Search for superconducting ternary hydrides by materials informatics based on evolutionary algorithms

(Coffee Break) 10:15 – 10:45

(Session 2) Chair: Yoshitada Morikawa (Osaka University, Japan)

10:45 – 11:15 Hyoung Joon Choi (Yonsei University, Korea)
Effect of surface doping on electron correlation in FeSe

11:15 – 11:45 Shiyou Chen (East China Normal University, China)
Effective Non-Radiative Recombination-Center Defects in Multinary and Low-Symmetry Semiconductors

11:45 – 12:15 Yoshitaka Tateyama (NIMS, Japan)
DFT Sampling Studies on Interface Ionics at Disordered Heterogeneous Solid-Solid Interfaces

(Closing Session)

12:15 – 12:30 Closing Remarks

Posters

P-1 Electronic structure of rare-earth nitrides calculated by quasi-particle self-consistent *GW* method
Kazunori Sato and Takao Kotani

P-2 Strain-induced electronic property modulation of monolayer tellurium: a first-principles study
Jinjin Wang, Yanrong Guo, Songyou Wang, Yu Jia and Wan-Sheng Su

P-3 Strain induced topological insulator phase in $CsPbBr_xI_{3-x}$ (x=0, 1, 2, and 3) perovskite: an *ab initio* study
Jen-Chuan Tung, Yu-Hsuan Hsieh and Po-Liang Liu

P-4 Noncollinear Spin Torque Effect in Magnetic Heterojunctions: Combined First-Principles Calculation and TB-NEGF Method
Yu-Hui Tang, Bao-Huei Haung, Chia-Chia Chao and Chao-Cheng Kaun

P-5 Metallic and Magnetic Edge States of $HfSe_2$ Nanoribbons
Hsin-Mei Ho, Kuan-Rong Chiang, Icuk Setiyawati and Yu-Hui Tang

P-6 Substrate-mediated umklapp scattering at the incommensurate interface of a monatomic alloy layer
Angus Huang, Santosh Chiniwar, W. W. Pai, S.-J. Tang and H.-T. Jeng

P-7 Electronic structure of a monoatomic Cu_2Si layer on a Si(111) substrate
C.-H. Chen, M. Cameau, R. Yukawa, A. Huang, H.-T. Jeng, M. D'angelo and I. Matsuda

P-8 Atomically precise bottom-up synthesis of π-extended [5]triangulene
J. Su, M. Telychko, P. Hu, G. Macam, P. Mutombo, H. Zhang, Y. Bao, F. Cheng, Z. Q. Huang, Z. Qiu, S. J. R. Tan, H. Lin, P. Jelínek, F. C. Chuang, J. Wu, J. Lu

P-9 Sparse sampling approach to efficient ab initio calculations at finite temperature
Jia Li, Markus Wallerberger, Naoya Chikano, Chia-Nan Yeh, Emanuel Gull and Hiroshi Shinaoka

P-10 Structure Perturbation in Black Phosphorus Driven by Atom Intercalation
Sheng-Hsiung Hung, Woei Wu Pai and Horng-Tay Jeng

P-11 Spinless Charged Particle Tunneling Effect under Uniform Magnetic Field
Shih-Chuan Lien, Bao-Huei Huang and Yu-Hui Tang

P-12 First-principles study on electric field control of magnetism in bilayer VI_3
T. P. T. Nguyen, K. Yamauchi, T. Oguchi

P-13 Origin of Dimeric and Trimeric Formations of NO on Cu(111) from Van der Waals Density Functional Calculations
Thanh Ngoc Pham, Yuji Hamamoto, Kouji Inagaki, Do Ngoc Son, Ikutaro Hamada and Yoshitada Morikawa

P-14 First-principles Study of Diamond Strain engineering
Chang-Ti Chou, Jyh-Pin Chou, Alice Hu, Yu-Chieh Lo

P-15 First-Principles Study of Piezoelectricity in Nanostructured Wurtzite Materials
Hiroyoshi Momida and Tamio Oguchi

P-16 The evidence of new unconventional antiferromagnetic accompanying with insulators and semi-conductors in double-perovskite $BiPbCrMnO_6$ and $BiPbCrTcO_6$
Po-Han Lee, Yu-Feng Chien, Po-Han Chen and Yin-Kuo Wang

P-17 Topology analysis for anomalous Hall effect in magnetic octupole Mn_3AN
Vu Thi Ngoc Huyen, Michi-To Suzuki, Kunihiko Yamauchi and Tamio Oguchi

P-18 First-principles study on the origin of structural stability of Mg-*M*-Y (*M* = Ni, Cu, Co, and Zn) alloys with long-period stacking ordered structure
Takao Tsumuraya and Tamio Oguchi

P-19 Direct and inverse magnetocaloric effects of FeRh alloy
Hung Tran Ba, Tetsuya Fukushima, Kazunori Sato and Tamio Oguchi

P-20 Electronic and Topological Properties in Layered Ternary Transition Metal Chalcogenides (ABX_4, A and B =Ti, Zr, or Hf; X=S, Se, or Te)
Ali Sufyan, Zhi-Quan Huang, Chia-Hsiu Hsu, Hsin Lin, Feng-Chuan Chuang

P-21 First-Principles Investigations on Photoabsorption Spectra of Oxyluciferin Anions in Aqueous Solution
Yoshifumi Noguchi, Miyabi Hiyama, Motoyuki Shiga, Hidefumi Akiyama and Osamu Sugino

P-22 First-principles calculation of superconductivity in hole-doped perovskite oxyhydride
Minjae Ghim, Nobuya Sato, Ryosuke Akashi, Seung-Hoon Jhi and Shinji Tsuneyuki

P-23 Magnetism and magneto-optical effects in bulk and multilayer CrI_3: An *ab-initio* study
Vijay Kumar Gudelli and Guang-Yu Guo

P-24 First-principles study on thickness dependent electronic properties of ZrX_2 (X = S, Se, or Te) thin films
Aniceto B. Maghirang III, John Symon C. Dizon, Rovi Angelo B. Villaos, Zhi-Quan Huang, Chia-Hsiu Hsu and Feng-Chuan Chuang

P-25 The origin of high-temperature ferromagnetism in (In,Fe)Sb
Hikari Shinya, Tetsuya Fukushima, Akira Masago, Kazunori Sato and Hiroshi Katayama-Yoshida

P-26 Magnetism and Charge Densiy Wave localized on One-Dimensional MoS_2 Grain Boundaries
Jun Jung, Yong-Hyun Kim

P-27 First-principles-based scanning Seebeck microscope simulation of epitaxial graphene on 6H-SiC
Euicheol Shin, Ho-Hyun Nahm and Yong-Hyun Kim

P-28 First-principles study on magnetism and phase stability of antiferromagnetic V_2 based Heusler alloys
F. Kuroda, T. Fukushima and T. Oguchi

P-29 First-principles magnetic dipole-dipole energy calculation: Application to magnetic chain, film, and bulk systems
Masao Obata, Indra Pardede, Daiki Yoshikawa and Tatsuki Oda

P-30 Spin-wave dispersion of 3*d* ferromagnets based on quasiparticle self-consistent *GW* calculations
Haruki Okumura, Kazunori Sato and Takao Kotani

P-31 A Novel Method of Removing Defects from α-T boron
K. Shirai, N. Uemura, J. Kunstmann, E. A. Ekimov, Y. B. Lebed

P-32 O_2-release and Structure Evolution of Layered $Li_{1.2}M_{0.4}M'_{0.4}O_2$ (M, M' = Cr, Mn, Ti) Cathodes for Li-Ion Batteries: First-Principles Calculations
Motoyuki Hamaguchi, Hiroyoshi Momida and Tamio Oguchi

P-33 A First Principle Study on Magneto-Optical effects and Magnetism in $Y_3Fe_5O_{12}$ and $Bi_3Fe_5O_{12}$
Wei-Kuo Li and Guang-Yu Guo

P-34 First-principles study of two-dimensional higher-order topology in monolayer graphdiyne
Rokyeon Kim, Eunwoo Lee, Junyeong Ahn and Bohm-Jung Yang

P-35 Understanding Ion Migration in Metal Halide Perovskites
Young-Won Woo, Young-Kwang Jung, Sunghyun Kim and Aron Walsh

P-36 Curvature-driven atomic localization and dipole alignment of quantum emitters in h-BN
Donggyu Yim, Mihyang Yu, Gichang Noh, Jieun Lee and Hosung Seo

P-37 A Strategy for Finding Better Oxygen-ion Conductors beyond Database
Joohwi Lee, Nobuko Ohba and Ryoji Asahi

P-38 First-principles Study of Superconducting Al-Zn-Mg Quasi-crystals: Comparison between 1/1 and 2/1 Approximants
Masaki Saito, Takuya Sekikawa, Yoshiaki Ōno

P-39 Accessing the Accuracy of Density Functional Theory through Structure and Dynamics of the Water–Air Interface
Tatsuhiko Ohto, Mayank Dodia, Jianhang Xu, Sho Imoto, Fujie Tang, Thomas D. Kühne, Yasuteru Shigeta, Mischa Bonn, Xifan Wu and Yuki Nagata

P-40 Control of Magnetic Interactions in Eu-doped GaN
Akira Masago, Tetsuya Fukushima, Hikari Shinya, Kazunori Sato and Hiroshi Katayama-Yoshida

P-41 Investigation of Interface Structures of Au(111)/Li_3PO_4 using High-Dimensional Neural Network Potential
Koji Shimizu, Wei Liu, Wenwen Li, Yasunobu Ando, Emi Minamitani and Satoshi Watanabe

P-42 Bulk Rashba Effect in Ferroelectric Transtion-Metal Oxides
Kunihiko Yamauchi, Paolo Barone and Silvia Picozzi

P-43 Topological crystalline insulator: from symmetry indicators to material discovery
Tay-Rong Chang, Hsin Lin and Liang Fu

P-44 The Oxidative Coupling of Methane Catalyzed by MgO; A First-Principle Based Microkinetics and Ab-initio Molecular Dynamics Study
A. Ishikawa and Y. Tateyama

P-45 First-principles theory of Cr-vacancy in $BaZrO_3$ as a solid-state qubit candidate
Jaewook Lee and Hosung Seo

P-46 Atomistic Study of Electronic Structure and Electron-Phonon Coupling in Twisted Graphene Layers
Young Woo Choi and Hyoung Joon Choi

P-47 First-Principles Calculation of DNA Energy Band Responsible for Superconductivity
Takuya Sekikawa, Hiroyuki Kawai and Yoshiaki Ōno

P-48 Oxidation of Diamond (100) Surface Studied Using Density Functional Theory
John Isaac Enriquez, Fahdzi Muttaqien, Masato Michiuchi, Kouji Inagaki, Ikutaro Hamada and Yoshitada Morikawa

P-49 Hydrogen Induced Caesium Desorption from Caesium-Decorated Tungsten(110) Surface
Allan Abraham B. Padama, Wilson Agerico Diño, Motoi Wada, Katsuyoshi Tsumori, Masashi Kisaki, Hideaki Kasai, Hiroshi Nakanishi, Mamiko Sasao and Nozomi Tanaka

P-50 Thermoelectric Properties of Nanoribbons of Phosphorene, Arsenene, Antimonene, and Bismuthene from Non-Equilibrium Green's Function Calculations
Masashi Yoshisato, Yasumitsu Suzuki and Kazuyuki Watanabe

P-51 Spin-Dependent O_2 Binding to Hemoglobin
Daiichi Kurokawa, Jessiel Siaron Gueriba, Wilson Agerico Diño

P-52 Structural investigation on ternary PdRuM (M=Pt, Rh or Ir) nanoparticles using first-principles calculations
Shih-Hsuan Hung, Taisuke Ozaki

P-53 Force Field Parameterization using Genetic Algorithm for Lithium-ion Battery Applications
Xichan Gao, Yoshitaka Tateyama and Kazuto Akagi

P-54 First-principles study on structures of crystalline Nd-Fe alloys as candidates for grain-boundary phases in Nd-Fe-B sintered magnets
Y. Ainai, Y. Tatetsu, A. Terasawa and Y. Gohda

P-55 Development of First-Principles Crystal Structure Search Method with High Precision and High Efficiency and Its Implementation
Masaaki Geshi and Hiroki Funashima

P-56 Intrinsic Doping Limit and Defect-Assisted Luminescence in Cs_4PbBr_6
Young-Kwang Jung and Aron Walsh

P-57 Machine Learning Kohn-Sham Density Functionals from Molecules
Ryo Nagai, Ryosuke Akashi and Osamu Sugino

P-58 Design of isostructural metal-insulator transition in VO_2
Bongwook Chung, Seulyoung Park, Daesu Lee, Si-Young Choi, Chang-Beom Eom and Jaichan Lee

P-59 Temperature Dependent Scattering Mechanism of ZrS_2 from First-principles Calculations
Hitoshi Mori, Masayuki Ochi and Kazuhiko Kuroki

P-60 Negatively charged carbon dimer defect as a potential spin qubit candidate in hexagonal boron nitride: an *ab-initio* study
Jooyong Bhang, Dong-gyu Yim, He Ma, Giulia Galli and Hosung Seo

P-61 Band gap engineered ternary semiconductor $Pb_xCd_{1-x}S$: first-principles study
Shang-Wei Lien, Tay-Rong Chang and Ming-Way Lee

P-62 First-principles study of Raman spactra of Yb silicates under pressure
Takafumi Ogawa, Noriko Otani, Taishi Yokoi, Craig A. J. Fisher, Akihide Kuwabara, Hiroki Moriwake and Satoshi Kitaoka

P-63 Anharmonicity and two-channel phonon transport in thermoelectric tetrahedrite
Terumasa Tadano and Koichiro Suekuni

P-64 AMP^2: A Package for Automated *Ab-initio* Calculation for Crystalline Materials
Yong Youn, Miso Lee, Changho Hong, Doyeon Kim, Kanghoon Yim, Yoshitaka Tateyama and Seungwu Han

P-65 Correlation effects seen in one-particle spectra by Green's function coupled-cluster singles and doubles method
Yu-ichiro Matsushita and Taichi Kosugi

P-66 Construction of Green's functions on a quantum computer: quasiparticle spectra of molecules
Taichi Kosugi and Yu-ichiro Matsushita

P-67 Why is the electronic density of states peaked in H_3S?
Ryosuke Akashi

P-68 AtomREM: Non-empirical seeker of the minimum energy escape paths on many-dimensional potential landscapes without coarse graining
Yuri S. Nagornov and Ryosuke Akashi

P-69 Enectrode potential at the metal electrode/electrolyte solution interface studied by DFT with reference interaction site method
Satoshi Hagiwara and Minoru Otani

P-70 Formic Acid Adsorption and Decomposition on the Cu(111) Surface : Monomeric and Polymeric Structures
S. E. M. Putra, F. Muttaqien, Y. Hamamoto, K. Inagaki, I. Hamada, Y. Morikawa

P-71 Antiferromagnetic topological insulator $EuSn_2P_2$
Hung-Ju Tien, Tay-Rong Chang, WeiWei Xie and Robert J. Cava

P-72 Machine learning analysis on tunnel magnetoresistance of Fe/disordered-$MgAl_2O_4$/Fe(001) magnetic tunnel junction
Shenghong Ju, Yoshio Miura, Kaoru Yamamoto, Keisuke Masuda, Ken-ichi Uchida and Junichiro Shiomi

P-73 Electronic structure characterization of $NiCo_2O_4$: QSGW *ab-initio* calculation
Hasan Al Rasyid, Masao Obata, Indra Pardede, Marleni Wirmas, Takao Kotani and Tatsuki Oda

P-74 First-principles study of Rashba effect in quantum well states of Ag/Au(111)
M. Kawamura, R. Noguchi, K. Kuroda, T. Kondo, T. Ozaki

P-75 Reaction of CO_2 and C on flat and step surfaces of Co metal
Yee Jie Wong, Nor Fazila Khairudin, Septia Eka Marsha Putra, Thanh Ngoc Pham, Abdul Rahman Mohamed and Yoshitada Morikawa

P-76 Strongly Fluctuating Atomic Volumes, Charges, and Stresses in BCC Multicomponent Alloys
Shoji Ishibashi, Yuji Ikeda, Fritz Körmann, Blazej Grabowski and Jörg Neugebauer

P-77 First-principles Study of the Interaction between Boron Nitride and H-terminated (111) Diamond Surface
Sushma Yadav and Tsuyoshi Miyazaki

P-78 First-principles analysis on superconductivity under strain in Li-intercalated bilayer MoS_2
Poobodin Mano, Emi Minamitani and Satoshi Watanabe

P-79 First-Principles Calculations of Point Defects and Proton Incorporation in Orthorhombic Perovskite $LaScO_3$
A.Taguchi, T. Ogawa, A. Kuwabara and C. A. J. Fisher

P-80 IrO_3 Desorbability of Iridium Alloys at High Temperatures from Thermodynamical Perspective
I. Seo, S. Yokota, Y. Imai and Y. Gohda

P-81 Calculated Large Seebeck Coefficients in Fe-doped Si-Ge Alloys
Ryo Yamada, Akira Masago, Tetsuya Fukushima, Hikari Shinya, Tien Quang Nguye and Kazunori Sato

P-82 Nuclear Quantum Effect for Hydrogen Adsorption on Pt(111)
Lei Yan, Yoshiyuki Yamamoto, Motoyuki Shiga and Osamu Sugino

P-83 Band Alignment and Reconstruction of ABO_3 (001) Surfaces
Ha-Jun Sung, Yasuhide Mochizuki and Fumiyasu Oba

P-84 Density Functional Theory-based Investigation of Nickel Selenide as an Electrocatalyst for Oxygen Reduction and Water Oxidation Reactions
Beatriz Andrea C. Tan, Ace Christian F. Serraon, Allan Abraham B. Padama, Ikutaro Hamada, Joey Ocon, Yoshitada Morikawa

P-85 First-principle calculation of superconducting transition temperatures of elemental transition metals including the effect of spin fluctuations
Kentaro Tsutsumi, Yuma Hizume, Mitsuaki Kawamura, Ryosuke Akashi and Shinji Tsuneyuki

P-86 Self-consistent first-principles method for extended Hubbard interactions
Sang-Hoon Lee and Young-Woo Son

P-87 Ground-State Structure Search for Pnictide Antiperovskites
Yasuhide Mochizuki, Ha-Jun Sung, Akira Takahashi, Yu Kumagai and Fumiyasu Oba

P-88 Single Platinum Atom Supported at Graphene Edges as a Promising Catalyst for CO Oxidation Reaction
Sasfan Arman Wella, Yuji Hamamoto, Ferry Iskandar, Suprijadi, Yoshitada Morikawa, Ikutaro Hamada

P-89 High Carrier Mobility of MoS_2 Nanoribbons Under Simultaneous Strain and Electric Field
Md Mokhlesur Rahman, Noki Lee, Saroj Kanal and Jaichan Lee

P-90 Classical Density Functional Theory Calculations of Distribution Function of Ne Liquid
Jun Haruyama and Osamu Sugino

P-91 Development of program code for the first-principles photoemission-spectrum calculation
Noriaki Hamada, Satoshi Nakamura, Kenta Takahashi and Tomohiko Saitoh

P-92 Impurity Diffusion via Nonadiabatic Charge State Change
Yoshiyuki Yamamoto and Osamu Sugino

P-93 Thickness and bilayer stacking dependence on the electronic properties of HfX_2 (X = S, Se, or Te)
Huynh Thi My Duyen, Gennevieve Macam, Harvey N. Cruzado, John Symon C. Dizon, Zhi-Quan Huang, Chia-Hsiu Hsu and Feng-Chuan Chuang

P-94 Structure Search and Property Analysis of Interfaces between Cathode and Solid Electrolyte in All-Solid-State Battery via DFT-CALYPSO Method
Bo Gao, Randy Jalem, Yanming Ma, Yoshitaka Tateyama

P-95 Parameter in a Descriptor for Efficient Crystal Structure Search Using the Bayesian Optimization
Nobuya Sato, Tomoki Yamashita, Tamio Oguchi, Koji Hukushima and Takashi Miyake

P-96 Theoretical Investigation on Vibrationally Enhanced Hydrogenation of CO_2 on Cu(111)
Fahdzi Muttaqien, Septia Eka Marsh Putra, Yuji Hamamoto, Kouji Inagaki, Ikutaro Hamada, and Yoshitada Morikawa

P-97 Crystal structure prediction of $Li(CB_9H_{10})$: an example of XRD-data-assimulated molecular dynamic simulation
Ryuhei Sato, Toyoto Sato, Toshiya Otomo, Shin-ichi Orimo and Shinji Tsuneyuki

P-98 Band Structure of Group IV-VI 2D Materials
A. Zaharo and M. Saito

P-99 First principles calculations of magnetocrystalline anisotropy of doped antiferromagnetic transition metal oxide
K. Miyamae, A.-M. Pradipto, T. Akiyama, T. Ito and K. Nakamura

P-100 First-principles Study of Anomalous Nernst Effect in The 2D Ferromagnetic Half-metal 1T-FeX_2 (X = Br, Cl)
Rifky Syariati, Susumu Minami, Hikaru Sawahata and Fumiyuki Ishii

P-101 First principals study for charge conductivity change due to the spin orbit coupling effect in metallic bilayer film system
Yutai Nagato, A.-M. Pradipto, T. Akiyama, T. Ito and K. Nakamura

P-102 Crystal Orientation Dependence of Lead Vacancy Stability and Defect State on $PbTiO_3$ Grain Boundary
Yuichi Motohashi and Takahiro Yamamoto

P-103 *Ab initio* study of contact behaviors at 2D/3D GaX(X = S, Se, Te)/Si(111) heterojunctions
Junghwan Kim, Kyung-Ah Min, Janghwan Cha and Suklyun Hong

P-104 Magneto-optical conductivity in 5d transition metal by first principles calculations
T. Shiraki, A.-M. Pradipto, M. Arifin, T. Akiyama, T. Ito and K. Nakamura

P-105 Spin-Polarized Cation Vacancies in Compound Semiconductors: First-principles Study
Muhammad Y. H. Widianto, Hana P. Kadarisman, Amran M. Yatmeidhy and Mineo Saito

P-106 Band alignment in graphene/WSe_2 heterostructures before and after oxygen plasma treatment
Janghwan Cha and Suklyun Hong

P-107 Implementation of computing anomalous Hall conductivity for high throughput screening of magnetic thermoelectric materials
Hikaru Sawahata, Naoya Yamaguchi, Susumu Minami and Fumiyuki Ishii

P-108 H_2 Nuclear Spin Transition on Metals: Physisorption Vs. Molecular Chemisorption
Elvis Arguelles, Koji Shimizu, Wilson Agerico Diño, Hiroshi Nakanishi and Hideaki Kasai

P-109 Large-scale DFT study on Pd@Ag core-shell nanoparticles
Ayako Nakata, David R Bowler and Tsuyoshi Miyazaki

P-110 Thickness dependent electronic structures of Pd dichalcogenides: a first principles study
Liang-Ying Feng, Rovi Angelo B. Villaos, Zhi-Quan Huang, Chia-Hsiu Hsu and Feng-Chuan Chuang

P-111 First-Principles Study of the Surface Alloys *M*/Ag (111)-$\sqrt{3}\times\sqrt{3}$ *R* 30°
Monika Nur, Naoya Yamaguchi and Fumiyuki Ishii

P-112 Diffusion of Carbon in α-Fe in the Presence of Vacancy
Tien Quang Nguyen, Ngoc Nam Ho, Kazunori Sato and Yoji Shibutani

P-113 Hydrogen on Reconstructed Gold Surface
Yuta Kataoka and Osamu Sugino

P-114 Electronic stress tensor density based on the quantum field theory in surface material systems
Masahiro Fukuda, Masato Senami and Tachibana Akitomo

P-115 Development and Validation of a Neural Network Potential for Identifying Stable Phases in the Y-Ti-O System
Ushio Matsumoto, Takafumi Ogawa, Craig A. J. Fisher, Satoshi Kitaoka, Hiroki Moriwake and Isao Tanaka

P-116 Intrinsic and anisotropic Rashba spin splitting in Janus monolayer transition metal dichalcogenides MXY (M = Pd, Te; X/Y = S, Se, Te)
Paul Albert L. Sino, Liang Ying Feng, Rovi Angelo B. Villaos, Zhi Quan Huang, Chia Hsiu Hsu and Feng-Chuan Chuang

P-117 Effect of External Electric Field on Methane Conversion on IrO_2(110) Surface: A Density Functional Theory Study
Chen-Hao Yeh, Thong Minh Le Pham, Santhanamoorthi Nachimuthu and Jyh-Chiang Jiang

P-118 Anisotropic Mechanical and Thermal Properties of Two Dimesional Borophene
Mehmet Emin Kilic and Kwang Ryeol Lee

P-119 Evaluation of solid-solution strengthening of alloys
R. Teshima, S. Yokota, Y. Imai and Y. Gohda

P-120 Jx: An open-source software for calculating magnetic interactions based on magnetic force theory
Hongkee Yoon, Taek Jung Kim, Jae-Hoon Sim and Myung Joon Han

P-121 A Study about the Possibility of Reducing Coercive Field in Pristine HfO_2 from the Ab-initio Calculation
Jinhyeong Jo, Hyun-Jae Lee, Hyemi Yang and Jun Hee Lee

P-122 First-principles Fully Relativistic Calculations of Insulators Under Finite Electric Fields by Using the LCAO Method
Naoya Yamaguchi and Fumiyuki Ishii

P-123 Cu_4 Complex in Silicon and Impurity Reaction between Cu_4 and Hydrogen
T. Fujimura and K. Shirai

P-124 First-principles calculation on defects in LiFeAs
Yushi Taruoka, Emi Minamitani and Satoshi Watanabe

P-125 Interlayer Exciton in WS_2
Dilna Azhikodan, Tashi Nautiyal and Sangeeta Sharma

P-126 First-principles study of van der Waals magnetic materials: CrOX (X = Cl, Br) bulk to monolayer
Juhyeok Lee, Seung Woo Jang, Hongkee Yoon, Yoon Gu Kang and Myung Joon Han

P-127 Logarithmic Violation of Mott Relation for Anomalous Nernst Effect
Susumu Minami, Fumiyuki Ishii, Motoaki Hirayama, Takuya Nomoto, Takashi Koretsune and Ryotaro Arita

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