List of Poster Presentations

Presenters assigned to **odd-numbered posters** are scheduled to present their posters on Monday, October 27, from 13:15 to 15:00. Those with **even-numbered posters** will present on Tuesday, October 28, during the same time slot. All presenters are kindly requested to remain at their assigned poster location for the entire duration of their session.

< DFT and Beyond DFT >

1. **Tunable In-Plane Anomalous Hall and Magneto-Optical Kerr Effect via Stacking Engineering in 2D Magnets**
   Li Huang (Southern University of Science and Technology)

2. **First-Principles Investigation of Defects in VSe_2**
   Hsuan Yu Kuan (National Taiwan University)

3. **Coupled Bogoliubov Equations of Electrons and Phonons**
   Chung-Yu Wang (Academia Sinica)

4. **Analysis of cRPA Methods for Calculating Hubbard *U* Parameters: A Comparative Study**
   Indukuru Ramesh Reddy (Kyungpook National University)

5. **Development of an *Ab Initio* Method for Non-coplanar Spin Texture and Topological Hall effect**
   Hsiao-Yi Chen (Tohoku University)

6. **Computational Discovery of Altermagnet CrO with Chiral Structural Features**
   Jieun Kim (Chungnam National University)

7. **Study on distinct charge density wave phases of LiVX2 (X = S, Se) within density functional theory**
   Jae Min Han (Chungnam National University)

8. **Analysis of Oxygen Vacancy Migration in 3*d* Transition-Metal Oxides via Modified Bond Valence Theory**
   Inseo Kim (Inha university)

9. **Identification of the shift current photovoltaic materials based on materials database: first-principles study**
   Jae Seong Lee (Soongsil University)

10. **Estimation of bcc-hcp Structural Phase Transition Temperatures from First Principles**
    Kota Hashimoto (Institute of Science Tokyo)

11. **First-Principles Study of Magnon in Altermagnet: Hexagonal FeS**
    Koki Kobayashi (Mie University)

12. **First-principles calculations of XMCD/XMLD: A case study for Fe/MgO, $D0_{22}$-Mn_3Ga and altermagnet RuO_2**
    Rikuto Takai (Mie University)

13. **Atomic Force Microscopy Imaging Simulation by Regional Chemical Potential Analysis with Distance Dependency**
    Masahiro Fukuda (The University of Tokyo)

14. **Flat Midgap States at Domain-wall Interfaces of 3D Stiefel–Whitney Insulators**
    Hongsik Shin (Sungkyunkwan University)

15. **Finite-temperature Density-functional Theory incorporating Three Types of Fluctuations**
    Go Tsuihiji (Metro, inc.)

16. **Direct determination of layer anomalous Hall conductivity using hybrid Wannier functions**
    Naoya Yamaguchi (Kanazawa University)

17. **First-Principles Calculation of Magnetization-Field Curves in $L1_0$-FePt Alloy**
    Ryoya Hiramatsu (National Institute of Advanced Industrial Science and Technology (AIST))

18. **Intrinsic Breakdown Strength: Theoretical Derivation and First-Principles Calculations**
    Shixu Liu (Fudan University)

19. **First-Principles Methods for Calculating Generalized Stacking Fault Energies in BCC Metals**
    Kazuhiko Ema (Kumamoto University)

20. **Diffusion Monte Carlo study on the photodetachment in Al_{13}^- anions and photoionization in Al_{13} neutrals**
    Meliton Chiong III (The University of Osaka)

21. **First-Principle Study of Topological Index in Finite System**
    Jingwen Yang (Kanazawa University)

22. **First-principles Calculation for Phonon dispersions of Polar Materials based on Self-screened Perturbations**
    Yoshihide Yoshimoto (The University of Tokyo)

23. **Reproducing Magnetization Easy-Axes in $RE_2Fe_{14}B$ by First-Principles Calculations**

Haruki Okumura (National Institute of Advanced Industrial Science and Technology (AIST))

24. **X-ray absorption spectroscopy calculation with the DFT-ΔSCF method**
Seokkyu An (The University of Tokyo)

25. **Current-Induced Transverse Spin and Orbital Magnetic Polarizations at Co/5d Heavy-Metal Interfaces**
Tomoki Ishihara (Mie University)

26. **Structural Analysis of SiO2 glass model using dimensionality reduction method**
Atsushi Tanaka (Nippon Electric Glass Co., Ltd)

27. **First-principles Calculation of Orbital Magnetization Using the Gauge-covariant Derivatives**
Shota Sasajima (Kanazawa University)

28. **Analytic Berry Connection (ABC) formula**
Taisuke Ozaki (The Univ. of Tokyo)

< Time-dependent DFT (TDDFT) >

29. **First-principles analysis of nonlinear optical response in silicon semiconducting nanostructures**
Mitsuharu Uemoto (Kobe University)

< Materials Informatics >

30. **Surface structure search for variable two-dimensional superlattice and composition**
Fumiaki Kuroda (National Institute of Advanced Industrial Science and Technology (AIST))

31. **Exploration of Anti-Perovskite-Type Solid Electrolytes by Combined High-Throughput DFT Calculations and Multi-Objective Bayesian Optimization Scheme**
Randy Jalem (National Institute for Materials Science (NIMS))

32. **First-Principles Inverse Magnetic Materials Design by Automatic Differentiation**
Kohei Ishii (The University of Tokyo)

33. **Exploration of High-Pressure Phases of Yttrium via a Data Assimilation Approach**
Yuuki Kubo (The University of Tokyo)

< Many-body Perturbation Theory >

34. **First ionization potentials from a first-principles self-interaction-corrected GWΓmethod**
Tamao Isago (Shizuoka University)

35. **Effects of Plasmon-Pole Models in Dyson's and Bethe-Salpeter Equations**
Yukitosameera Karunarathna (Shizuoka University)

36. **Time-Dependent *GW* Molecular Dynamics: A New Possible Paradigm for Accurately Traversing The Excited-State Dynamical Landscape**
Aaditya Manjanath (National Institute for Materials Science (NIMS))

37. **Multiplet Excitations of Transition Metal Luminescent Centers via the Quasiparticle Self-Consistent *GW* Method**
Harutaka Saito (The University of Osaka)

38. **Benchmarking Superconducting Transition Temperature through Fully Ab Initio Eliashberg Method**
Alwan Abdillah Darussalam (Tohoku University)

< Exchange-correlation Functional Development >

39. **A Computationally Efficient Nonlocal Descriptor for Machine-Learning Exchange-Correlation Functionals**
Ryo Nagai (Preferred Networks, Inc.)

< Machine Learning Potentials >

40. **Machine Learning Empirical Pseudopotentials for Total Energy and Electronic Energy Bands**
Sungmo Kang (Korea Institute for Advanced Study)

41. **The High-Value Thermoelectric Properties of Ruby-Silver Ores Ag3XS3 (X = As, Sb): A Combined Density Functional Theory and Machine Learning Approach**
Alfredo Ranes Coro III (National Sun Yat-sen University)

42. **Dynamically Training Machine Learning Based Force Fields for Strongly Anharmonic Materials**
Martin Callsen (Academia Sinica)

43. **Accurate Screening of Functional Materials with Machine-Learning Potential and Transfer-Learned Regressions: Heusler Alloy Benchmark**
Enda Xiao (National Institute for Materials Science (NIMS))

44. **Application of Machine Learning Potential to Design of Intermetallic Catalysts: Zn-doped PtCo**
Jae Hyun Ryu (Seoul National University)

45. **From atomic energy decomposition as a gauge to a theory of ionic thermoelectricity**
Byeoksong Lee (Daegu Gyeongbuk Institute of Science and Technology (DGIST))

46. **Development of Global Atomic Structure Descriptor**
Hyunwook Ha (Daegu Gyeongbuk Institute of Science and Technology (DGIST))

47. **Employing Machine Learning Molecular Dynamics to Probe Diamond Tool Degradation in Iron Cutting**

Bao-Anh Nguyen-Trinh (The University of Osaka)

48. **Understanding Cu/amorphous-Ta_xN Interfaces with Machine Learning Interatomic Potentials: Stoichiometry and Interface Construction Effects**
Jaehoon Kim (Seoul National University)

49. **r^2SCAN level universal neural network potential for diverse systems**
Chikashi Shinagawa (Preferred Networks, Inc.)

50. **Efficient Machine Learning Force Fields Building for Structural Relaxation of Magic-Angle Twisted Bilayer Graphene**
Shigetomo Yanase (Kanazawa University)

51. **An efficient forgetting-aware fine-tuning framework for pretrained universal machine learning interatomic potentials**
Jiho Lee (Seoul National University)

52. **Modeling water-triggered degradation pathways in Organotin materials using Deep Potential Molecular Dynamics**
Seungtae Kim (Seoul National University)

53. **Neural Network-Driven Molecular Insights into Alkaline Wet Etching of GaN: Toward Atomistic Precision in Nanostructure Fabrication**
Purun-hanul Kim (Seoul National University)

54. **Anomalous Water Penetration of Al3+ Dissolution**
Jihoon You (Seoul National University)

55. **Non-Equilibrium Molecular Dynamics of Li-Ion Conduction in $Li_{10}GeP_2S_{12}$ with Equivariant Neural Network Models of Interatomic Potentials and Born Effective Charge Tensors**
Saori Minami (Toyota Central R&D Labs., Inc.)

56. **Long-range-corrected Deep Potential Molecular Dynamics for Acid Dissociation in Water**
Rizka Nur Fadilla (The University of Osaka)

57. **Machine Learning Potential for Predicting Thermal Transport in Defective AlN**
Ying Dou (Institute of Science Tokyo)

58. **Simulating Electrochemical Interfaces under Bias Voltage Using an Ionic Charge Imbalance Method with a Universal Interatomic Machine Learning Potential**
Taisuke Hasegawa (Matlantis corporation)

59. **Modelling Nuclear Quantum Effects in Sub- and Supercritical Water**
Bo Thomsen (Japan Atomic Energy Agency)

60. **Stability of Intermetallic Phases from Universal Machine Learning Potential**
Wenhao Zhang (National Institute for Materials Science (NIMS))

61. **Crystal Structure Prediction with a Universal Machine Learning Interatomic Potential PFP and Efficient Search Algorithm for the Entire Convex Hull**
Yuta Aoki (Matlantis Corporation)

62. **Robust and Transferable Thermal Expansion Calculation with Refined Approximations and Universal Machine Learning Interatomic Potentials**
Yujin Will Kang (Seoul National University)

< Parallelization and HPC >

63. **Reducing Numerical Precision Requirements in Electronic Structure Calculations**
William Dawson (RIKEN)

< Workflow Automation >

64. **Advanced Automation of Crystal Structure Prediction using AiiDA**
Reo Morii (Nagaoka University of Technology)

< Multiscale Simulation >

65. **Spin-Cluster Expansion and its Application to Evaluating the Dzyaloshinskii-Moriya Interaction**
Tomonori Tanaka (Institute of Science Tokyo)

66. **Non-equilibrium Stochastic modeling and Molecular Dynamics Toward Ion Jamology**
Yasunobu Ando (Institute of Science Tokyo)

67. **Probing Photoluminescence of WSe2/AuNP Plasmonic Hybrid Nanostructures using FDTD simulation**
Hido Woo (Seoul National University)

< Other Methods >

68. **Prediction of accurate enough k-point samplings using machine learning**
Donggeon Lee (Sungkyunkwan University)

69. **Effect of Pressure on Silica Studied with Locally Averaged Atomic Fingerprints and Unsupervised Learning**
Anh Khoa Augustin Lu (The University of Tokyo)

70. **Machine Learning Model of Dipole Moments in Liquids Considering Long-Range Interaction**
Yutaro Okamoto (The University of Tokyo)

71. **Filling-Enforced Obstructed Atomic Insulators in Three-Dimensional Stacked Su–Schrieffer–Heeger Chains**
SungKyun Ahn (Sungkyunkwan University)

72. **Emerging Isotropic Chiral Interactions from Triangular Lattices**
Hiroshi Katsumoto (The University of Osaka)

73. **Qubit encoding of maximal-fidelity Lorentzian orbitals for quantum chemistry in real space**
Taichi Kosugi (Quemix Inc.)

74. **Imaginary Time Evolution for XAFS Spectral Calculations on a Quantum Computer**
Yu-ichiro Matsushita (The University of Tokyo)

75. **Real-space decomposition of longitudinal electrical conductivity in slab Bi_2Se_3 using the Closest Wannier function**
Jin Inoue (Kanazawa University)

< 2D Materials and Heterostructures >

76. **Surface-State-Driven Tunneling in hcp-Co/*h*-BN/hcp-Co Magnetic Tunnel Junctions**
Ivan Kurniawan (National Institute for Materials Science (NIMS))

77. **Metamorphic Quantum Dot Arrays in Twisted Trilayer Hexagonal Boron Nitride**
Kunihiro Yananose (Korea Institute for Advanced Study)

78. **A refined method for magnetic anisotropy energy calculation: Application to polarization control at a PtCoO/ZnO interface**
Takumi Katsuta (Kanazawa University)

79. **Transition-Selective Photocurrents in Floquet-Driven Monolayer $MoSe_2$**
Hongguk Min (Sungkyunkwan University)

80. **Phonon- and Charge-Transfer-Assisted Stabilization of Monolayer High-Entropy 1H-XS_2 Compounds**
Chi-Cheng Lee (Tamkang University)

81. **Dual Electronic Nature in Bulk and Monolayer 1T-$CrTe_2$: A Hund Metal with Self-Doped Double-Exchange Ferromagnetism**
Dong Hyun David Lee (Korea Advanced Institute of Science and Technology (KAIST))

82. **DFT calculation of High-Entropy MXene**
Rikuto Shogan (Yokohama National University)

83. **Effect of Strain and Interfacial States on Tunneling Magnetoresistance in van der Waals Cr_2C/TMDs/Cr_2C Magnetic Tunnel Junctions**
Sakshi Goel (Indian Institute of Technology Mandi)

84. **Computational Chemistry Insights into Substrate-Dependent Moisture Stability of Monolayer TMDCs**
Yeone Kim (Kumoh National Institute of Technology)

85. **Light-Wave Control of Selective Single Q-Valley Polarization in Transition Metal Dichalcogenides**
Youngjae Kim (Korea Institute for Advanced Study)

86. **Structural Stability and Electronic Properties of T-C_2N_1: A Novel T-Graphene Based Two-Dimensional Monolayer**
Sangho Yoo (Konkuk University)

87. **Bright Dipolar Excitons in Monolayer Ti_2SiCO_2**
Haozhe Li (Fudan University)

< Topological Materials >

88. **Reveling 2P Interlayer Excitons through Hybridization in Bilayer MoS_2**
Raj Kumar Paudel (National Cheng-Kung University)

89. **Atomic Reconstructions with Machine Learning Interatomic Potential and Electronic Structure of Twisted Bilayer WSe_2**
Syifa Fauzia Hariyanti Putri (Kanazawa University)

90. **First-Principles Study of Electronic Properties and Anomalous Hall Effect in Noble-Metal-Capped Fe(001) Surfaces**
Nur Anggita Sari (Kanazawa University)

91. **Strain Tuned Magnetic and Optoelectronic Properties of Monolayer CrS2 for CO2 Reduction A First Principles Approach**
PRASENJIT MONDAL (National Taipei University of Technology)

92. **First-Principles Calculation on Electronic Structures of NiFe/graphene heterointerface**
Naohiro Matsumoto (Kobe University)

93. **Revealing Orbital Chern Insulators in Two-dimensional Pnictogens by Orbital Topology**
Yueh-Ting Yao (National Cheng Kung University)

94. **Higher-fold topological excitations in phononic and electronic phases of chiral-type BaXY (X=Pt, Pd; Y= P, As, Sb, Bi) materials: a first-principles investigation**
Bibhash Paul (National Sun Yat-sen University)

95. **Topological Insulating Phase in Nonsymmorphic Bulk AX_2 (A = Ca, Sr, or Ba; and X = As, Sb, or Bi) Compounds**
Winda Purwitasari (National Sun Yat-sen University)

96. **Topological Dirac semimetallic phase in Heusler-type Li_2YZ (Y = Zn or Cd; and Z = Ge, Sn, or Pb) compounds: a first-principles investigation**
Fareeha Waheed (National Sun Yat-Sen University)

97. **Prediction Of Dirac Line Semi-Metallic Phase In HfSnTe: A First-Principles Study**
Fehmeeda no Shaheen (National Sun Yat-sen University)

98. **Ab initio Study on Linear Optics of Topological Kagome Materials: Optical Anisotropy, Magneto-Optical Effect, and Quantum Geometry**
Ming-Chun Jiang (RIKEN)

99. **Ab Initio Study of Nonlinear Optical Responses of an Ideal Weyl Semimetal: Cu_2SnSe_3**
Aatif Ahmad (National Taiwan University)

100. **Type-II Weyl Fermions in Chiral $NbSi_2$**
Hsuan-I Wu (National Cheng Kung University)

101. **Single Dirac band induced quantum metric non-linear Hall effect in $EuSn_2As_2$ thin films**
Tay-Rong Chang (National Cheng Kung University)

102. **First-principles calculations of weak-type Stiefel-Whitney insulators in two dimensions**
Sunam Jeon (Sungkyunkwan University)

103. **Tunable Magnetism and Anomalous Hall Response in Flat-Nodal-Line Fe_3GaTe_2**
Yoon-Gu Kang (Korea Advanced Institute of Science and Technology (KAIST))

104. **Normal Dirac Semimetal Phase and Zeeman-Induced Topological Fermi Arc in $PtSr_5$**
Inkyou Lee (Sungkyunkwan University)

105. **Microscopic Mechanism of Obstruction-Driven Strong Optical Absorption in Hexagonal Transition Metal Dichalcogenides**
Seungil Baek (Korea Advanced Institute of Science and Technology (KAIST))

106. **Tunable high spin Chern-number insulator phases in strained Sb monolayer**
Po-Yuan Yang (National Cheng Kung University)

107. **Topological Insulating Phases and Anisotropic Rashba Spin Textures in Monolayer Ternary Zintl Bismuthide ALiBi (A = Ca, Sr, Ba, Eu, or Yb)**
Aniceto III Balmes Maghirang (National Sun Yat-sen University)

108. **Persistent Thermoelectric Signal of Topological Edge States in Bilayer Graphene**
Jaeuk Seo (Korea Advanced Institute of Science and Technology (KAIST))

< Magnetic Materials >

109. **Theoretical Studies of Topological Properties in Self-intercalated Magnetic Systems**
Yusheng Hou (Sun Yat-Sen University)

110. **First-Principles Study of the Physical Properties of the Ferromagnetic Semiconductor (In,Fe)Sb**

Ryo Matsuzawa (The University of Tokyo)

111. **Tailoring Magnon Dirac Gap in 2D van der Waals CrI_3/As Bilayers: First-Principles Study**
Andi Gumarilang Cakti Ahmadi (Mie University)

112. **Proposal for new d-wave altermagnetic metallic candidates based on density functional theory calculations**
Jeong-Hyeon Park (Chungnam National University)

113. **Two-dimensional Magnetic Properties of EuOX (X=F,Cl,Br,I)**
Sheng Hsiung Hung (National Tsing Hua University)

114. ***Ab Initio* Study and Magnetic Symmetry Analysis of Altermagnetic Candidate Materials**
Kunihiko Yamauchi (The University of Osaka)

115. **Understanding Magnetism in $NiPS_3$: A First-Principles Study**
Pritam Sardar (National Taiwan University)

116. **Competing Layer-by-Layer Magnetic Anisotropy in Bulk and Ultra-thin Cr_2Te_3**
Wan-Sheng Tang (National Central University)

117. **Spin-Orbit-Driven Phenomena in Magnetic Materials**
Chu-Pu Lee (National Central University)

118. **Ab Initio Study on Magneto-optical Kerr Effect of Co-intercalated Transitional Metal Dichalcogenides $Co_{1/3}NbS_2$ and $Co_{1/3}TaS_2$**
Tsun-Sung Kuo (National Taiwan University)

119. **Voltage-controlled and perpendicular magnetic anisotropy in Fe/MgO system with Nitride and Fluoride interface modifications**
Masato Tsuchida (Mie university)

120. **First-Principles Investigation of Pressure-Driven Structural, Magnetic, and Electronic Changes in CrSBr**
Seulbi Kim (Kyung Hee University)

121. **Fractional Quantum Multiferroics from Coupling of Fractional Quantum Ferroelectricity and Altermagnetism**
MAOQIANG Dong (Fudan University)

122. **Dzyaloshinskii-Moriya Interaction in Helimagnet CrIX (X = Cl, Br) Monolayer: First-Principles Study**
Hanif Yuandi Widyandaru (Institute of Science Tokyo)

123. **First-Principles Study of the Stability of 120° and Inverse-120° Magnetic Structures in Mn_3X Noncollinear Antiferromagnets**
Kohei Kuwano (Tohoku University)

< Semiconductors >

124. **Sustainable Doping via Molecular Adsorption on Thin-film Semiconductor Bi_2O_2Se**
Tai-Ting Lee (National Taiwan University)

125. **Atomistic Insights into Hydrogen Migration in IGZO from Machine-Learning Interatomic Potential**
Hyunsung Cho (Seoul National University)

126. **Atomic Layer Deposition Simulation of Silicon Nitride Using Stochastic Parallel Particle Kinetic Simulator**
Woojin Kang (Seoul National University)

127. **Multistability of Interstitial Magnesium and Its Carrier Recombined Migration in Gallium Nitride**
Yuansheng Zhao (Quemix Inc.)

128. **Polaron Dynamics in TiO_2 from Hybrid Density Functional Theory and Machine Learning**
Christian S Ahart (Westlake University)

< Superconductors >

129. ***Ab initio* study on magnetism suppression, anharmonicity, rattling mode, and superconductivity in Sc_2MTe_2 (M = Fe, Co, Ni)**
Guang-Yu Guo (National Taiwan University)

130. **Ab initio many-body theory of superconductivity in electron-doped cuprate $La_{1.9}Ce_{0.1}CuO_4$**
Yun-Chen Liao (National Taiwan University)

131. **Evolutionary Search for Superconducting Phases in the La-N-B-H System under High Pressure**
Takahiro Ishikawa (The University of Tokyo)

132. **Finite-Temperature *ab Initio* Structural Optimization of the Bilayer Nickelate Superconductor $La_3Ni_2O_7$**
Ryoma Asai (The University of Tokyo)

133. **Spin Fluctuations in Hydride Superconductors from First Principles**
Shaocong Lu (The University of Tokyo)

< Oxides / Perovskites >

134. **First-principles Electron-Phonon Coupling Calculation of Tin Halide Perovskite**

Kazuki Morita (Helmholtz Zentrum Berlin)

135. **First-principles analysis for optical properties and one-particle spectra in transparent metal-oxide $LiTi_2O_4$**
Haruya Niwa (Kanazawa University)

136. **Structure Prediction of ABO_{3-x} Using Universal Machine Learning Potential and *Ab* Initio Calculations**
Yu Takatsuka (Nagaoka University of Technology)

137. **Electronic and Optical Properties of In_2O_3 Polymorphs from First Principles Calculations within GGA + *U* Frameworks**
Muhammad Arifin (Gadjah Mada University)

138. **Theoretical Elucidation of Local Atomic Structures and Colossal Permittivity Properties of Nb-doped TiO_2**
Dung Ngoc Dinh (The University of Osaka)

139. **Anisotropic Multi-centered Polarons in $BiVO_4$**
Seyeon Park (Kyungpook National University)

140. **First-principles study of strain effects and thickness dependence of electronic and magnetic properties in $SrRuO_3$ thin films**
Md Joynadul Hosain (Kanazawa University)

141. **Electronic structure and magnetic properties of doped $LaMnO_3$ under extreme strain**
Ju Hyeon Lee (Kyungpook National University)

142. **Theoretical Study on Dopant Effects in the Stability and Electronic Properties of Ti/Zr and TiO_2/ZrO_2**
Masato Fukushima (Hiroshima University)

143. **First-Principles Study of Anomalous Hall Conductivity in $La_{1-x}Sr_xMnO_3$ and $LaMnO_3/SrMnO_3$ Perovskites**
MUHAMMAD AHMED (Kanazawa University)

< Energy Materials (batteries, solar cells, thermoelectrics) >

144. **Hydrogen Storage in TM-Intercalated Bilayer Graphene with Mechanical Force-Driven Control of Binding Energy**
Jongdeok Kim (Konkuk University)

145. **Ion Diffusions Driven by Dynamic Lattice Deformations in Perovskite Solid Electrolyte**
Bo Gao (Jilin University)

146. **A density functional theory analysis of defect characteristics and transport properties in NiO**

Na-Young Lee (Sungkyunkwan University)

147. **Visualization of concerted ion migration in Superionic conductors**
Ryuhei Sato (The University of Tokyo)

148. **Electronic Band Gap of Kesterite Materials Predicted by Machine Learning**
Ji-Sang Park (Sungkyunkwan University)

149. **Active Learning-Guided Accelerated Discovery of Ultra-Efficient High-Entropy Thermoelectrics**
Wooseok Lee (Seoul National University)

150. **Enhanced Interfacial Kinetics and SEI formation of Single-Atom Cu-Modified Hard Carbon for Fast-Charging Li-ion Battery Anodes**
Minhee Park (Seoul National University)

151. **Exploring Lithium Superionic Behavior and Defect Tolerance in $LiNbOCl_4$ via Density Functional Theory Molecular Dynamics**
Halimah Harfah (National Institute for Materials Science (NIMS))

152. **Adiabatic Potential Barriers for Interlayer Cs and K Diffusion in Weatherd Biotite**
Rina Yabuta (Wakayama University)

153. **Li-ion Diffusion Mechanisms in $Li_{2-2x}Mg_{1+x}Cl_4$ Studied by Molecular Dynamics Simulations**
Kaito Kosugi (Nagaoka University of Technology)

154. **Microscopic insights into interfaces formed by $Li_{1+x}Al_xTi_{2-x}(PO_4)_3$ (LATP) electrolyte and its intermediate phases by ReaxFF molecular dynamics simulations**
Sudeshna Madhual (National Institute for Materials Science (NIMS))

155. **Operando-Style MD Structural Analysis of Li-ion Diffusion in the Solid Electrolytes $LiNbCl_6$ and $LiNbOCl_4$**
Wonzee Jung (Korea Institute of Energy Research)

156. **Molecular Dynamics with Machine-Learned Potentials: Metal Deposition on Carbon-Based Hosts in Anode-Free Batteries**
Moonwon Lee (Korea Institute of Energy Research)

157. **The Total Capacitance Profile of Dielectric Nanoscale Capacitor: First-Principles Study**
Ahmad Sohib (Kanazawa University)

158. **Structure and Ion Dynamics of Superionic Glass AgI-As_2Se_3 Investigated by Machine Learning Interatomic Potential**
Taisei Arakawa (Yamagata University)

159. **Mechanism of Na Cluster Formation and Na-ion Diffusion in Hard Carbon Nano-pores: a DFT-MD Study**
Che-an Lin (Institute of Science Tokyo)

160. **Framework Distortions and Coupled Ion–Polaron Transport in Prussian Blue**
Dan Ito (Waseda University)

161. **Anomalous blueshift in nitrile electrolyte: combined analysis of universal interatomic potential and quantum chemistry**
Ryoma Sasaki (Institute of Science Tokyo)

162. **Electric polarization-controlled of bulk photovoltaic effect in van der Waals Janus WSSe**
Yedija Yusua Sibuea Teweng (Kanazawa University)

163. **DFT Study of Interface between Hard Carbon Anode and Solid Electrolyte Interphase in Na-ion Battery**
An Niza El Aisnada (Institute of Science Tokyo)

164. **Various Magnetic Properties of Transition Metal Atoms doped $CoSb_3$ Thin Films**
Kazuaki Kobayashi (National Institute for Materials Science (NIMS))

165. **Structure Exploration and Electronic States Analysis of Argyrodite/Li-GICs Interfaces for All-Solid-State Battery**
Rikiya Mizobuchi (Institute of Science Tokyo)

166. **First-Principles Study on the Interlayer Coupling Effects in Thermoelectric Properties of Layered $CaGe_2$ and $CaSi_2$**
Ahmad Al Ghiffari (Kanazawa University)

167. **Molecular Dynamics Study on The Stokes-Einstein Picture of Highly Concentrated Electrolytes**
Riku Kitano (Institute of Science Tokyo)

168. **Thermoelectric Properties of Perovskite Chalcogenides Ba*TM*S_3 (*TM* = Zr, Hf) with Low Thermal Conductivity**
Xinyi He (Kanagawa Institute of Industrial Science and Technology (KISTEC))

169. **First-Principles Study of Thickness-Dependent Thermoelectric Properties of SnSe using Green's Function Method**
Zohan Syah Fatomi (Kanazawa University)

< Catalysis and Surface Chemistry >

170. **Dopant-derived Synergistic Effect for Enhancement of Electrocatalytic Nitrogen Reduction Reaction**
Ukjung Kang (Jeonbuk National University)

171. **First-Principles Study of Strain-Controlled Band Alignment in Chemiresistive Materials for Gas Sensing Enhancement**
Meng Yin (Tohoku University)

172. **The role of Ni in stabilizing the surface terminations of $BaZrO_3$ in Ni/$BaZrO_3$ cermet: DFT analysis**
Maxim Shishkin (Institute of Science Tokyo)

173. **Theoretical Insight into Alkane Hydrogenolysis Based on Free Energy Landscape**
Kenshin Takei (The University of Tokyo)

174. **Composition Optimization of High-Entropy Alloy Nanoparticle Catalysts using Machine Learning**
Koki Otsuka (The University of Tokyo)

175. **CO Coadsorption Effects on Water-Gas Shift Reaction on Cu Clusters Supported on Cu(111)**
Muhammad Fadhlan Anshor (The University of Osaka)

176. **Theoretical study by large-scale DFT and machine learning on electronic structures of nanoscale materials**
Shengzhou Li (National Institute for Materials Science (NIMS))

177. **Active Sites Evolution in Cu Catalysts: Insights from Machine Learning Molecular Dynamics**
Harry H. Halim (The University of Osaka)

178. **Surface Reconstruction in Non-metallic Spinel Oxides: Structure Prediction, Chemical Trends, and Surface Reactivity**
Tianwei Wang (Institute of Science Tokyo)

179. **First-Principles Study of CO_2 Reduction on Strained $CrSe_2$ Monolayer**
Syeda Aqsa Hassan (National Taiwan University)

180. **Theoretical Analysis of the Stability of Water Clusters on Transition Metal Surfaces**
Ren Yamaoka (Hiroshima University)

181. **Dopant-Driven Surface Stabilization Against Moisture in Garnet LLZO: A First-Principles Study**
Feye-Feng Lu (Institute of Science Tokyo)

< Defects and Interfaces >

182. **Assessing *p*-Type Dopability in Oxygen 2*p*-Dominated Electronic States**
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183. **Hetero junction for Diamond NV center modulation doping**

Sangwoo Kim (Konkuk University)

184. **The effect of stress on nitrogen-vacancy center in diamond**
Hyungwoo Lee (Inha University)

185. **First-principles calculation of native point defects in CaO**
Yunhwa Jo (Inha University)

186. **Unsupervised analysis of defects in gallium nitride**
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187. **Electron Trapping in Sn(IV)-Based Oxides and Sulfides: A First-Principles Study**
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188. **Elucidation of the Intermixing mechanism in AlN/GaN interfaces**
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189. **Triboelectrification driven by thermoelectricity**
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190. **Probing Stability and Crystallinity in Fe/MgO/Fe Interfaces Using a Machine Learning Potential Trained on Density Functional Theory**
Andi Muhammad Nur Fitrah Syamsul (Mie University)

191. **Crystal Structure Prediction and Stacking Fault Energies of Non-Basal Slip Systems in Mg-Y Alloys Using Machine Learning Potentials**
Eiki Kosakamoto (Kumamoto University)

192. **Molecular Dynamics Study of a-$(SiO_2)_x(Al_2O_3)_{1-x}$/GaN Interface Using Machine Learning**
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193. **First Principle Study of Ordered Defect Structure of MAX Phases**
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195. **Enhancing the Screening of Metal-Organic Frameworks for CO_2 Direct Air Capture using Machine Learning Force Field**
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196. **Orientation-Dependent Hot Carrier Relaxation in TiN Thin Films Facilitated by Electron–Phonon Scattering**

Hemant Verma (Academia Sinica)

197. **Temperature-dependent band structure of bulk 1T-$TiSe_2$ in charge-density-wave phase from first principles**
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198. **First-Principles and Cluster Expansion Study on the Stability of Laves Phases in Mg-Al-Ca Alloys**
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