List of Poster Presentation 1 (Sep. 5, 17:00–19:00)

*: Student Poster Prize Nominee

5Po-01* **Woojin Park** (Kyungpook National University, Korea)
Mixed-Reference Spin-Flip (MRSF) Time-Dependent Density Functional Theory for Accurate X-ray Absorption Spectroscopy

5Po-02* **Maryam Farmani** (Kyungpook National University, Korea)
Photochemistry of Thymine in Solution and DNA Revealed by an Electrostatic Embedding QM/MM Combined with Mixed-Reference Spin-Flip TDDFT

5Po-03* **Mitradip Das** (Tata Institute of Fundamental Research, India)
Emergence of Reaction Coordinates in Protein Simulations

5Po-04* **Nidhi Gupta** (IIT Kanpur, India)
Growth of Silicene on Ag(111) Surface: A Kinetic Monte Carlo and DFT-Based Study

5Po-05* **Ramsha Javed** (Indian Institute of Technology Kanpur, India)
Bucket Sampling: A New Sampling Approach to Sample High Dimensional Free Energy Landscapes

5Po-06 (cancelled)

5Po-07* **Supratim Ghosh** (IIT Bombay, India)
Role of Noncovalent Interactions in an Asymmetric Reductive Deoxygenation of Alcohol Involving a Planar Carbocationic Intermediate

5Po-08* **Abdullah Bin Faheem** (Kunsan National University, Korea)
Development of a Reliable Neural-Network Potential for Molten LiCl/KCl Salts

5Po-09 **Airi Kawasaki** (Gunma University, Japan)
Low-rank geminal theory for strongly correlated systems

5Po-10* **Kenta Yoneyama** (Shizuoka University, Japan)
All-electron first-principles *GW* simulations for core-electron binding energies

5Po-11 **Taro Udagawa** (Gifu University, Japan)
DFT study on the nuclear quantum effect in the reaction between phenol and hydroxyl radical

5Po-12 **Masahiro Tsuda** (Osaka University, Japan)
Theoretical study on magnetic properties of mononuclear transition metal complexes on graphene

5Po-13* **Chinami Takashima** (Waseda University, Japan)
Long-range corrected density functional theory calculation with the infinite-order two-component Hamiltonian

5Po-14 **Yoshio Nishimoto** (Kyoto University, Japan)
Analytic First-Order Derivatives of CASPT2 in OpenMolcas

5Po-15* **Ryusei Nishimura** (Waseda University, Japan)
Main Configuration Analysis for Divide-and-Conquer Excited-State Calculations using Frequency-Dependent Polarizability

5Po-16 **Yutaka Nagahata** (Hokkaido University, Japan)
Challenges for finding bottleneck of energy landscape

5Po-17* **Ryuto Kambara** (Hokkaido University, Japan)
Theoretical study on nonadiabatic dissociation dynamics of OCS^{2+} induced by direct photo-ionization

5Po-18* **Akihiro Mutsuji** (Hokkaido University, Japan)
A theoretical analysis of electron self-exchange reactions of transition metal complexes by an energy extrapolation approach

5Po-19 **Rejwan Ali** (City University of New York & BHSEC, USA)
Electronic Energy Singularities of Weakly H-bonded Ammonium Dimer

5Po-20* **Subhadip Mondal** (Indian Institute of Technology (IIT) Kanpur, India)
Polariton chemistry: Insights into Cavity-Mediated Vibrational Energy Flow Pathways

5Po-21 **Davor Margetic** (Rudjer Boskovic Institute, Croatia)
Computational Study of Reaction Mechanism of Formation of Boc-2-amino-quinazolin-4(3*H*)-ones from Aryl-$(Boc)_2$Guanidines

5Po-22* **Shakir Ali Siddiqui** (Shiv Nadar Institution of Eminence, India)
Local Electric Field Controlled Engineering of Porphyrin-Based Cage for Efficient Catalysis

5Po-23 **Taiji Nakamura** (Kyushu University, Japan)
Theoretical study of proton-coupled electron transfer in nitrogen fixation using metallocene: Analysis of reaction mechanism and electronic structures

5Po-24 (cancelled)

5Po-25* **Takuma Ito** (Hokkaido University, Japan)
Reaction path search and kinetic simulation for a Diels-Alder reaction including dynamical bifurcations

5Po-26* **Sangmin Jeong** (POSTECH, Korea)
Tunability of Photoisomerization Behavior via B-N Functionalization of Benzene

5Po-27 **Yoshifumi Nishimura** (Waseda University, Japan)
Extension and acceleration of nanoreactor molecular dynamics based on species-selective algorithm and linear-scaling tight-binding quantum chemical computations

5Po-28* **Eunji Park** (The Catholic University of Korea, Korea)
Theoretical investigation of photo and thermal reaction mechanisms of *p*-hydroxyphenacyl diethyl phosphate (HPDP)

5Po-29 **Aditya Wibawa Sakti** (Waseda University, Japan)
Density-Functional Tight-Binding Molecular Dynamics on Deciphering Lithium Dendrite Formation in Li-S Battery

5Po-30* **Takumi Koshiba** (Tohoku University, Japan)
Classical and quantum dynamics of vibrational relaxation in H_3O^+Ar

5Po-31 **Chao Xu** (South China Normal University, China)
Ultrafast Internal Conversion Dynamics Through the on-the-fly Simulation of Transient Absorption Pump-Probe Spectra with Different Electronic Structure Methods

5Po-32 **Ryohei Kishi** (Osaka University, Japan)
Theoretical study on structure-excitation property relationships in non-alternant isomers of [*n*]acenes

5Po-33 **Takeshi Yoshikawa** (Toho University, Japan)
Theoretical Study on Fluorescence Properties of Pyridine with Dithiophene

5Po-34* **Kaichi Shimada** (Osaka University, Japan)
Theoretical study on structures and electronic states of covalently-linked bis-periazulenes

5Po-35* **Naoki Negishi** (The University of Tokyo, Japan)
Solvatochromic effect to broadening of absorption spectra in solution

5Po-36 **Hajime Miyamoto** (Osaka University, Japan)
Theoretical study on singlet fission dynamics in one-dimensional molecular aggregates: Effects of local changes of intermolecular interactions

5Po-37 **Fengyi Liu** (Shaanxi Normal University, China)
Photodynamics of Criegee intermediates: The expected and unexpected findings

5Po-38 **Yosuke Sumiya** (Kyushu University, Japan)
Comprehensive analysis for tensile, shear, and peel adhesion strength of epoxy resin based on quantum chemical calculations

5Po-39* **Koki Masuda** (Osaka University, Japan)
Theoretical study on relationship between structure and magnetic anisotropy in Tb complexes

5Po-40* **Takahiro Uwabe** (Kyushu University, Japan)
Elucidating effects of chemisorbed waters on adhesive interactions of epoxy resin to γ-alumina surface

5Po-41* **Tamotsu Uchiyama** (Gunma University, Japan)
Theoretical study of the Si/C mixed analogues of polyhedral compounds

5Po-42* **Naoka Amamizu** (Osaka University, Japan)
Theoretical study on electronic structure and electron conductivity of annulene as molecular parallel circuit models

5Po-43* **Yuta Hayashi** (Osaka University, Japan)
Theoretical study of frontier orbitals of binuclear Ir^{III}-M^{II} (M^{II} = Mn, Fe, Co, Ni, Cu, Zn) complexes that provides hydride in the reaction

5Po-44* **Chihiro Nakasuji** (Osaka University, Japan)
Theoretical study on electronic structure of open-shell germylenes stabilized by a phenalenyl-based ligand

5Po-45* **Yuki Shirasawa** (Nagoya University, Japan)
Ionic conductivity in the solid electrolyte interphase film of the Li-ion battery during charging and discharging processes: 3D-RISM and Q-learning analysis

5Po-46 **Rabindranath Lo** (Czech Academy of Sciences, Czech Republic)
The impact of changing solvent polarity on the stability of covalent dative bonds

5Po-47 **Debashree Manna** (Czech Academy of Sciences, Czech Republic)
Dative Covalent Complexes: Role of the Solvent Dielectric Constant

5Po-48 **Shi Jun Ang** (Agency for Science, Technology and Research, Singapore)
Generating tandem mass spectra of natural products with *ab initio* molecular dynamics

5Po-49 **Shintaroh Kubo** (The University of Tokyo, Japan)
Molecular dynamics simulation of proton-transfer coupled rotations in ATP synthase Fo motor

5Po-50* **Shreya Rastogi** (Indian Institute of Technology Kanpur, India)
Intramolecular Proton Transfer in Pyridoxal 5'-phosphate Schiff Bases and Free Energy Landscape for Transimination Reaction at the Active site of Ornithine Decarboxylase

5Po-51* **Rounak Nath** (Indian Association for the Cultivation of Science, India)
Decoding Regioselective Reaction Mechanism of the Gentisic Acid Catalyzed by Gentisate 1,2-Dioxygenase Enzyme

5Po-52 **Yusuke Kanematsu** (Hiroshima University, Japan)
Characterization of P450nor by using statistical analysis and quantum chemical calculation

5Po-53 **Vladislav Vasilyev** (The Australian National University, Australia)
In silico Tuning of Binding Selectivity of Existing Drugs and Drug Candidates

5Po-54 **Thanyada Rungrotmongkol** (Chulalongkorn University, Thailand)
Exploring Novel Wild-type and Mutant EGFR Tyrosine Kinase Inhibitors from Furopyridine-Based Compounds: In Silico and In Vitro Study

5Po-55* **Daisuke Terada** (FUJI FILM Corporation & Keio University, Japan)
Theoretical study of enzymatic C-glycosylation of Phloretin catalyzed by glycosyltransferase *GgCGT*

5Po-56 **Michal Michalski** (University of Warsaw, Poland)
Exploring the structure and dynamics of influenza hemagglutinin transmembrane domain

5Po-57 **Kaori Ueno-Noto** (Kitasato University, Japan)
Theoretical Study of the Protein-Glycan Interaction in FimH Adhesin

5Po-58 **Victor Bernstein** (Technion - Israel Institute of Technology, Israel)
Comparative molecular dynamics study of C_{60} impact interactions with low mass targets

5Po-59 **Yusaku Abe** (Yokohama City University, Japan)
Theoretical study of isotope effect on phase transition in lead hydrogen phosphate

5Po-60* **Sara Suzuki** (Kyoto University, Japan)
Influence of microscopic solute-solvent interaction on the radical cyclization reaction

5Po-61 **Manussada Ratanasak** (Hokkaido University, Japan)
Mechanistic DFT Study of BPh_3-Catalyzed *N*-Methylation of Amines with CO_2 and $PhSiH_3$

5Po-62 **W. M. C. Sameera** (Hokkaido University, Japan)
On the mechanism of the N_2 reduction by a $[Mo_3S_4Fe]$ cluster

5Po-63 **Sarinya Hadsadee** (Hokkaido University, Japan)
DFT Exploration of the Catalytic Active Site of CoN_4C_x on KB for Electroreduction of CO_2 to CO

5Po-64* **Krish Jhurani** (Homestead High School, USA)
Investigating the Role of Quantum Coherence in Transition Metal Catalyzed Reactions

5Po-65 **Patcharaporn Khajondetchairit** (Chulalongkorn University, Thailand)
A DFT study on how transition metal affects hydrogen storage kinetics in magnesium nickel hydride

5Po-66 **Tinnakorn Saelee** (Chulalongkorn University, Thailand)
On the enhanced performance of Pt-based high-entropy alloys catalyst during water-gas shift reaction: A density functional theory study

5Po-67* **Chanthip Wangphon** (Chulalongkorn University, Thailand)
How can the PtPd-based high-entropy alloy triumphs conventional TWC catalyst during the NO reduction? A Density Functional Theory Study

5Po-68* **Arini Amalia Choir** (Bandung Institute of Technology, Indonesia)
A Comparative Site-Specific Interactions of $Ga_{12}Y_{12}$ (Y= N, P, As, Sb) Nanocages on The Adsorption of CO_2 and H_2 Molecules

5Po-69 **Gehoon Chung** (Seoul National University, Korea)
Oleophilicity induced by ultraviolet irradiation of titanium surface

5Po-70* **Sapajan Zakirovich Ibragimov** (Gdansk University of Technology, Poland)
Geometry and electronic structure of iron(III) oxides and its reduced forms.

5Po-71* **Kazuki Honjo** (Osaka University, Japan)
Theoretical study on proton transfer to the M-cluster of nitrogenase

5Po-72* **Hitoshi Nabata** (Hokkaido University, Japan)
Systematic reaction path search for thermal formic acid decomposition on the anatase TiO_2 (101) surface

5Po-73* **Daiki Asada** (The University of Tokyo, Japan)
Deoxydehydration reaction by monomeric and dimeric molybdenum oxide catalysts supported on TiO_2: A density functional theory study

5Po-74 **David Samuel Rivera Rocabado** (Hiroshima University, Japan)
Unlocking the secrets of CO interaction and activation on Ru nanoparticles supported on Al_2O_3: harnessing the predictive power of the electronic structure decomposition approach

5Po-75* **Jewel Hossen** (Tokyo Metropolitan University, Japan)
Theoretical study of structure control mechanism of $[Pd_6Si_2]$ cluster

5Po-76* **Milan Kumar Jena** (IIT Indore, India)
Development of an Artificially Intelligent Nanopore for High-Throughput DNA Sequencing with a Machine-Learning-Aided Quantum-Tunneling Approach

5Po-77* **Sneha Mittal** (IIT Indore, India)
Decoding Both DNA and Methylated DNA Using a MXene-Based Nanochannel Device: Supervised Machine-Learning-Assisted Exploration

5Po-78 **Pavel Sidorov** (Hokkaido University, Japan)
Predicting Highly Enantioselective Catalysts Using Machine Learning

5Po-79 **Yuya Nakajima** (ENEOS Corporation, Japan)
Atomic clustering based on molecular properties considering surrounding environments and its application to accuracy verification

5Po-80* **Ryo Fujisawa** (Waseda University, Japan)
Development of machine-learned electron correlation model including the fourth-row elements

5Po-81 **Yu Takano** (Hiroshima City University, Japan)
Prediction of Heme Protein Function with Random Forest Classifier Based on Porphyrin Distortions and Axial Ligands of Heme

5Po-82 **Soichi Shirai** (Toyota Central R&D Labs., Inc., Japan)
Computational analysis of chemical reactions using a variational quantum eigensolver method without specifying spin multiplicity

5Po-83 **Chihiro Osaku** (The University of Tokyo, Japan)
Quantum simulation of entangled electron-nuclear dynamics of molecular hydrogen ions using a quantum computer

5Po-84 **Kajjana Boonpalit** (VISTEC, Thailand)
Graph Neural Networks Accelerated High-throughput Screening of Dual-atom Catalyst for Hydrogen Evolution Reaction

List of Poster Presentation 2 (Sep. 7, 17:00–19:00)

*: Student Poster Prize Nominee

7Po-01* **Satoka Yamada** (Shizuoka University, Japan)
Development of Full GW Electron-Hole Interaction Kernel

7Po-02* **Soichiro Nishio** (Kyoto University, Japan)
Development of multireference theory for excited states of π-conjugated molecular aggregates and its application

7Po-03 **Ryo Fujiki** (University of Tsukuba, Japan)
3D-RISM Theory for Biological System: QM and MM

7Po-04* **Hiroaki Okada** (Hokkaido University, Japan)
On accelerating substrate optimization using computational Gibbs energy barriers: A numerical investigation utilizing an extensive reaction barrier dataset of Claisen rearrangement

7Po-05* **Lihao Qu** (Hokkaido University, Japan)
Reaction pathway and AIMD trajectory analysis and visualization of organic reactions using data science algorithms

7Po-06* **Ryota Sato** (Hokkaido University, Japan)
Tacticity dependence on polystyrene structure: A theoretical analysis based on systematic structure search

7Po-07* **Kosuke Imamura** (Kyoto University, Japan)
Open-boundary cluster model with a parameter-free complex absorbing potential

7Po-08* **Yutaro Otani** (Tokyo Metropolitan University, Japan)
Development of DMRG-DOCI-PT2 method

7Po-09 **Satoi Wada** (Hokkaido University, Japan)
Intersystem crossing dynamics based on spin-pure and spin-mixed potential energy surfaces

7Po-10 **Manabu Kanno** (Tohoku University, Japan)
A structure-based Gaussian expansion for quantum reaction dynamics: Application to hydrogen tunneling in malonaldehyde

7Po-11 **Jun Yang** (The University of Hong Kong, Hong Kong)
Downfolded Configuration Interaction for Correlated Electronic States

7Po-12* **Rei Oshima** (Waseda University, Japan)
Solving unstable behavior of divide-and-conquer self-consistent field calculations using level shift technique based on pair-excited perturbative selection

7Po-13* **Jeheon Woo** (KAIST, Korea)
Neural network-based pseudopotential: development of a transferable local pseudopotential

7Po-14* **Shoya Kondo** (Hokkaido University, Japan)
Exploring structural transitions in molecular crystals using AFIR combined with molecular mechanics force fields

7Po-15* **Yuki Kanamaru** (University of Tsukuba, Japan)
Analysis of solvent electrostatic potential described by solvation models in charged systems

7Po-16* **Burai Murayama** (Hokkaido University, Japan)
Characterizing Reaction Route Map of Realistic Molecular Reactions Based on Weight Rank Clique Filtration of Persistent Homology

7Po-17* **Hiroki Sakagami** (Yokohama City University, Japan)
Development of combined plane wave and localized basis sets method toward theoretical analysis of H/D isotope effect of molecule adsorption on metal surface

7Po-18 **Masanori Yamanaka** (Nihon University, Japan)
Calculation of index of quantum evolution of biological macromolecules by density functional theory

7Po-19 (cancelled)

7Po-20* **Keita Mataki** (Hokkaido University, Japan)
Reaction Space Projector Analysis for Ambimodal Pericyclic Reactions: Visualization of Potential Energy Landscape and Dynamics in Reduced Dimension

7Po-21* **Wataru Kanna** (Hokkaido University, Japan)
Reaction Development of Catalytic Olefin Aminocarboxylation with CO_2 Based on Potential Energy Surface Crossing Points for Single Electron Transfer Steps

7Po-22 **Bastian Bjerkem Skjelstad** (Hokkaido University, Japan)
A Computational Study on the Early-Stage Self-Assembly of the SIFSIX-3-Zn Metal-Organic Framework

7Po-23* **Tomislav Rozic** (University of Copenhagen, Denmark)
Insights into non-statistical chemical reactivity from a vibrational relaxation model

7Po-24* **Maximilian C. Poverlein** (Stockholm University, Sweden)
QM/MM Free Energy Calculations of Long-Range Biological Protonation Dynamics

7Po-25* **Friederike Allgower** (Stockholm University, Sweden)
Mechanism of Water Oxidation of Proton Release in Photosystem II

7Po-26* **Ryoichi Tanaka** (Hokkaido University, Japan)
An analysis of Chemical Reaction Dynamics in DImensionally Reduced Phase Space

7Po-27* **Hyunho Kim** (Stockholm University, Sweden)
Proton-coupled Electron Transfer Dynamics in the Alternative Oxidase of *Trypanosoma brucei*

7Po-28 **Daniel Riepl** (Stockholm University, Sweden)
Long-Range Charge Transfer Mechanism of the III_2IV_2 Mycobacterial Supercomplex

7Po-29* **Shuhei Kanesato** (Nagoya University, Japan)
All-atom simulation of chain-transfer alkene polymerization reaction of (pyridylamido)Hf catalyst: Microscopic steric effects on polymerization properties

7Po-30 **Hiroshi Teramoto** (Kansai University, Japan)
Reproducing Reaction Route Map on the Shape Space from its Quotient by Complete Nuclear Permutation-Inversion Group

7Po-31* **Moe Murata** (Yokohama City University, Japan)
Molecular Dynamics Simulations for Analysis of Substituent Effects in Self-Assembled Gear-Shaped Amphiphile Molecules with/without Methyl Groups

7Po-32 **Kenji Okada** (Osaka University, Japan)
Low-lying excited states of fused-ring diphenoquinones and their potential applications to singlet fission molecules

7Po-33 **Osamu Takahashi** (Hiroshima University, Japan)
Structure of aqueous ethanol solution: Soft X-ray emission spectroscopy measurements and theoretical calculations

7Po-34* **Marina Mizuno** (Hokkaido University, Japan)
Development of Circularly Polarized Luminescent Materials with Axially Chiral Binaphthyl Framework Based on Theoretical Calculations of Their Excited States

7Po-35* **Wataru Yoshida** (Osaka University, Japan)
Theoretical study on charge density distributions of cationic multimers of π-conjugated molecules

7Po-36 **Hiroki Uratani** (Kyoto University, Japan)
Kinetics of thermally activated delayed fluorescence in amorphous aggregates: effects of structural disorder

7Po-37 **Yuichi Tanaka** (Nagoya University, Japan)
Electrode potential effect on the formation process and stability of SEI film in lithium-ion batteries

7Po-38* **Hikaru Tanaka** (Gifu University, Japan)
Nuclear quantum effect on aromaticity: A path integral molecular dynamics study

7Po-39* **Mitsuhiro Nishida** (Osaka University, Japan)
Theoretical study of heteroatom substitution effect on current-voltage characteristics of polyacenes

7Po-40* **Seiya Tsuchida** (Osaka University, Japan)
Theoretical studies on electronic structures of open-shell π-extended pentalenes

7Po-41* **Ryota Sugimori** (Osaka University, Japan)
Calculations of magnetic response properties of π-stacked dimers of antiaromatic molecules.

7Po-42* **Tomohito Shinozuka** (Kyoto University, Japan)
Computational study on the enhancement of the negative second hyperpolarizability in mixed-valence molecules

7Po-43 **Takashi Kawakami** (RIKEN, Japan)
Theoretical studies on magnetic interactions in trinuclear manganese complexes by UNO CAS-based methods

7Po-44* **Yuika Baba** (Japan Womens University , Japan)
Electronic State of Sumanene Derivative Bowl-Shaped Molecules

7Po-45 **Yuriko Ono** (Hokkaido University, Japan)
Anharmonic vibrational state computations to reveal disappearance mechanism of the fundamental peak of noble gas complex

7Po-46* **Keisuke Sasaki** (Osaka University, Japan)
Theoretical Study on Redox Control of Paddlewheel-type Diruthenium Complexes by Introducing π-electron Groups

7Po-47* **Mitsuhiro Bandai** (Ibaraki University, Japan)
Evaluation of the effects of mutations in Cp*Rh(III) complex-linked artificial metalloenzyme Nitrobindin^{HLH}-Cp*Rh(III) by MD simulation

7Po-48 **Tomoki Nakayoshi** (Hiroshima City University, Japan)
Computational estimation of the activation energy for the peptide-bond flip induced by active-center reduction of plant-type ferredoxin

7Po-49* **Mio Takakuwa** (Yokohama City University, Japan)
Theoretical study on hydrogen-bonded structures of the green fluorescent protein with multi-component density functional theory

7Po-50* **Ayaka Sato** (University of Tsukuba, Japan)
Theoretical analysis of the electronic and geometrical structures of the active center of a high-potential iron-sulfur protein and its influence from surrounding amino acids

7Po-51 **Koichi Miyagawa** (University of Tsukuba, Japan)
Relative stability and electronic structure in the S_1 state of the $CaMn_4O_5$ cluster of the PSII by DFT and CC calculations

7Po-52 **Kizashi Yamaguchi** (Osaka University, Japan)
Theory of Chemical Bonds in Metalloenzyme XXV —OEC of PSII—

7Po-53 **Kowit Hengphasatporn** (University of Tsukuba, Japan)
FMO-Guided Design of Darunavir Analogs as HIV-1 Protease Inhibitors

7Po-54* **Haruka Yotsuya** (Nagoya University, Japan)
Structural regulation of hemoglobin by the histidine protonation state depending on pH: a theoretical analysis

7Po-55* **Koki Adachi** (Waseda University, Japan)
Molecular dynamics study on the roles of K-loop of KIF1A in the binding to microtubule

7Po-56 **Koichi Yamashita** (Yokohama City University, Japan)
Optical Properties and Defect Structures of Double Perovskite Cs_2SnGeI_6

7Po-57* **Tomoya Iwashita** (Kyushu University, Japan)
The Decomposition of Friction Coefficients for Analysis of Solvation Effects on Diffusion Coefficients

7Po-58 **Kazuaki Kuwahata** (Yokohama City University, Japan)
Nuclear quantum effect in the phase transition from Ice VII to Ice X

7Po-59 **Deepak Ojha** (Tohoku University, Japan)
Vibrational Dynamics of Liquid Water in an External Field

7Po-60* **Nan He** (Tokyo Metropolitan University, Japan)
DFT and CASPT2 studies of Fe-catalyzed coupling reaction: Effect of electron correlation

7Po-61* **Kai Oshiro** (Hokkaido University, Japan)
Mechanistic study of the alkali tolerance mechanism of H_2SO_4/Fe_CeO_2 catalyst for NH_3-SCR

7Po-62* **Tomohisa Yonemori** (Osaka University, Japan)
Theoretical investigation on the role of moisture in the process of CO oxidation reaction by Au/Polyoxometalate catalyst

7Po-63 **Wei-Chih Chen** (Providence University, Taiwan)
Effect of Alkali Metal Ions on the Reduction Mechanism of Phosphinous Acid-Ligated Pd(II) Precatalysts in Suzuki-Miyaura Cross-Coupling Reactions

7Po-64* **Noriyuki Takai** (Hokkaido University, Japan)
Electronic theory analysis of Pd-catalyzed cross-coupling reaction based on reactive orbital energy theory

7Po-65 **Tatsushi Ikeda** (The University of Tokyo, Japan)
Long-Range Proton and Hydroxide Ion Transfer Dynamics at Water/CeO_2 Interface in Nanosecond Regime: Molecular Dynamics Simulations with Neural Network Potential

7Po-66* **Kota Oishi** (The University of Tokyo, Japan)
Computational analysis of Al site-directing ability of organic structure-directing agents in FER and CHA zeolites

7Po-67* **Takaaki Endo** (The University of Tokyo, Japan)
Free energy analysis of nitrile hydration reaction using cerium oxide catalysts

7Po-68* **Tomoya Kanno** (The University of Tokyo, Japan)
Grand Canonical Monte Carlo Simulations for Hydrogen Adsorption on Metal Surfaces with Neural Network Potentials

7Po-69* **Yuta Kataoka** (The University of Tokyo, Japan)
Calculation of hydrogen diffusion coefficients on metal surfaces using density functional based potential

7Po-70* **Narumi Fujiwara** (Japan Womens University , Japan)
Theoretical study on reaction mechanism of water splitting process on Cobalt-Oxo Cubane Clusters

7Po-71 **Azusa Muraoka** (Japan Womens University , Japan)
Charge Separation Process in PTB7/BTAx Nonfullerene Organic Solar Cells

7Po-72* **Yuzuka Minami** (Japan Womens University , Japan)
Comparison of Charge Transfer Distance in PDCBT/BTA Non-Fullerene Organic Solar Cells

7Po-73* **Luxuan Guo** (KU Leuven, Belgium)
Computational Modelling of Microscopic Reactivity of Phenylferrate Ions

7Po-74 **Motoji Sakai** (Nagoya University, Japan)
Learning Organo-Transition Metal Catalyzed Reactions by Graph Neural Networks

7Po-75* **Lian Duan** (Unversity of Tsukuba, Japan)
Convolutional Neural Network Model for Predictive Screening of Cyclic Peptides in Drug Design and Development

7Po-76* **Ryosuke Sasaki** (Waseda University, Japan)
Utilization of image recognition for chemical experiments toward development of automated electronic laboratory notebook

7Po-77 **Philippe Gantzer** (Hokkaido University, Japan)
Representation of Reaction Networks by Generative Topographic Mapping

7Po-78* **Takuya Isoda** (Waseda University, Japan)
A Feasibility Study of Symbolic Regression Algorithms for Chemical Laws

7Po-79* **Seonghwan Kim** (KAIST, Korea)
Reliable generative AI for Chemical reaction exploration

7Po-80 **Dmitry Zankov** (Hokkaido University, Japan)
Multi-Instance learning approach to the modeling of enantioselectivity of conformationally flexible organic catalysts

7Po-81* **Jun Hyeong Kim** (Korea Advanced Institute of Science and Technology, Korea)
Discovery of Thermally Activated Delayed Fluorescence Materials Using the Deep Generative Model

7Po-82* **Ryoya Kondo** (Hokkaido University, Japan)
Development of Information Theoretical Analysis Based on Spatial Heterogeneity for Raman HISTOLOGY

7Po-83 **Changduk Yang** (UNIST, Korea)
Universal Volatile Additives to Realize Polymer Batch Insensitive Organic Solar Cells

7Po-84 **Supanida Piyayotai** (King Mongkuts University of Technology Thonburi , Thailand)
Predicting small molecule bioactivity with machine intelligence

7Po-85* **Akanksha Mishra** (Babasaheb Bhimrao Ambedkar University, India)
Illuminating the Path of Inhibited Acetylcholinesterase by Unravelling the Dynamics of Biochemical Pathways of CNS