Poster Session 1 – 19:30-21:30, Monday, 14 October 2024

PO1-1	Highly coarse-grained patchy ellipsoid particle model of glucose	Bin Li
PO1-3	Atomistic insights on recognition of transcription factor binding motif in DNA through bZIP domain	Piya Patra
PO1-4	Structure and catalytic properties of Cu-Au nanoparticles under high CO and O coverage	Anastasiia Mikhailova
PO1-5	Computational screening of doped-$V_3C_2O_2$ for propane dehydrogenation using DFT-based microkinetic simulations	Aqsa Abid
PO1-6	Modeling realistic structures of trimetallic nanoalloy catalysts using chemically meaningful descriptors	Arravind Subramanian
PO1-7	Accurate adsorption energy predictions using many-body methods with quantum embedding	Changsu Cao
PO1-8	TBA	Congqiao Xu
PO1-9	Illuminating tandem reactions characterized by temporal separation of catalytic activities via DFT calculations: A case study of Ni-catalyzed alkyne semihydrogenation	Dongju Zhang
PO1-10	Effect of ZnO support and nanostructuring on catalytic activity of noble metals: Insights from Sabatier principle	Fernando Buendia Zamudio
PO1-11	Theoretical insights into the ammonia and hydrogen-induced structural evolution of Pt clusters in mordenite	Gang Feng
PO1-12	Mean-field QM/MM simulations for electrochemical interfaces	Hyungjun Kim
PO1-13	Structure-driven tuning of adsorption properties of core-shell nanoparticles: a density functional theory study	Ilia Chepkasov
PO1-14	Controlling active phase and interface interactions in bimetallic Ru-Pd catalyst via CO oxidation	Janobiddinkhuja Bahodurov
PO1-15	Delayed fluorescence from inverted singlet and triplet excited states in heptazine analogues HzT-FEX2 studied by mixed-reference spin-flip time-dependent density functional theory (MRSF-TDDFT)	Alireza Lashkaripour
PO1-16	Advances in Q-Chem 6.2	Andrew Gilbert
PO1-17	Extension of the charge stabilization method beyond energies	Charlotte Titeca
PO1-18	Noncollinear functionals for real-time TDDFT and gradients of spin-flip TDDFT	Hao Li
PO1-20	Unraveling the mechanism of a switchable acid catalyzed COT oxide contraction towards homoallylic alcohols	Manuel Pedrón

PO1-21	Some restrictive open-shell excited-state ΔSCF methods	Peng Bao
PO1-22	Electronic structure of periodic systems containing strongly correlated transition metals	Ilya Popov
PO1-23	Density-based many-body expansion as a case study on interoperability	Kevin Focke
PO1-24	Developments of approaches for structural relaxation of excited states of materials based on embedded cluster model	Teng Zhang
PO1-25	Nonadiabatic field on quantum phase space	Baihua Wu
PO1-26	Mechanistic insights into twisted intramolecular charge transfer in CBP and its derivatives	Donghwan Im
PO1-27	Building accurate molecular simulation models for studying warm cloud seeding	Guangzhi He
PO1-28	Correlation functions from tensor network influence functionals: The case of the spin-boson model	Haimi Nguyen
PO1-29	Time-dependent density matrix renormalization group method for quantum transport with phonon coupling in molecular junction	Hengrui Yang
PO1-30	Solvated electron from first principles and machine learning	Jinggang Lan
PO1-31	Real-time time-dependent density functional theory for X-ray absorptions	Linfeng Ye
PO1-32	TBA	Paul Robinson
PO1-33	Non-unique Hamiltonians for discrete symplectic dynamics	Liyan Ni
PO1-34	An electronic spin on geometric phase effects in molecular systems	Martin van Horn
PO1-35	Excursions in polaritonic chemistry: From relaxation in liquids to chemical kinetics	Muhammad Risyad Hasyim
PO1-36	Early stages of battery electrolytes degradation: Theory and experiment	Alia Tadjer
PO1-37	Stability and ion conductivity of novel Li_6PIO_5 : A DFT study	Areg Hunanyan
PO1-38	Disordered structure reduces the bandgap of double perovskite Cs_2 AgBiBr$_6$ t hrough wavefunction localization	Bayan Amer Abzakh
PO1-39	A theoretical study on proton transfer reactions in anthracene-urea derivatives	Changbang Long
PO1-40	Theoretical study on the effect of ring modification in cuprous halide complexes on the TADF mechanism	Guangyu Wang
PO1-41	Review on improving the performance of SiOx anodes for a lithium-ion battery through insertion of heteroatoms: State of the art and outlook	Hai Li
PO1-42	Theoretical study on singlet fission dynamics in finite-size molecular aggregates with various intermolecular interaction strengths and structures	Hajime Miyamoto
PO1-43	A molecular dynamics simulation on the stress corrosion cracking mechanism of BCC-FCC type dual-phase high-entropy alloys	Haoyu Zhao

PO1-44	Modelling of sodium clusters in various conjugated carbonaceous structures	Hristo Rasheev
PO1-45	Assessing short-range charge transfer character of potential MR-TADF emitters with wavefunction descriptors	Mariana Telles do Casal
PO1-46	XEDA: An efficient and flexible energy decomposition analysis (EDA) toolkit	Yueyang Zhang
PO1-47	Sub- and supercritical water structure calculated using the self-learning path integral hybrid Monte Carlo method	Bo Thomsen
PO1-48	Towards ML- and QML-accelerated discovery of catalytic materials and mechanisms	Dennis Salahub
PO1-49	Breaking the size limitation of non-adiabatic molecular dynamics in condensed matter systems with local descriptor machine learning	Dongyu Liu
PO1-50	Reciprocal prediction of multimodal spectral and structural descriptors for incomplete data	Guokun Yang
PO1-51	Spectra-based clustering of high-entropy alloy catalysts: Improved insight over use of atomic structure	Huirong Li
PO1-52	A simple approach to rotationally invariant machine learning of a vector quantity	Jakub Martinka
PO1-53	Machine learning photodynamics uncover blocked non-radiative mechanisms in aggregation-induced emission	Jingbai Li
PO1-54	Density functional theory and machine learning exploration of disorder in materials	Jingrui Li
PO1-55	Stochastic resolution of identity to CC2 for large systems	Chongxiao Zhao
PO1-57	Quantum simulation with cluster embedding strategy for surface chemisty	Dedong Wan
PO1-59	Development of a compact and dynamic ansatz for enhanced quantum efficiency	Dipanjali Halder
PO1-60	Nuclear quantum effects enhance hydrogen evolution reaction on graphene-embedded transition metal atoms	Erxun Han
PO1-61	Development of quantum embedding computing for Quantum Chemistry	Wafa Makhlouf
PO1-62	Chemoexcited formation and radiationless decay dynamics of firefly chromophore	Maryam Farmani
PO1-63	Theoretical study of lanthanide single-ion magnet: Electronic structure, magnetic anisotropy and relaxation	Bing Yin
PO1-64	The automated design of chemical reactions program	Guoao Li
PO1-65	A workflow for reaction datasets construction by layer-based modification modeling process.	Hexiang Qi
PO1-66	Mapping hydrogen positions along proton transfer pathway in organic crystals by computational X-ray spectra	Guoyan Ge

PO1-67	A Green's-function-based many-body perturbation theory approach to electron-vibration coupling in molecular systems	Haoyu Qi
PO1-68	Reveling the ultrafast energy transfer pathways in energetic materials: Time-dependent and quantum state-resolved	Jia Liu
PO1-69	Second-order Møller–Plesset perturbation theory with pair natural orbitals for periodic systems	Andrew Zhu
PO1-71	Equation-of-motion block-correlated coupled cluster method for excited electronic states of strongly correlated systems	Haodong Zhang
PO1-72	Toward a systematic and high-precision ab initio framework for metallic solids	Hung Pham
PO1-73	The truncation schemes for unitary coupled-cluster based polarization propagator theory	Junzi Liu
PO1-74	A moiety-based charge-transfer decomposition for exploring the charge-transfer character and exciton binding energies in dye-sensitized solar cells	Lena Szczuczko
PO1-75	DC-MP2-PBC: Fast and accurate quantum chemical calculation for large-scall periodic systems	Ogawa Gen
PO1-76	Unveiling the local structure of liquid water via X-ray spectroscopy simulations employing multiconfigurational wave function theory	Alekos Segalina
PO1-77	U≡C triple bonds in fullerene compounds	Jing Zhao
PO1-78	Design strategy of MR-TADF materials with tunable Stokes shift and narrow spectra band through-space conjugation	Meihui Liu
PO1-79	Million-atom molecular dynamics simulations on the splitting mechanism of Ni particles within the anode of solid oxide fuel cells	Yixin Su
PO1-80	Relativistic effects in ultrafast light induced spectroscopy	Torsha Moitra
PO1-81	Time evolving matrix product operator (TEMPO) method in a non-diagonal basis set based on derivative of the path integral expression	Shuocang Zhang
PO1-82	MC23: A New Meta-GGA On-Top Functional for Hybrid Multiconfiguration Pair-Density Functional Theory with Improved Accuracy	Jie Bao
PO1-83	First-principles calculation of the enhancement of oleic acid collector molecule adsorption by surface oxygen vacancy defects in hematite	Jing Wen