Poster Session 2 – 19:30-21:30, Tuesday, 15 October 2024

PO2-1	Rare event kinetics in complex systems with Milestoning	Ru Wang
PO2-2	How transcription factor NF-κB RelA recognize a central base pair: Computational insights into transient interactions	Tianjie Li
PO2-3	Accurate carbohydrate-binding site prediction	Xi Cheng
PO2-4	Probing the orientation and membrane permeation of Rhodamine Voltage Reporters through molecular dynamics and free energy calculations	Yajing Qi
PO2-5	CO_2 t o methanol conversion on Cu/ZnO catalyst: Unveiling the role of catalyst architecture and binding affinity	Jie Zhao
PO2-6	Tailoring active-site spacing of single-atom catalyst for CH_4-to-CH_3O H conversion: Co_1/UiO-66 MOF as an exemplary model	Karim Harrath
PO2-7	Inverted region in electrochemical reduction of CO_2 i nduced by potential-dependent Pauli repulsion	Leyu Liu
PO2-8	Effective screening descriptors of metal−organic framework supported single-atom catalysts for electrochemical CO_2 reduction reactions	Lihui Mou
PO2-9	Towards systematic initiations of minimum energy path calculations	Maike Muecke
PO2-10	A theoretical study on the asymmetric site of CO_2 h ydrogenation to methanol on Cu-based catalysts	Mingcan Chen
PO2-11	CO_2 e lectroreduction to CO on ultrasmall Ag nanoparticles supported on polymeric carbon nitride (PCN)	Mohammed Aliasgar
PO2-13	The oxidation of CO on step interfaces between ZnO deposits and metal supports	Paulo de Carvalho Dias Mendes
PO2-14	Small molecule activation by uranium and group 6 metal complexes, a theoretical study	Qingjiang Pan
PO2-16	Explicitly density-dependent noncollinear and nonlocal exchange-correlation functional	Tai Wang
PO2-17	A tuning method for range-separated hybrid functionals based on charge transfer density-based indexes	Tianhong Yan
PO2-18	Energetic information from information-theoretic approach in density functional theory as quantitative measures of physicochemical properties	Xin He
PO2-19	Exact properties of multi-state density functional theory	Yangyi Lu
PO2-20	Exploring the range-separation schemes in the range-separated hybrid functionals	Ye Li

PO2-21	Towards consistent projection-based wavefunction in density functional theory embedding	Yitian Zhu
PO2-22	Comparison of solvent electrostatic potential and improvement proposal for polarizable continuum model	Yuki Kanamaru
PO2-23	Role of electronic polarization in the primary charge-transfer states of the purple bacteria reaction center: A polarizable QM/MM study with the integral-exact direct reaction field method	Yuquan Cao
PO2-24	Application of quantum embedding theory on lanthanide-based materials	Zewei Li
PO2-25	Excitonic energy transfer under strong coupling from a semi-classical surface hopping perspective	Priyam Kumar De
PO2-26	Ab-initio study on the effect of dipolar spin-spin interactions in singlet fission	R. K. Kathir
PO2-27	Radiosensitizing potential of halo-uracils via low-energy electrons: A simulation study	Raj Roy
PO2-28	Describing nuclear quantum effects in coupled nuclear-electron dynamics at gas-metal surface: A ring polymer molecular dynamics extension to electronic friction	Ruihao Bi
PO2-29	First-principles demonstration of nonadiabatic Thouless pumping of electrons in a molecular system	Ruiyi Zhou
PO2-30	A grid-based gauge-invariant non-perturbative solution of the Schrodinger equation for electrons and nuclei in strong magnetic fields	Sangita Sen
PO2-31	Non-adiabatic molecular dynamics on ultrafast relaxation of ortho-nitrophenol upon photoexcitation	Satoi Wada
PO2-32	Theoretical study of the spin transition processes of molecular systems	Shuming Bai
PO2-33	Phonon-mediated ultrafast energy- and momentum-resolved hole dynamics in monolayer black phosphorus	Siyuan Gao
PO2-34	Large-scale nonadiabatic dynamics study of doping process within PbSe quantum dots	Tenghui Li
PO2-35	Multi-scale modeling of hydroxyl radical reactions with isoprene in the gas phase and at the air-water interface	Tianren Zhu
PO2-36	Ab initio investigation of the features of $Sr_3Ti_3(BO_6)_2$	Mikayel Sahakyan
PO2-37	Study of the influence of the grain boundary structure on the properties of $CsPbBr_3$ perovskite	Mikhail Samatov
PO2-38	Time-domain ab initio analysis of facet-dependent carrier dynamics in Cuprous oxide	Minjae Kwen
PO2-39	Mechanism of lithium dendrite growth on iron surfaces toward high-performance and safe anode-free lithium metal batteries	Nannan Li
PO2-40	Computational screening of multi-resonance thermally activated delayed fluorescence (MR-TADF) molecules for lasing application	Rongrong Li
PO2-41	Theoretical study on open-shell electronic structures of through-bond through-space hybrid conjugated systems	Ryohei Kishi

PO2-42	Computational study on high-performance memristors utilizing nanomanipulation and device architecture design	Shuang Chen
PO2-43	Theoretical studies of 0D-perovskite based luminescent materials	Songqi Cao
PO2-44	Intrinsic defects in B- site columnar-ordered halide double perovskites Cs_2 AgPdBr_5	Wenjun Chu
PO2-45	Growth kinetics of single-crystal covalent organic frameworks	Xiangkun Yu
PO2-46	Do Zimmermann-Traxler transition states always have strong explanatory power? --A combined experimental and computational 'archaeology of chemistry' study.	Zongchang Han
PO2-47	Analysis of organic reactions by combinatorial optimization and dimension reduction method	Lihao Qu
PO2-48	Mechanistic insights into water autoionization through metadynamics simulation enhanced by machine learning	Ling Liu
PO2-49	Enhancing molecular data through quantum chemical calculations: An overview of the PubChemQC project	Maho Nakata
PO2-50	Predicting heat capacity of molecular fluids using interpretable machine learning models: Application of the Fluid_Thermo database	Simin Li
PO2-51	Scalable and accurate chemical property predictions using universal neural network potentials as atomic descriptors	Tomoya Shiota
PO2-52	Machine learning force field construction of organmetallic complex materials: An equilibrium molecular dynamics study on thermal conductivity calculation of copper phthalocyanine	Wenjie Zhang
PO2-53	Development of programs for identifying active sites on catalyst surfaces and constructing databases for transition states	Xiao Ma
PO2-54	An AI-assisted pure density-based nonlocal functional	Xiaoyu Zhang
PO2-55	Fragment-based deep learning for simultaneous prediction of polarizabilities and NMR shieldings of macromolecules and their aggregates	Dongbo Zhao
PO2-56	Unveiling the impact of the air-water interface on altering reaction mechanisms: Incorporating DFT, AIMD, and CMD	Mohammad Hassan Hadizadeh
PO2-58	Calculating potential energy surfaces with the variational quantum eigensolver	Shizheng Zhang
PO2-59	Enhancing variational quantum eigensolver with clifford transformation and robust parameter optimization	Weitang Li
PO2-60	Grid-based quantum simulation of photoexcited pyrazine	Xiaoning Feng
PO2-61	The application of Hardware heuristic ansatz in periodic system	Xiaopeng Li
PO2-62	How to experimentally detect planar tetracoordinate hydrogen within the indium framework? An answer from quantum dynamics theory	Xingyu Zhang

PO2-63	Uranium dioxide-mediated carbon dioxide photoreduction	Xuelian Jiang
PO2-64	Automated review generation method based on large language models	Shican Wu
PO2-65	Coupling simulations of spatiotemporal electromagnetic fields with simulations of ultrafast photoinduced dynamics	Lorenz Grünewald
PO2-66	Femtosecond pump-probe-spectra in the heptazine-H_2O complex: A computational study	Sebastian Viktor Pios
PO2-67	Simulating transient X-ray spectra of molecules and crystals from snapshots along the potential energy surfaces	Weijie Hua
PO2-68	Accurate and efficient NMR shielding calculation with parallel, fully RI-boosted finite 1st derivative framework	Xiao Liu
PO2-69	Linear response pCCD-based methods	Paweł Tecmer
PO2-70	Individual and cooperative superexchange enhancement in cuprates	Tonghuan Jiang
PO2-71	Block-correlated coupled cluster theory for accurate static correlation of strongly correlated systems	Xiaochuan Ren
PO2-72	Excitonic model for excited state processes in molecular aggregate	Xiaoyu Xie
PO2-73	When do tripdoublet states fluoresce? A theoretical study of copper(II) porphyrin	Xingwen Wang
PO2-74	QUEST#4X: an extension of QUEST#4 for benchmarking multireference wavefunction methods	Yangyang Song
PO2-75	Triple electron attachments with a new Intermediate-Hamiltonian Fock-space coupled-cluster method	Yanmei Hu
PO2-76	Exhaustive screening of topological high-fold degenerate semimetal with chiral structure	Yan Wang
PO2-77	Magnetic topological Weyl fermions in half-metallic In_2CoSe_4	Qiunan Xu
PO2-78	The description of atom and bond reactivity in the language of conceptual density (matrix) functional theory	Bing Wang
PO2-79	Structure and dynamics at Pt/water interfaces revealed by machine learning molecular dynamics	Feiteng Wang
PO2-80	Dimensionality reduction in electronic structure theory via nonlinear dynamics and machine learning: Classical and quantum computing aspects	Chayan Patra
PO2-81	Multivalent interactions in sequence mediated spontaneous association of short RNA chains	Manas Mondal
PO2-82	Quantitative Studies of the Key Aspects in Selective Acetylene Hydrogenation on Pd(111)	Wenbo Xie
PO2-83	A stochastic Schrödinger equation and matrix product state approach to carrier transport in organic semiconductors with nonlocal electron-phonon interaction	Liqi Zhou
PO2-84	TD-DMRG study of exciton dynamics with both thermal and static disorders for Fenna-Matthews-Olson complex	Zirui Sheng