Poster Session 3 – 19:30-21:30, Thursday, 17 October 2024

PO3-1	Multiscale regulation of light-harvesting and quenching in LHCII protein	Yingjie Wang
PO3-2	Long-range electron tunneling through protein junctions	Zdenek Futera
PO3-3	Accelerating reliable multiscale quantum refinement of protein–drug systems enabled by machine learning	Zeyin Yan
PO3-4	ReaxFF force field parameter optimization based on enhanced sampling algorithm	Shuang Li
PO3-5	Stability of Ru@Sn_9 Z intl cluster on a CeO_2 (111) surface and its catalytic activity in Water-Gas-Shift (WGS) reaction.	Sourav Mondal
PO3-6	Theoretical investigation of Fe-based perovskite for chemical looping partial oxidation of methane	Tingting Yang
PO3-7	Importance of material surface structure for photocatalytic reactions in water	Wenhui Ding
PO3-8	Computational insights into how Co/Mn dopants stabilize RuO_2 catalyst under OER conditions	Wenrui Ma
PO3-9	Theory-driven catalyst design for propane dehydrogenation	Xin Chang
PO3-10	Properties of metal-supported ZnO films and their application in water splitting	Yizhen Song
PO3-11	Kinetic simulations of methanol steam reforming and CO_2 h ydrogenation	Yongjie Jiang
PO3-12	How to achieve both stability and activity in Fe-N-C electrocatalysts for ORR: Unifying roles of O and S doping	Yuan Yuan
PO3-13	Efficient and flexible approach for local distortion: Distortion distribution analysis enabled by fragmentation	Yunteng Liao
PO3-14	The role of bases and silver(I) additives in the ligand-promoted β-C(sp^3)-H heteroarylation of free carboxylic acids	Zhewei Li
PO3-15	Noncollinear functional construction schemes in different dimensions	Yu Jing
PO3-16	From collinear functionals to noncollinear functionals	Yunlong Xiao
PO3-17	Exact constraint of density functional approximations at the semiclassical limit	Yunzhi Li
PO3-18	A pointwise machine learning correction to eliminate error cancellation in density functional approximation	Zipeng An
PO3-19	Snap-shots of cluster growth: Electronic structures of a Zintl ion with a linear Fe_3 core, $[Fe_3Sn_{18}]^{4-}$	Zisheng Li
PO3-20	Exact factorization-based density functional theory beyond the Born-Oppenheimer approximation: Case study of a model system	Zixuan Wang
PO3-21	Dynamic correlation in single-ion magnets using density matrix embedding theory	Zhebin Guan

PO3-22	Dynamical mean-field theory of the Holstein polaron: Solving the impurity Green's function by discretizing the hybridization function	Zhecun Shi
PO3-23	Towards realistic simulation of material with ab-initio correlated method	Zigeng Huang
PO3-25	Dual-mode floquet quantum master equation for electronic transport in a bichromatic-driven quantum dot	Vahid Mosallanejad
PO3-26	Machine learning assisted first-principles simulation of tunneling phenomena in spectroscopy	Wei Fang
PO3-27	Memory kernel coupling theory: Obtain time correlation function from higher-order moments	Wei Liu
PO3-28	New insights into phase space representations for finite-state quantum systems and applications in nonadiabatic transition dynamics	Xiangsong Cheng
PO3-29	The exact solution to the finite size one dimension model	Yang He
PO3-30	Theoretical analysis of X-ray spectra of water	Yihao Zhao
PO3-31	Stability of quantum systems beyond canonical typicality	Yu Su
PO3-32	Mechanisms of the interlayer charge transfer in two-dimensional heterostructures: nonadiabatic molecular dynamics investigations	Yuli Lei
PO3-33	The electronic friction effects of strongly correlated systems	Yunhao Liu
PO3-34	Photo-induced dynamics with continuous and discrete quantum baths	Zhaoxuan Xie
PO3-36	Theoretical calculation of organic host-guest doped materials with room temperature phosphorescence	Xiaoli Wang
PO3-37	Hierarchical approximation and question-driven strategy for efficient computation of charge transport in molecular devices	Xuan Ji
PO3-39	Design of bipolar organic matrices for rechargeable redox reactions in non-aqueous electrolytes	Yanislav Danchovski
PO3-40	Device engineering optimization of organic photovoltaic assisted by machine learning	Yaping Wen
PO3-41	Theory of electron spin resonance spectroscopy in scanning tunneling microscopy	Lyuzhou Ye
PO3-42	Modelling the emissive properties of NIR-emitters	Yixuan Li
PO3-43	Simultaneous intra- and intermolecular singlet fission through macrocyclic structures	Zhangxia Wang
PO3-44	PM6/L8-BO thin films through layer-by-layer engineering: Formation mechanism, energetic disorder, and carrier mobility	Zihao Wen
PO3-45	Machine learning-assisted dual-atom sites design with interpretable descriptors unifying	Xiaoyun Lin

PO3-46	DPA-Semi:Machine-learning-based interatomic potentials for group IIB to VIA semiconductors: Towards a universal model	Xingchen Zhang
PO3-47	Machine learning-aided in-situ structure identification of low-dimensional carbon nanomaterials from STM images	Yanbo Li
PO3-48	Predicting regioselectivity in functionalized fullerenes and carboncones using deep learning	Yang Wang
PO3-49	Active learning for fast and robust dynamics simulations	Yifan Hou
PO3-50	Stability prediction of gold nanoclusters with different ligands and doped metals by deep learning	Yuming Gu
PO3-51	UAIQM – the new generation of universal AI models	Yuxinxin Chen
PO3-52	Performance prediction for all small-molecule-based organic solar cells	Zhiwen Zhao
PO3-53	DC-PUHF: Toward large-scale quantum chemical calculation including static correlation	Masatsugu Nishida
PO3-54	Accurate and efficient CCSD(T)/CBS: Development and application for complicated molecules up to 1000 atoms	Peter Nagy
PO3-55	Accurate chemical reaction modeling on noisy intermediate-scale quantum computers using a noise-resilient wavefunction ansatz	Xiongzhi Zeng
PO3-56	Variational quantum computation for large molecules using matrix product state inspired ansatz	Yi Fan
PO3-57	Quantum equation-of-motion method with triple excitations reduced by perturbation and symmetry	Yuhan Zheng
PO3-58	Quantum structure search for molecular ground-state energy computation	Yunong Li
PO3-59	A hybrid framework for simulating molecular systems on quantum computers	Zhanou Liu
PO3-60	Integrating self-initialized local thermalizing lindblad operators for variational quantum algorithm with quantum jump: Implementation and performance	Zhihao Lan
PO3-61	Circuit-efficient Qubit-excitation-based variational quantum eigensolver	Zhijie Sun
PO3-62	Kylin-V: An open-source package calculating the dynamic and spectroscopic properties of large systems	Yihe Xu
PO3-63	Metal-centered boron-wheel cluster of $Y©B_{11}^{2-}$ with rare D_{11h} Symmetry	Xinran Dong
PO3-64	Theoretical studies on strong coupling mechanism between surface plasmon and molecules	Xueyang Zhen
PO3-65	Analytical derivative approaches for vibro-polaritionic structures and properties	Xunkun Huang
PO3-66	Electronic absorption and circular dichroism spectra of one-dimensional bay-substituted chiral PDIs: Effects of intermolecular interactions, vibronic coupling and aggregate size	Yuchuan Xu
PO3-67	Quantum chemical approaches based on renormalized states for strongly correlated systems	Yifan Cheng
PO3-68	Towards an exact description of Compound I in P450	Yifei Huang

PO3-69	Parallel and GPU-accelerated implementation of density matrix renormalization group	Yingqi Tian
PO3-70	Kylin 1.2: An advanced ab-initio density matrix renormalization group program	Yinxuan Song
PO3-71	A multi-reference random phase approximation theory	Yuqi Wang
PO3-72	Diffusion quantum Monte Carlo studies multi-reference systems	Zhiru Huang
PO3-73	Exact analytic solutions of Schrödinger equations with non-separable variables: A case study of 1D quartic potential	Zhiyuan Yin
PO3-74	Formally exact and practically useful analytic solution of harmonium	Wenqing Yao
PO3-75	Distinct single-electron actinide−actinide bonding and fullerene-enhanced magnetism in two-dimensional diactinide endohedral metallofullerene monolayers	Xiaokun Zhao
PO3-76	Molecular descriptors for high-throughput screening of inverted singlet−triplet gap materials	Yu Pang
PO3-77	Employing uncertainty-driven active learning strategies to construct full-dimensional intermolecular potential energy surfaces within spectroscopic accuracy	You Li
PO3-78	Learning molecular conformational energies using semi-local density fingerprints	Zhuofan Shen
PO3-79	Development of a compact Ansatz via operator commutativity screening to avoid local traps and barren plateaus	Dibyendu Mondal
PO3-80	Tools for Overcoming Reliance on Energy-Based Measures in Chemistry: a Tutorial Review	Tianlv Xu
PO3-81	Response of the Mechanical and Chiral Character of Ethane to Ultra-Fast Laser Pulses	Tianlv Xu
PO3-82	Ultra-fast laser pulses as a probe of electron dynamics:A next generation QTAlM perspective	Huan He
PO3-83	Chirality reversal with the carrier-envelope phase: A next generation QTAlM interpretation	Xinjie Zhou
PO3-84	TBA	Xun Wu
PO3-85	Sublinear NMR spin-spin coupling	Bohan Yan