

PROGRAM

June 29

9:00 ~ 22:00 **Registration & Reception**

June 30

8:30 ~ 8:50 **Opening (Chair: Keli Han)**

8:50 ~ 9:00 Photo

Chair **Guozhong He**

9:00 ~ 9:30 Semiclassical Treatment of Non-adiabatic Chemical Dynamics

Hiroki Nakamura

9:30 ~ 10:00 Free Energies of Chemical Reactions in Solution and in Enzymes with *Ab Initio* QM/MM Methods

Weitao Yang

10:00 ~ 10:30 Developing polarized protein-specific charges for accurate protein structure and dynamics

John Z. H. Zhang

10:30 ~ 10:45 Coffee Break

Chair **Daiqian Xie**

10:45 ~ 11:15 An Inhomogeneous Model of Proteins' Dielectric Response and its Applications to Solvation Dynamics and Protein-protein Interactions

Xueyu Song

11:15 ~ 11:45 Quantum Instanton Approach for Calculations of Chemical Reaction Rate Constants

Yi Zhao

11:45 ~ 12:15 Born-Oppenheimer *ab initio* QM/MM Molecular Dynamics Simulations of Enzyme Reactions

Yingkai Zhang

12:15 ~ 14:00 Lunch

Chair **Jinlong Yang**

14:00 ~ 14:30 An efficient computational approach for electronic structure of nanomaterials

Yi Luo

| | |
|---------------|--|
| 14:30 ~ 15:00 | Dissipative particle dynamics simulation technique: A promising mesoscopic simulation tool to help the research in soft condensed matters Zhongyuan Lü |
| 15:00 ~ 15:30 | Multi-aspects of Carbon: C ₆₀ , Carbon Nanotubes, and their Hybrids Haibin Su |
| 15:30 ~ 15:45 | Coffee Break |
| Chair | Xiangyuan Li |
| 15:45 ~ 16:15 | Sparse Numerical Integration Grids for Density Functional Theory Paul Ayers |
| 16:15 ~ 16:45 | Design of new organic semiconductors having improved Anisotropic hole mobilities Weiqiao Deng |
| 16:45 ~ 17:15 | <i>Ab initio</i> studies of S ₀ , S ₁ , and S ₂ equilibrium geometries of pyrazine and simulation of absorption spectra Chaoyuan Zhu |
| 17:15 ~ 17:45 | A reactant-coordinate based time-dependent wave packet approach to triatomic state-to-state reaction dynamics: An application to the H+O ₂ reaction Donghui Zhang |
| 18:15 ~ 19:45 | Banquet |

July 1

| | |
|---------------|--|
| Chair | Jiushu Shao |
| 8:30 ~ 9:00 | Magnetism in graphene systems Jinlong Yang |
| 9:00 ~ 9:30 | Solvent reorganization energy for self-exchange electron transfer reactions between tetra-n-alkylhydrazines and their cations Xiangyuan Li |
| 9:30 ~ 10:00 | Hydrogen-bonding in liquid alcohols from Raman spectroscopy Shilin Liu |
| 10:00 ~ 10:30 | Combined QM/MM Study on Substrate Specificity and Reaction Mechanism of the Enzymatic Aldose-Ketose Isomerization Zexing Cao |
| 10:30 ~ 10:45 | Coffee Break |

| | |
|---------------|---|
| Chair | Wenjian Liu |
| 10:45 ~ 11:15 | Stochastic Formulation of Quantum Dissipative Dynamics Jiushu Shao |
| 11:15 ~ 11:45 | Direct Dynamic Simulation of Adenine Deactivation Zhenyi Wen |
| 11:45 ~ 12:15 | Theoretical simulations on the structures and properties of some functional materials Cheng-Bo Liu |
| 12:15 ~ 14:00 | Lunch |
| Chair | Donghui Zhang |
| 14:00 ~ 14:30 | Rational Drug Design and Discovery through High-Performance Supercomputing Chang-Guo Zhan |
| 14:30 ~ 15:00 | First-Principle Study of Carbon Monoxide Oxidation in Excess of Hydrogen Wei-Xue Li |
| 15:00 ~ 15:30 | Multilayer Multiconfiguration Time-Dependent Hartree Theory with Second Quantization Haobin Wang |
| 15:30 ~ 15:45 | Coffee Break |
| Chair | Hong-Xing Zhang |
| 15:45 ~ 16:15 | Test and modification of the Van der Waal's radii employed in the default PCM model De-Cai Fang |
| 16:15 ~ 16:45 | High resolution spectroscopy of molecules with vibrational and electronic coupling: challenge to nonadiabatic theoretical calculations Yuxiang Mo |
| 16:45 ~ 17:15 | Photon Statistics of Single Quantum System via Generating Function Approach Yujun Zheng |
| 17:15 ~ 17:45 | Attosecond resolution quantum dynamics calculations for atoms and molecules in strong laser fields Keli Han |
| 18:00 ~ 19:30 | Dinner |
| 19:30 ~ 21:30 | Poster Session |

July 2

| | |
|---------------|---|
| Chair | Zexing Cao |
| 8:30 ~ 9:00 | Relativistic Theory for NMR Parameters Wenjian Liu |
| 9:00 ~ 9:30 | Extending the applicability of B3LYP Xin Xu |
| 9:30 ~ 10:00 | Computational Design and Discovery of Conformationally Flexible Inhibitors of Acetohydroxyacid Synthase to Overcome Drug Resistance Associated with W586L Mutation Guang-Fu Yang |
| 10:00 ~ 10:20 | Award Ceremony for Poster Winner (Chairs: Xuebin Chi and Keli Han) |
| 10:20 ~ 10:45 | Coffee Break |
| Chair | Zhong Jin |
| 10:45 ~ 11:00 | GridMol: A Grid Application for Molecular Modeling and Visualization Yanhua Sun |
| 11:00 ~ 11:30 | Ground state tunneling splitting of malonaldehyde using an accurate ab initio potential energy surface: full dimensional quantum calculations v.s. one dimensional reaction path Yimin Wang |
| 11:30 ~ 12:00 | Molecular Dynamics Simulations of the Detoxification of Paraoxon Catalyzed by Phosphotriesterase (PTE) Yirong Mo |
| 12:00 ~ 14:00 | Lunch |
| Chair | Xin Xu |
| 14:00 ~ 14:30 | Potential energy surfaces and infrared spectra for van der Waals complexes: dependence on one intramolecular mode Daiqian Xie |
| 14:30 ~ 15:00 | Molecular Dynamics Simulations in Drug Design Weiliang Zhu |
| 15:00 ~ 15:30 | Quantum mechanical study of atomic hydrogen adsorption and transmission in nano-structures Hong Zhang |
| 15:30 ~ 15:45 | Coffee Break |

| | |
|---------------|--|
| Chair | Cheng-Bo Liu |
| 15:45 ~ 16:15 | The preliminary results on creating our software package of computational chemistry |
| | Jianguo Yu |
| 16:15 ~ 16:45 | Metallophilic Attraction and Luminescence of d^8 and d^{10} Transition Metal Complexes: An Quantum Theoretical Study |
| | Hong-Xing Zhang |
| 16:45 ~ 17:15 | Is there a density functional theory for atoms and molecules |
| | Shubin Liu |
| 17:15 ~ 17:45 | $d-d$ Transitions and optical nonlinearity in coordination metal clusters |
| | Kechen Wu |
| 18:00 ~ 19:30 | Dinner |

July 3

ALL DAY **Excursion to Qingdao's attractions**