Mini Workshop on Nonadiabatic Chemistry

Time\Date	19-May	20-May
8:10-8:30	Opening	
Morning Session	Session Chair: Zhigang Shuai	Session Chair: Jiali Gao
8:30-9:15	William Miller	Weitao Yang
9:15-10:00	Weihai Fang	Zhigang Shuai
10:00-10:20	Coffee Break	Coffee Break
	Session Chair: William Miller	Session Chair: Weihai Fang
10:20-11:05	Kazuo Takatsuka	GuanHua Chen
11:05-11:50	Chaoyuan Zhu	Chao-Ping Hsu
11:50-12:20	Yi Zhao	Jun Jiang
12:20-14:00	Lunch Break	Lunch Break
Afternoon Session	Session Chair: Jiushu Shao	Session Chair: Weitao Yang
14:00-14:45	Yoshitaka Tanimura	Wenjian Liu
14:45-15:30	Yijing Yan	Jiali Gao
15:30-15:50	Coffee Break	Coffee Break
	Session Chair: Kazuo Takatsuka	Session Chair: Yoshitaka Tanimura
15:50-16:20	Xin Chen	Zhenggang Lan
16:20-16:50	Haibo Ma	Zhennan Zhou
16:50-17:20	Qiang Shi	Linjun Wang
	Dinner	Banquet

Scan the QR code to access the conference website

会议地点:

北京大学镜春园78号（怀新园）

北京国际数学中心77201室

Room 77201, #78 Jingchunyuan (Huaixinyuan)

Peking University, Beijing

Mini Workshop on Nonadiabatic Chemistry

19-May

8:30-9:15 William Miller

Classical molecular dynamics simulations of electronically non-adiabatic processes

9:15-10:00 Weihai Fang

Quantum trajectory mean-field approach and its numerical implementation for exploring non-adiabatic effect on the mechanistic photochemistry

10:20-11:05 Kazuo Takatsuka

Recent progress in nonadiabatic electron wavepacket dynamics

11:05-11:50 Chaoyuan Zhu

TDDFT with and without spin-flip in global switching trajectory surface hopping method: Cis-trans azobenzene photoisomerization

11:50-12:20 Yi Zhao

Time-dependent wavepacket diffusion method and its application to nonadiabatic dynamics of carrier in materials

14:00-14:45 Yoshitaka Tanimura

The multi-state quantum hierarchal Fokker-Planck Equation approach to nonadiabatic wave packet dynamics in multi-dimensional spectroscopies

14:45-15:30 Yijing Yan

Advancing the quasi-particle approach to quantum transport and quantum dissipation

15:50-16:20 Xin Chen

Unified understanding of resonance energy transfer and electronically Non-Adiabatic Relaxation Dynamics under the thermal evanescent field

16:20-16:50 Haibo Ma

Density matrix renormalization group quantum chemistry and quantum dynamics

16:50-17:20 Qiang Shi

Generalized master equations: exact memory kernel, high order perturbation, and applications

20-May

8:30-9:15 Weitao Yang

Electronic excited states from pairing matrix fluctuations and particle-particle random phase approximation

9:15-10:00 Zhigang Shuai

Time-dependent matrix product states for exciton-phonon model in aggregates

10:20-11:05 GuanHua Chen

Time-dependent density-functional theory for open quantum systems

11:05-11:50 Chao-Ping Hsu

Diabatic states as determined by molecular properties: singlet fission as an example

11:50-12:20 Jun Jiang

A theoretical study of nonlinear spectroscopy

14:00-14:45 Wenjian Liu

iCI towards full CI

14:45-15:30 Jiali Gao

Diabatic states by construction through generalized singular value decomposition

15:50-16:20 Zhenggang Lan

Nonadiabatic dynamics in polyatomic molecular systems

16:20-16:50 Zhennan Zhou

Surface hopping algorithms in quantum dynamics and thermal equilibrium sampling

16:50-17:20 Linjun Wang

Trajectory surface hopping methods for complex nonadiabatic dynamics with high density of states