

Workshop

Structure, Dynamics, Spectroscopy

Hangzhou Dianzi University, Hangzhou, July 1-4, 2021



The aim of this interdisciplinary workshop is to bring together specialists in *ab initio* quantum chemistry, quantum/semiclassical/quasiclassical dynamics and experimental ultrafast spectroscopy to discuss recent advances, challenges, and future developments at the interface of these three disciplines.

No registration fee

Workshop venue and accommodation:

HDU campus, Shujinag hotel.

Rooms for the participants (380 RMB/night) are reserved.



Workshop schedule:

July 1-3: Scientific activities.

July 4: Discussion of ongoing/future projects, round-table discussion, social program.

Organizers:

Maxim Gelin (Hangzhou Dianzi University, China, maxim@hdu.edu.cn)

Kewei Sun (Hangzhou Dianzi University, China, skw79724@hdu.edu.cn)

Gagik Gurzadyan (Dalian University of Technology, China, gurzadyan@dlut.edu.cn)

Lipeng Chen (Max Planck Institute for the Physics of Complex Systems, Germany, lchen@pks.mpg.de)

Yang Zhao (Nanyang Technological University, Singapore, YZhao@ntu.edu.sg)

Local organizers:

Bai Yiting, Yang Jianmin, Zhan Siying, and Cunzhi Dou
(Hangzhou Dianzi University, China)

Program of invited talks

July 1

8:45-9:00. [Jiangrong Xu](#) (Vice President of HDU)

Opening

9:00-9:45. [Yoshitaka Tanimura](#) (Kyoto University)

Numerically “exact” simulations of entropy production and non-equilibrium work: Boltzmann entropy vs. von Neumann entropy [\[online\]](#)

9:45-10:30. [Yijing Yan](#) (USTC, Hefei)

Noise resolved quantum Langevin equation and system--bath entanglements

10:30-11:00. [Coffee break](#)

11:00-11:45. [Yang Zhao](#) (NTU, Singapore)

Schrodinger-cat states in Landau-Zener-Stueckelberg-Majorana interferometry [\[online\]](#)

11:45-12:30. [Jianzhang Zhao](#) (DUT, Dalian)

Singlet and Triplet Energy Transfer In Pt(II) Complexes Showing Strong Absorption of Visible Light and Long-Lived Triplet Excited State

12:30-14:00. [Lunch](#)

14:00-14:45. [Dmitry Shalashilin](#) (University of Leeds)

A brief overview of Coherent State based methods of quantum nonadiabatic dynamics [\[online\]](#)

14:45-15:30. [Xiao Zheng](#) (USTS, Hefei)

Low-temperature dissipative dynamics of strongly correlated quantum impurity systems

15:30-16:00. [Coffee break](#)

16:00-16:45. [Lipeng Chen](#) (Max Planck Institute for the Physics of Complex Systems, Germany)

Wavepacket dynamics at conical intersection and its spectroscopic manifestation [\[online\]](#)

16:45-17:30. [Gagik Gurzadyan](#) (DUT, Dalian)

Relaxation Processes from Upper Excited States: Breaking Kasha-Vavilov Rule

18:00-19:00. [Dinner](#)

July 2

9:00-9:45. **Yi Zhao** (Xiamen University)

Stochastic Schrodinger equation and its application to ultrafast quantum dynamics

9:45-10:30. **Wei Zhuang** (Fuzhou IAS)

Simulating THz Optical Kerr Spectra of a solvated Lysozyme-Inhibitor Binding Complex

10:30-11:00. **Coffee break**

11:00-11:45. **Chuancun Shu** (CSU, Changsha)

Quantum Dynamics Identification for Visualizing Hidden Quantum Processes

11:45-12:30. **Guichao Kuang** (Changsha, CSU)

Single component BODIPY derivatives as white light emission materials

12:30. **Lunch**

14:00-14:45. **Raffaele Borrelli** (University of Turin)

Non-Equilibrium Thermo Field Dynamics of Closed and Open System Evolution: Theory, Implementation and Application **[online]**

14:45-15:30. **Linjun Wang** (Zhejiang University)

Nonadiabatic Dynamics in Extended Systems

15:30-16:00. **Coffee break**

16:00-16:45. **Hong-Guang Duan** (UHH and EuXFEL)

Quantum Coherent Dynamics in Natural/Artificial Photoactive Complexes **[online]**

16:45-17:30. **Yiyang Yan** (Zhejiang University of Science and Technology, Hangzhou)

Variational approach to time-dependent emission spectrum of a strongly driven qubit

18:00-20:00. **Conference dinner**

July 3

9:00-9:45. Haibo Ma (Nanjing University)

Spectroscopy and ultrafast excited state dynamics in organic semiconductor: a theoretical simulation

9:45-10:30. Pavlo Dral (Xiamen University)

Efficient excited-state simulations with machine learning and semiempirical methods

10:30-11:00. Coffee break

11:00-11:25. Wenjun Ni (DUT, Dalian)

Ultrafast relaxation pathways in perylene film: excimer formation versus singlet fission

11:25-11:50. Xue Zhang (DUT, Dalian)

Dependency of the Charge Transfer and Intersystem Crossing on Molecular Geometry and Electronic Coupling in Compact Anthracene-Naphthalimide Dyads

11:50-12:15. Yuqi Hou (DUT, Dalian)

Efficient Spin-Orbit Charge Transfer Intersystem Crossing (SOCT ISC) in Compact Bodipy-Carbazole Electron Donor-Acceptor Dyads

12:30. Lunch

14:00-14:45. Zhiguo Lv (Shanghai Jiaotong University)

Plateau dynamics with quantized oscillations of a strongly driven qubit: Counter-rotating hybridized rotating-wave method **[online]**

14:45-15:30. Wenjie Dou (Westlake University, Hangzhou)

Excited-state electronic structure and non-adiabatic dynamics as applied to chemisorption and photochemistry

15:30-16:00. Coffee break

16:00-16:45. Jing Liu (HUST, Wuhan)

Operational definition of the quantum speed limit

16:45-17:30. Wenbo Yang (DUT, Dalian)

Excited state dynamics in photosensitizers

17:30-18:15. Dinner

18:15.-22:30. Boat trip along the Qiantang River & Grand Canal