

# **International (CECAM–CN) Workshop**

## **on Excited States and Dynamics in Condensed Phases**

**May 15~16, 2024**

**Beijing, China**



# International (CECAM-CN) Workshop on Excited States and Dynamics in Condensed Phases

## Program

May 15 (Wednesday), 2024   Conference Room I, 1st Floor, CSRC Building	
<b>Morning Session Chair I: Shiwu Gao</b>	
09:00-09:10	<b>Opening</b> Welcome remarks by Su-Huai Wei
09:10-09:40	<b>The DFT-NEGF approach to electronic and atomic structure under electronic current</b> Mads Brandbyge (Technical University of Denmark)
09:40-10:10	<b>Subnanometer resolved single-molecule optical spectroscopy</b> Zhen-Chao Dong (University of Science & Technology of China)
10:10-10:40	<i>Photography; Coffee &amp; Tea Break</i>
<b>Morning Session Chair II: Su-Huai Wei</b>	
10:40-11:10	<b>Excited electronic states calculated by converging on saddle points on the energy surface generated by a self-interaction corrected density functional</b> Hannes Jonsson (University of Iceland)
11:10-11:40	<b>Theoretical study of chemical processes at the water interface</b> Chong-Qin Zhu (Beijing Normal University)
11:40-14:00	<i>Lunch (Canteen, B1) &amp; Rest</i>

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May 15 (Wednesday), 2024   Conference Room I, 1st Floor, CSRC Building	
<b>Afternoon Session Chair I: Bing Huang</b>	
14:00-14:30	<b>Harnessing hot-carrier transfer: new insights in ethylene epoxidation catalysis</b> Anders Hellman (Chalmers University of Technology)
14:30-15:00	<b>Computational study on the dome-like phase diagram of several superconductors</b> Kai Liu (Renmin University of China)
15:00-15:30	<i>Coffee &amp; Tea Break</i>
<b>Afternoon Session Chair II: Jun Kang</b>	
15:30-16:00	<b>Ab initio real-time quantum dynamics of charge carriers in momentum space</b> Qi-Jing Zheng (University of Science & Technology of China)
16:00-16:30	<b>Electron-phonon coupling and anomalous phonon transport</b> Wu Li (Eastern Institute of Technology, Ningbo)
17:15-18:15	<i>Dinner (Canteen, B1)</i>

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## Program

May 16 (Thursday), 2024   Conference Room I, 1st Floor, CSRC Building	
<b>Morning Session Chair I: Peng-Fei Guan</b>	
09:00-09:30	<b>Basis-error-free RPA correlation energies for atomic and diatomic systems based on the Sternheimer equation</b> Xin-Guo Ren (Institute of Physics CAS)
09:30-10:00	<b>Nonadiabatic dynamics and time resolved spectra</b> Zheng-Gang Lan (South China Normal University)
10:00-10:30	<i>Coffee &amp; Tea Break</i>
<b>Morning Session Chair II: Zijing Ding</b>	
10:30-11:00	<b>Theoretical study on coherent spin dynamics of magnetic molecules on surfaces</b> Xiao Zheng (Fudan University)
11:00-11:30	<b>Quantum dynamics and non-adiabatic effects simulated by the initial value representation method</b> Xin-Zheng Li (Peking University)
11:30-14:00	<i>Lunch (BI Canteen) &amp; Rest</i>

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May 16 (Thursday), 2024   Conference Room I, 1st Floor, CSRC Building	
<b>Afternoon Session Chair I: Kai Liu</b>	
14:00-14:30	<b>Exciton-phonon coupling in semiconductors</b> Jun Zhang (Institute of Semiconductors CAS)
14:30-15:00	<b>Light control of phase transitions</b> Sheng Meng (Institute of Physics CAS)
15:00-15:30	<i>Coffee &amp; Tea Break</i>
<b>Afternoon Session Chair II: Shiwu Gao</b>	
15:30-16:00	<b>Gilbert damping of low-dimensional ferromagnetic materials</b> Zhe Yuan (Fudan University)
16:00-16:30	<b>Density-matrix embedding theory based multi-configurational wavefunction approach to strongly correlated single-impurity systems</b> Hong Jiang (Peking University)
16:30-17:00	<b>Closing</b> Concluding remarks by Shiwu Gao
17:15-18:15	<i>Dinner (Canteen, B1)</i>