

**International Conference on Algorithms and Applications for
Excited State Electronic Structure Theories**

August 8-10, 2016

Location: Conference room II, 3rd floor, CSRC Building

Day 1: August 8, 2016 (Monday)	
8:00am-8:50am	Registration
8:50am-9:00am	Opening Remark
Morning Session (Chaired by Weitao Yang)	
9:00am-10:00am	Plenary Lecture by Prof. Roberto Car: Overview of DFT development
10:00am-10:40am	Group photo and coffee break
10:40am-11:20am	Prof. Zhigang Shuai: Theory and application of excited state decay rate formalism for OLEDs
11:20am-12:00am	Prof. Gang Lu: Charge Stripe Formation in Perovskite Photovoltaics – A Large-Scale TDDFT Study
12:00-2:00pm	Lunch Break
Afternoon Session (chaired by Limin Liu)	
2:00pm-2:40pm	Prof. Wibe Albert de Jong: Advancing Algorithms of Correlated and Dynamical Electronic Structure Simulations
2:40pm-3:20pm	Prof. Xinzheng Li: Quantum simulation of hydrogen and hydrogen bonds

3:20pm-3:40pm	Coffee break
3:40pm-4:20pm	Prof. Sheng Meng: Excited state electron-ion dynamics in condensed matter
4:20pm-5:00pm	Prof. Shiwu Gao: Quantum aspects of plasmonic excitations
Day 2, August 9, 2016 (Tuesday)	
Morning Session (Chaired by Lin Lin)	
9:00am-9:40am	Prof. Weitao Yang: Electronic Excited States from Pairing Matrix Fluctuations and Particle-Particle Random Phase Approximation
9:40am-10:20am	Prof. Lixin He: First principles investigation of plasmons on graphene
10:20am-10:40am	Coffee break
10:40am-11:20am	Prof. Stefano Baroni: Excited states without virtual orbitals
11:20am-12:00	Prof. Chao Yang: Low rank approximation in G0W0 calculations
12:00-2:00pm	Lunch
Afternoon Session (chaired by Zhigang Shuai)	
2:00pm-2:40pm	Prof. Thomas Frauenheim: Recent DFTB extension for improving accuracy and boosting the efficiency for computational applications to nanomaterials
2:40pm-3:20pm	Prof. Lin Lin: Adaptively compressed exchange operator
3:20pm-3:40pm	Coffee break
3:40pm-4:20pm	Prof. Fabien Bruneval: Electronic excitations in molecules with many-body perturbation theory

4:20pm--5:00pm	Prof. Hong Jiang: Towards first-principles approaches to electronic band structure of complex materials
Day 3: August 10, 2016 (Wednesday)	
Morning Session (Chaired by Thomas Frauenheim)	
9:00am-9:40am	Prof. Eberhard Kurt Ulrich Gross: Ultrafast laser-induced demagnetization of solids: Understanding the mechanism with real-time TDDFT
9:40am-10:20am	Prof. Xifan Wu: X-ray absorption spectra of H-bonded materials by many-body perturbation theory
10:20am-10:40am	Coffee break
10:40am-11:20am	Prof. Zhenyu Zhang: Spintronics and half-metallicity based on monolayered nanoribbons
11:20am-12:00	Prof. Chi-Yung Yam: Nanoscale optoelectronics: the interaction of nanoscale junctions with light
12:00-2:00pm	Lunch
Afternoon Session (Chaired by Stefano Baroni)	
2:00pm-2:40pm	Prof. Guanhua Chen: Quantum simulation of open quantum systems
2:40pm-3:20pm	Prof. Gilberto Teobaldi: Linear-scaling, self-consistent projector constrained DFT approximations to charge-transfer at extended interfaces
3:20pm-4:00pm	Prof. Suhuai Wei: Design of 2D Materials for Energy Related Applications
Conference Adjourn	