Program

Jan 11 (Wed.), 2017

08:45	~	09:00	Opening session

Session 1 Chair: Wenjian Liu (Peking Univ)

09:00	~	09:50	**Seung Kyu Min (UNIST)** A new approach to non-adiabatic molecular dynamics based on exact factorization: Theory and Applications
09:50	~	10:00	**Tea Break**
10:00	~	10:50	**Ganglong Cui (Beijing Normal Univ)** Methodological Developments of Conical Intersection Optimization and Trajectory-Based Nonadiabatic Dynamics Simulation
10:50	~	11:00	**Tea Break**

Session 2 Chair: Muneaki Kamiya (Gifu Univ)

11:00	~	11:50	**Yu Harabuchi (Hokkaido Univ)** Automated search for minimum energy conical intersection and seam of crossing geometries: Application to photoreactions
11:50	~	14:30	**Lunch**

Session 3 Chair: Young Min Rhee (POSTECH)

14:30	~	15:20	**Eunji Sim (Yonsei Univ)** Avoiding Self-Interaction-Errors in Density Functional Theory
15:20	~	15:30	**Tea Break**
15:30	~	16:20	**Satoru Iuchi (Nagoya Univ)** Model electronic Hamiltonian for transition metal complexes: application to molecular dynamics simulation of light-induced spin crossover
16:20	~	16:30	**Tea Break**
16:30	~	17:20	**Takeshi Yoshikawa (Waseda Univ)** Excited-state calculation method using dynamical polarizabilities for large systems based on divide-and-conquer method
17:20	~	20:00	Dinner

Program

Jan 12 (Thu.), 2017

Session 1			Chair: Jin Yong Lee (Sungkyunkwan Univ.)
09:00	~	09:50	**Takeshi Sato (Univ of Tokyo)** Development and applications of time-dependent ab initio wavefunction methods for intense-laser driven multielectron dynamics of atoms and molecules
09:50	~	10:00	**Tea Break**
10:00	~	10:50	**Yi Zhao (Xiamen Univ.)** Time-dependent wavepacket diffusive method and its applications to carrier quantum dynamics in organic materials
10:50	~	11:00	**Tea Break**
Session 2			Chair: Koji Ando (Kyoto Univ.)
11:00	~	11:50	**Kyoung Koo Baeck (GWNU)** A Practical Scheme to Construct Diabatic States and to Evaluate Nonadiabatic Coupling Terms by Using Adiabatic Energies Only
11:50	~	14:30	**Lunch**
14:30	~	17:20	**Excursion (Buyeo)**
17:20	~	20:00	Banquet

Program

Jan 13 (Fri.), 2017

Session 1			Chair: Hiromi Nakai (Waseda Univ.)
09:00	~	09:50	**Haibo Ma (Nanjing Univ.)** Electronic Excited States in Organic Semiconductors
09:50	~	10:00	**Tea Break**
10:00	~	10:50	**Cheol Ho Choi (KNU)** Efficient Implementations of Nonadiabatic Molecular Dynamics in GAMESS
10:50	~	11:00	**Tea Break**
Session 2			Chair: Shinji Saito (IMS)
11:00	~	11:50	**Jian Liu (Peking Univ.)** A unified theoretical framework for mapping models for multi-state Hamiltonian
11:50	~	14:30	**Lunch**
Session 3			Chair: Michio Katouda (RIKEN AICS)
14:30	~	15:20	**Joonsuk Huh (POSTECH)** Quantum computing of vibronic transition
15:20	~	15:30	**Tea Break**
15:30	~	16:20	**Xiao Zheng (Univ. of Science and Technology of China)** An accurate and universal hierarchical dynamics approach to open quantum systems
16:20	~	16:30	**Tea Break**
16:30	~	17:20	**Takatoshi Fujita (IMS)** Quantum Dynamics of Molecular Excitons
17:20	~	18:00	Panel Discussion
18:00	~	20:00	Dinner