Program

March 7

9:00 - 9:10	Kiyotaka Asakura (CRC, Hokkaido)	Opening Address
9:10 - 9:20	Chantal Daniel (Strasbourg)	Welcome Address

Chair, Koichi Yamashita (Tokyo)

9:20 - 10:05	William H. Miller (Berkeley)	Using the Initial Value Representation of Semiclassical Theory to Add Quantum Effects to Classical Molecular Dynamics Simulations
10:05 - 10:40	George C. Schatz (Northwestern)	Coupling Quantum Mechanics to Classical Electrodynamics

Coffee Break

Chair, Emmanuel Fromager (Strasbourg)

11:00 - 11:35	Joel M. Bowman (Emory)	Unusual Reaction Dynamics in High Dimensional Systems
11:35 - 12:00	Chantal Daniel (Strasbourg)	Inorganic Photoisomerization The Case Study of Rhenium (I) Complexes

Lunch

Chair, Agustí Lledós (Barcelona)

14:00 - 14:35	Kimihiko Hirao (RIKEN)	Long-range-corrected Density Functionals
14:35 - 15:10	Gernot Frenking (Marburg)	Reaction Pathways for Activation of Small Molecules by Amido Substituted Ditetrylenes R_2N-EE-NR_2 (E = Si - Sn)
15:10 - 15:45	Odile Eisenstein (Montpellier)	Optimizing a Catalytic Cycle: the Case of the Schrock Olefin Metathesis Catalysts

Coffee Break

Chair, Shigeyoshi Sakaki (Kyoto)

16:15 - 16:50	William A. Goddard III (Cal. Tech.)	First-Principles Based Multiscale Multiparadigm Methods for Applications to Complex Systems
16:50 - 17:35	Keiji Morokuma (Kyoto)	Fascinating World of Chemical Reactions: Theory and Simulations

Group Photo

19:30 - 21:30	Banquet	Maison Kammerzell (16 place de la cathédrale)

March 8

Chair, Jun-ya Hasegawa (CRC, Hokkaido)

9:30 - 9:55	Tetsuya Taketsugu (Hokkaido)	Theoretical Study on Photo-Isomerization Pathways of Azobenzene: AIMD Simulations and Excited-State Potential Energy Surfaces
9:55 - 10:20	Feliu Maseras (Catalonia)	Oxidative Addition to Pd(0): a Simple Step with Many Nuances

Coffee Break

Chair, Tom Ziegler (Calgary)

10:50 - 11:25	Walter Thiel (Max-Planck-Inst.)	Theoretical Studies of Enzymatic Reactions
11:25 - 12:00	Per E. M. Siegbahn (Stockholm)	The Mechanism for Water Oxidation in Photosystem II

Lunch

Chair, Joel M. Bowman (Emory)

14:00 - 14:25	Djamaladdin G. Musaev (Emory)	Knowledge-based Catalyst Designing: From Solar-to-Chemical Conversion to Stereoselective C-H Bond Functionalization. Interplay of Theory and Experiment
14:25 - 15:00	Hiroshi Nakatsuji (QCRI)	Solving Three Big Quantum Principles Governing Complex Chemistry

Coffee Break

Chair, Kiyotaka Asakura (CRC, Hokkaido)

15:30 - 16:05	Iwao Ohmine (IMS)	Water Dynamics; Fluctuation, Phase Transitions and Chemical Reactions
16:05 - 16:50	Martin Karplus (Harvard)	Biomolecular Motors: Insights from Simulations

16:50 - 17:00	Shigeyoshi Sakaki (Kyoto)	Closing Remarks