Version: April 6, 2012

JST International Symposium on Multi-scale Simulation of Condensed-phase Reacting Systems

Program

May 10 (Thr)

9:00 - 9:30 **Opening address**

Session I: Quantum Chemistry of Reacting Systems (Chair: Koji Yasuda)

9:30 - 10:05 **Nobuaki Koga** (Nagoya University)
"σ Bond Cleavages in the Coordination Sphere of Transition Metals"

10:05 - 10:40 **Masaharu Nakamura** (Kyoto University)
"Development of Metal-Catalyzed C–C Bond Forming Reactions:
An example of interplay of computational modeling and experiment"

10:40 - 11:00 *Coffee Break*

11:00 - 11:35 **Cherumuttathu H. Suresh** (National Institute for Interdisciplinary Science and Technology)
"Application of Transferable and Additive Quantum Chemical Properties to Chemical Reactivity"

11:35 - 12:10 **Stephan Irle** (Nagoya University)
"Autocatalytic Networks of Chemical Reaction Processes in High-temperature Materials Science"

12:10 - 13:30 *Lunch*

13:30 - 15:00 **Poster Session**

Session II: Computational Biophysics and Biochemistry: Part 1 (Chair: Takahisa Yamato)

15:10 - 15:45 **Seiji Mori** (Ibaraki University)
"Recent Advances on Computational Studies of Mechanistic Insight into Prostaglandin Synthases"

15:45 - 16:20 **Masahide Terazima** (Kyoto University)
"Biologically Important Protein Reaction Dynamics"

16:20 - 16:40 *Coffee Break*

16:40 - 17:15 **John E. Straub** (Boston University)
"Dynamics of Methionine Ligand Rebinding in Cytochrome c"

17:15 - 17:35 **Masayoshi Takayanagi** (Nagoya University)
"Theoretical Study on the Incipient Relaxation Process of Photolyzed Carbonmonoxy Myoglobin by Perturbation Ensemble Molecular Dynamics Method"

May 11 (Fri)

Session III: Computational Biophysics and Biochemistry: Part 2 (Chair: Ikuo Kurisaki)

9:00 - 9:35 **Isseki Yu** (Aoyama Gakuin University)
"Space-Time Characteristics of the Protein Thermodynamic Quantities under the Cytoplasmic Condition of Extremophiles: Kirkwood-Buff Approach on the Preferential Hydration, Partial Molar Volume, and Transfer Free Energy"

9:35 - 10:10 **Masayoshi Nakasako** (Keio University)
"Static and Dynamical Pictures of Protein Hydration - To Understand Why Water is Indispensable for Structures and Functions of Proteins"

10:10 - 10:30 *Coffee Break*

Session III (Chair: Pornpan Pungpo)

10:30 - 11:05 **Manuel Angel Aguilar** (University of Extremadura)
"Solvent and Counterion Effects on the Absorption and Emission Spectra of a Model of the Rhodopsin Chromophore"

11:05 - 11:40 **Supa Hannongbua** (Kasetsart University)
"QM/MM Investigation on the Enzymatic Reaction of HIV-1 Reverse Transcriptase"

11:40 - 12:15 **Takeshi Ishikawa** (Tohoku University)
"Quantum Chemical Study for Condensed-phase System Based on the Fragment Molecular Orbital Method: Applications to Geometry Optimization and Molecular Dynamics Simulation"

12:15 - 13:30 *Lunch*

13:30 - 15:00 **Poster Session**

Session IV: Quantum Chemistry of Biomacromolecules (Chair: Susumu Okazaki)

15:10 - 15:55 **Kazuo Kitaura** (Kobe University)
"Calculations of Binding Free Energy Between Protein and Ligand Using the Fragment Molecular Orbital Method"

15:55 - 16:15 *Coffee Break*

Session V: Computational Chemistry of Condensed-phase Reacting Systems: Part 1 (Chair: Yuko Okamoto)

16:15 - 16:50 **Ignacio Fdez**. **Galván** (University of Extremadura)
"Electronic Excited States in Solution: An Averaged QM/MM Treatment"

16:50 - 17:25 **Nobuyuki Matubayasi** (Kyoto University)
"Extended Concept of Solvation toward Unified Understandings of Molecular Binding in Weakly Ordered Systems"

17:25 - 18:00 **Manuel F. Ruiz-López** (Nancy University)
"Chemical Reactivity at the Air/Water Interface: Insights from QM/MM Molecular Dynamics Simulations"

18:30 - **Reception Party**

May 12 (Sat)

Session VI: Computational Chemistry of Condensed-phase Reacting Systems: Part 2
(Chair: Norifumi Yamamoto)

9:30 - 9:50	**Norio Takenaka** (Nagoya University) "Theoretical Study on Hydration Structure and Charge Distribution of Zwitterionic Glycine in Aqueous Solution via the Number-Adaptive Multiscale QM/MM-MD Method"
9:50 - 10:25	**Toshio Asada** (Osaka Prefecture University) "Computational Approach to the Optimization Method of the Reaction Pathway on the Free Energy Surface"
10:25 - 11:00	**Hao Hu** (The University of Hong Kong) "Developments and Applications of QM/MM Free Energy Simulations of Important Biochemical Processes"
11:00 - 11:20	*Coffee Break*

Session VI (Chair: Atsushi Yamada)

11:20 - 11:55	**Satoru Iuchi** (Nagoya University) "Molecular Dynamics Simulation Study of Electronic Excited States of Transition Metal Complexes in Aqueous Solution"
11:55 - 12:15	**Kenta Yamada** (Nagoya University) "An Efficient Ewald Method for First-Principles QM/MM Calculations"
12:15 - 12:35	**Yoshiyuki Koyano** (Nagoya University) "Reaction Path Tracing via Free Energy Gradient Method for Ammonia Ionization Process in Aqueous Solution"
12:35 -	**Closing address**