Satellite Meeting of ICMS2013 in Nagoya:
Large-Scale Molecular Simulations in Biology, Chemistry, and Physics

Date: Nov. 16 (Sat), 2013

Venue: ES Bldg., Nagoya University

Organizers: Susumu Okazaki and Yuko Okamoto

Sponsored by: 'Campus Asia Program: A Cooperative Asian Education Gateway for a Sustainable Society: Expanding the Frontiers in Science and Technology of Chemistry and Materials', Nagoya University & Tohoku University

Computational Materials Science Initiative (CMSI)

The Molecular Simulation Society of Japan

Program

Time	Speaker	Title
9:30 - 9:50	Masaki SASAI	Dynamical energy landscape theory of protein functioning
9:50 - 10:20	Charles L. BROOKS III	Multi-scale explorations of virus maturation dynamics and mechanics
10:20 - 10:40	Yuji SUGITA	Molecular mechanisms for drug releasing from multi-drug transporter MATE
10:40 - 11:00	Coffee Break	
11:00 - 11:20	Masataka NAGAOKA	Statistical Approaches of Relaxations and Reactions in Proteins
11:20 - 11:50	Jeffery B. KLAUDA	Force Field Development and Molecular Simulations of Model Lipid Membranes
11:50 - 12:10	Stephan IRLE	What can we learn from MD simulations of carbon nanotube and graphene growth?
12:10 - 12:40	John E. STRAUB	Protein association and aggregation in micelles and membranes: Roles of solvation and confinement
12:40 - 14:10	Lunch	
14:10 - 14:30	Noriyuki YOSHII	Molecular dynamics study of formation and solubilization of micelles
14:30 - 15:00	Li Suan MAI	Mechanical stability of proteins: from coarse-grained to all-atom simulations
15:00 - 15:20	Takahisa YAMATO	Molecular mechanism of allosteric communication in proteins: Computational analysis of energy flow
15:20 - 15:50	Giovanni LA PENNA	Extending first-principles simulations to the nanoscale: learning with Quantum-Espresso
15:50 - 16:20	Coffee Break	
16:20 - 16:40	Hironori KOKUBO	Two-dimensional replica-exchange method for predicting protein-ligand binding structures
16:40 - 17:10	Huai SUN	Reactive force field and its applications
17:10 - 17:30	Yoshimichi ANDOH	Molecular dynamics study of biomembranes: A challenge to plasma membrane simulation
17:30 - 18:00	Robert BEST	How important are non-native contacts for determining protein folding mechanisms?
18:00 - 18:20	Motonori OTA	Hierarchical description of protein structural change by Motion Tree
18:20 - 19:00		
19:00 - 21:00	Banquet	