Program

Monday, November 10 (Day 1)		
8:30−		**Registration**
9:00− 9:10		Opening Remarks
		Chair: Wataru Shinoda (Nagoya University)
9:10− 9:50	O-01	**Shuichi Nosé: An Appreciation** Michael L. Klein (Temple University)
9:50−10:30	O-02	**Molecular Simulation of Complex Transitions** Bernd Ensing (University of Amsterdam)
10:30−10:50		Break
		Chair: Motoyuki Shiga (JAEA)
10:50−11:30	O-03	**Extending the classical phase space: Free energies from molecular dynamics with very large time steps** Mark E. Tuckerman (New York University)
11:30−12:10	O-04	**Sampling Rare Events in Biomolecular Simulations** Luca Maragliano (Istituto Italiano di Tecnologia)
12:10−13:10		**Lunch**
13:10−14:50		**Poster Session 1**
		Chair: Hisashi Okumura (Institute for Molecular Science)
15:00−15:40	O-05	**Extended-Ensemble Simulations of Some (Spin) Glass Models in Finite Dimensions** Koji Hukushima (The University of Tokyo)
15:40−16:20	O-06	**Exploring Free Energy Surfaces with Generalized-Ensemble Algorithms** Ayori Mitsutake (Keio University)
16:20−16:40		**Break**
		Chair: Masaharu Isobe (Nagoya Institute of Technology)
16:40−17:20	O-07	**Large Deviations and Glass Transitions** Juan P. Garrahan (University of Nottingham)
17:20−18:00	O-08	**Logarithmic Mean-Force Dynamics (LogMFD) for Sampling Rare Events** Tetsuya Morishita (AIST)
18:15−20:15		**Banquet**

Tuesday, November 11 (Day 2)		
8:30–		**Registration**
9:10– 9:50	O-09	Chair: Yoshitaka Tateyama (NIMS) **A Variational Approach to Enhanced Sampling and Free Energy Calculations** Michele Parrinello (ETH Zurich)
9:50–10:30	O-10	**Electrochemistry from First-Principles Molecular Dynamics** Osamu Sugino (The University of Tokyo)
10:30–10:50		Break
10:50–11:30	O-11	Chair Ayori Mitsutake (Keio University) **λ-Dynamics Free Energy Calculations: An Extended Lagrangian Approach** Charles L. Brooks III (University of Michigan)
11:30–12:10	O-12	**Path Search and Sampling Methods for Biomolecular Systems** Hiroshi Fujisaki (Nippon Medical School)
12:10–13:20		**Group Photo** **Lunch**
13:20–15:00		**Poster Session 2**
15:10–15:50	O-13	Chair: Tetsuya Morishita (AIST) **Sampling Using Stochastic Nosé Devices: From Molecular to Fluid Dynamics** Benedict J. Leimkuhler (University of Edinburgh)
15:50–16:30	O-14	**A Legacy of Shuichi Nosé's 1984 Work** William G. Hoover (Ruby Valley Research Institute)
16:30		Closing Remarks