

Molecular Dynamics Simulation on Micro/Nano Systems (August 4 ~ 12, 2008 at APCTP Headquarters, Pohang)

August 4, 2008 (Mon) (Chair: Sang-Rak Kim)

12:00 ~ 13:45 Registration with Coffee

13:45 ~ 13:55 Opening speech (Sang-Rak Kim)

13:55 ~ 14:00 Welcoming from APCTP (Seunghwan Kim)

14:00 ~ 16:00 Wonmuk Hwang (Texas A&M University)

Biomolecular simulation HOWTO

16:00 ~ 16:20 Coffee Break

16:20 ~ 18:20 Wonmuk Hwang (Texas A&M University)

The tug-of-war sampling for calculating molecular forces

18:20 ~ Welcoming Dinner

August 5, 2008 (Tue) (Chair: Hawoong Jeong)

11:00 ~ 12:00 Wonmuk Hwang (Texas A&M University)

Force generation by molecular motors: A case study for kinesin

15:00 ~ 17:00 Bae-Yeun Ha (University of Waterloo)

DNA organization in a living cell

Basic concepts in polymer physics

19:00 ~ 21:00 Free Discussions

August 6, 2008 (Wed) (Chair: Youngkyun Jung)

10:00 ~ 12:00 Bae-Yeun Ha (University of Waterloo)

Intermolecular interactions in biology and biophysics

Can peptide charge rescue multicellular organisms?

12:00 ~ 12:10 Photo

14:00 ~ 18:00 Free Discussions

18:00 ~ Dinner & Beer

August 7, 2008 (Thu) (Chair: Sang Bub Lee)

10:00 ~ 11:00 Jiyong Park (SNU)

Pattern selection of steric zipper patterns in the amyloid cross- β spine

11:00 ~ 12:00 Chanil Jeon (KAIST)

Diffusion of adsorbed polymer on a corrugated surface

14:00 ~ 16:00 Kyu Kwang Han (Paichai University)

Multiensemble Sampling Method (why and how to implement on MC and MD)

16:00 ~ 17:00 Free Discussions

19:00 ~ 21:00 Free Discussions

August 8, 2008 (Fri) (Chair: Hyungtae Kook)

10:00 ~ 12:00 Xin Zhou (APCTP)

*Dual-resolution coarse-grained simulations in polymer melts**Accelerated molecular dynamics for slow dynamics*

14:00 ~ 16:00 Xin Zhou (APCTP)

*New scheme to bridge different-level coarse-grained models**Fast adaptive calculation of density of state for enhanced sampling in large systems*

16:00 ~ 17:00 Free Discussions

19:00 ~ 21:00 Free Discussions

August 9, 2008 (Sat)

Tour or Hiking

August 10, 2008 (Sun) (Chair: Kyu Kwang Han)

10:00 ~ 11:00 Hyungtae Kook (Kyungwon University)

Brownian motor

11:00 ~ 12:00 Sangui Lee (Kyungpook Nat'l University)

A seamless approach to multiscale complex fluid simulation

12:00 ~ 13:00 Meesoon Ha (KAIST)

Flow control through polymer-grafted smart nanofluidic channels

15:00 ~ 17:00 Free Discussions

19:00 ~ 21:00 Free Discussions

August 11, 2008 (Mon) (Chair: Sangui Lee)

10:00 ~ 11:00 Sang Bub Lee (Kyungpook Nat'l University)

DNA bending stiffness on small length scales

11:00 ~ 12:00 Hawoong Jeong (KAIST)

Dynamics of entangled linear polymer melts

15:00 ~ 16:00 Juin Kim (KAIST)

Diffusion/reaction in confined polymer chain

16:00 ~ 17:00 Youngkyun Jung (KISTI)

Relaxation of self-avoiding polymer

19:00 ~ 21:00 Free Discussions

August 12, 2008 (Tue) (Chair: Meesoon Ha)

10:00 ~ 11:00 Sungyun Kim (APCTP)

Computability of entropy and information in classical Hamiltonian systems

11:00 ~ 12:00 Sang-Rak Kim (Kyonggi University)

The validity of samplings in molecular dynamics

12:00 ~ 13:30 Lunch

13:30 ~ 14:00 Closing