Singapore-MIT Alliance for Research and Technology

BIOSYSTEMS AND MICROMECHANICS

**Focused Seminar Series on Computational Techniques**

15 Feb — 11 Apr 2016, Level 5 Seminar Room, Enterprise Wing @ UTown, S'138602

# Seminar 3: Computer Simulations of Biomolecules and Their Interactions

**Dr Dai Liang**

Singapore-MIT Alliance for Research and Technology

**Date:** 29 Feb 2016, Monday

**Time:** 4pm to 5pm

**Venue:** Perseverance Room, Enterprise Wing Level 5 @ UTown

## Abstract

In this talk, I will briefly describe the methods of molecular dynamic (MD) simulations and discuss their applications in biological research via a few case studies, including (1) protein-ligand binding for drug design (2) penetration of biomolecules into cell membranes (3) quantum mechanics/molecular mechanics (QM/MM) calculation for biological catalysis, *i.e.*, how enzymes speeds up reactions.

## Biography

Dr Dai Liang is currently a Research Scientist in BioSystems and Micromechanics Inter-Disciplinary Research Group of Singapore-MIT Alliance for Research and Technology (SMART). Dr Dai pursued the undergraduate study from 2000 to 2004 in the physics department of University of Science and Technology of China (USTC), followed by a PhD study from 2004 to 2008 in the physics department of National University of Singapore (NUS). Before joining SMART in 2010, Dr Dai was a postdoc in the Center for Computational Biology and Bioinformatics of Indiana University. Dr. Dai applies multi-scale modelling, from atomistic to coarse-grained, and statistical mechanics to perform research in soft matter physics and biophysics, with close collaboration with experimental groups in MIT and NUS. Dr Dai has received a number of awards, including the 2009 Chinese Government Award for Outstanding Self-Financed Students Abroad, and the 2004 USTC award for the outstanding undergraduate thesis.