Stockholm/Uppsala molecular simulation workshop

Date: Thursday April 28, 2011

Location: Albanova University Center, Stockholm

Talks: The Svedberg Hall (FD5), entrance from level 4 next to the lecture rooms, or from level 5 next to the elevators on the right side of the main entrance
Coffee, Lunch and Dinner: round tables in the back of the restaurant on floor 3

How to get there: see www.albanova.se

Program

9:20	Introduction	
9:30	Johan Sund (UU)	Free energy calculations on the ribosome
10:00	Olof Allnér (KI)	Nucleotide modifications and tRNA anticodon-mRNA codon interactions on the ribosome and Mg2+ RNA interactions
10:30	Coffee	
11:00	Jack Lidmar (KTH)	Strategies for efficient sampling in rough energy landscapes
11:30	Patrik Henelius (KTH)	Of models and magnets - The dipolar model magnet LiHoF
12:00	Lynn Kamerlin (SU)	Renormalizing Enzyme Dynamics: Do Protein Motions Drive Chemistry?
12:30	Lunch	
13:30	Richard Tjörnhammar (KTH)	Mixed Classical and Quantum mechanical Simulations of Biological Systems
14:00	Erik Marklund (UU)	Proton transfer in classical molecular dynamics: Instantaneous Charge Exchange (ICE)
14:30	Joakim Jämbeck (SU)	An All-atom Force Field for Biological Membranes
15:00	Coffee	
15:30	Anatoly Belonoshko (KTH)	Mechanism of temperature-induced stabilization of dynamically unstable transition metals phases
16:00	Sten Sarman (SU)	Nonequilibrium Molecular Dynamics Simulation of Liquid Crystals
16:30	Sander Pronk (KTH)	How to fold a protein in 30 hours: the Copernicus framework
17:00	Discussion	
18:00	Dinner	

For more information contact Berk Hess (hess@kth.se)