UNIVERSITY OF CALGARY

Complexity Science Seminar

Wednesday, March 26, 2008

ICT 618B 4:00PM

Dr. Raymond Kapral

Chemical Theory Group

Department of Chemistry

University of Toronto

Molecular Machines and Synthetic Self-Propelled Particles

Molecular machines and molecular motors play important roles in biological systems. Proteins acting as molecular machines can undergo cyclic internal conformational motions that are initiated by the energy brought by a ligand. In response to binding of a ligand, the machine performs cyclic hinge motions strongly affected by hydrodynamical coupling to the solvent. The effects of hydrodynamics on molecular machine motion will be discussed. Recently, synthetic molecular motors have been constructed and studied experimentally. These motors, like their biological counterparts, operate in the regime of low Reynolds number hydrodynamics. The talk will describe simple mesoscopic models for the motion of such nanomotors. The motor consists of two linked spheres, one of which catalyzes the conversion between two chemical species. The chemical species interact differently with the the two spheres in the dimer. Simulations allow one to explore the mechanisms of the chemically powered motion and the effects of fluctuations on the motor dynamics.