Berlin Center for Studies of Complex Chemical Systems

Fritz-Haber-Institut der Max-Planck-Gesellschaft, Humboldt-Universität, Max-Delbrück-Centrum für Molekulare Medizin, Otto-von-Guericke-Universität Magdeburg, Physikalisch-Technische Bundesanstalt, Technische Universität Berlin, Universität Potsdam.

Seminar

Complex Nonlinear Processes in Chemistry and Biology

Honorary Chairman: G. Ertl.
Organizers: M. Bär, C. Beta, H. Engel, M. Falcke, M. J. B. Hauser, J. Kurths, A. S. Mikhailov, P. Plath, L. Schimansky-Geier, and H. Stark.

Friday, 27th April, 2012, 16:00 s.t.
Address: Richard-Willstätter-Haus, Faradayweg 10,14195 Berlin, U-Bahnhof Thielplatz (U3).

Prof. Raymond Kapral

Chemical Physics Theory Group, Department of Chemistry, University of Toronto

Protein Dynamics, Diffusion and Molecular Crowding

Proteins often execute cyclic internal conformational motions that are coupled to ligand binding and dissociation events in the course of carrying out their catalytic functions as enzymes. Under physiological conditions the binding process is often diffusion limited. Enzyme kinetics involves a disparate set of times scales that arise from the diffusive approach of the substrate to the enzyme, the conformational changes in the enzyme and the catalytic reactions it carries out. Such protein machines operate in highly fluctuating cellular environments, which may be crowded by obstacles and other macromolecular species. These environmental factors also influence how enzymes operate.

The talk will describe how to model enzyme kinetics under physiological conditions in a way that accounts for the long-time-scale diffusive encounters between substrate and enzyme, as well as the cyclic protein conformational changes induced by substrate binding and product release in the presence of solvent. The manner in which molecular crowding influences the catalytic activity and transport properties of enzymes will also be described. The results will be illustrated by simulations of the dynamics of two enzymes: phosphoglycerate kinase and adenylate kinase.

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