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

Berlin Center for Studies of Complex Chemical Systems

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, January 06, 2017, at 16:00
Address: Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Eugene-Paul-Wigner-Gebäude EW 733

Dr. Holger Flechsig

Hiroshima University (Japan)

A generalised structural and dynamical model of allosteric proteins

The phenomenon of allosteric interactions is ubiquitously present in proteins and therefore raises important questions of the fundamental nature of the underlying mechanisms. In my recent work I attempted to address this topic by establishing a generalized structural model of an allosteric system. To this end elastic-network structures which, as the principal element of allostery, encode pronounced coupling among two remote binding sites were designed *in silico* through evolutionary optimization. I will first explain how a strategy of iterative evolution was developed and applied to stepwise improve, starting from a random elastic network, the allosteric response in the emerging structures. In the designed structures allosteric communication is then analyzed in terms of the propagation of strain and its spatial distribution is used to identify pathways through which remote interactions are established. Moreover, the effect of mutations is demonstrated and robustness of allosteric performance in the designed structures examined. As it turned out, the designed structures of allosteric systems provide realistic counterparts of real allosteric proteins, showing similar dynamics features: i) the structures contain clusters of rigid parts connected by flexible linkers; ii) allosteric communication is established through a set of residues which constitute allosteric pathways; iii) critical mutations can knockout allostery completely. Hence, the obtained structures may serve as a toy models of complex allosteric structures, such as proteins.

Information: Dr. Steffen Martens, Tel. (030) 314 23001, email: steffen.martens@tu-berlin.de