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, November 13, 2015, at 16:00
Address: Richard-Willstätter-Haus, Faradayweg 10, 14195 Berlin, U-Bahnhof Thielplatz (U3)

Dr. Jeffrey Noel

Max-Delbrück-Centrum, Berlin
Fritz-Haber-Institut, Berlin

Energy landscapes of biomolecular machines: Capturing transition paths for conformational rearrangements in the ribosome

The energy landscape theory of protein folding is now a widely accepted view for understanding how relatively weak molecular interactions lead to rapid and cooperative protein folding. I will review this theoretical framework and discuss how it can be extended to describe large-scale functional motions observed in molecular machines. Based on these theoretical concepts, we develop simplified molecular Hamiltonians tailored for molecular dynamics simulations, and analyze large-scale aminoacyl-transfer RNA (aa-tRNA) rearrangements during accommodation on the ribosome. By projecting the dynamics along experimentally-accessible atomic distances, we can identify coordinates along which rearrangements are accurately described as diffusive movements across a one-dimensional free-energy profile, and therefore, provide the theoretical foundation required for single-molecule techniques to uncover the energy landscape governing aa-tRNA selection by the ribosome. Finally, I will discuss implications of this new view of aa-tRNA motion on the fidelity of mRNA translation.

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