Donnerstag, 20.11.2014 **Hörsaal C, Chemie Zentralbau, 17:15 Uhr**

Sprecher: Gerhard Stock
Universität Freiburg

Thema: Energy and Signal Flow in Biomolecules

Abstract:

In biomolecules, the transport of heat and vibrational energy occurs within (tens of) picoseconds. The propagation of conformational change in intramolecular signaling, on the other hand, is believed to occur on a much longer time scale of say, nano- to milliseconds. Interestingly, recent experiments and simulations indicate a possible connection between these fast and slow processes, e.g., via the notion that allosteric interactions may be of dynamical nature. To investigate these intriguing phenomena, transient infrared experiments on photoswitchable peptides and proteins are a powerful approach. Accompanying theses experimental studies, nonequilibrium molecular dynamics simulations allow us to study the mechanisms of energy transport and the transport of conformational change. We show that the energy flow in biomolecules is indeed fast and anisotropic, and can affect resides quite distant from the heat source. Transport of conformational change in a photoswitchable PDZ2 domain, on the other hand, is found to occur in various stages from pico- to microseconds, which may reflect elastic deformation, (de-)stabilized interactions and conformational transitions.

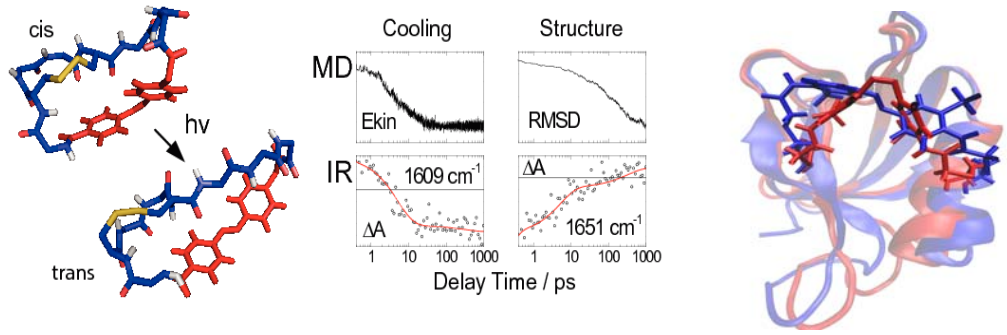

Figure 1: Photoinduced conformational change of a small peptide (left) and the PDZ2 domain (right) triggered by an azobenzene photoswitch. The measured (IR) and calculated (MD) response of the peptide is shown in the middle panel.

References

[1] H. Nguyen, H. Staudt, J. Wachtveitl, and G. Stock, "Real time observation of ultrafast peptide conformational dynamics: MD simulation vs. IR experiment" *J. Phys. Chem. B 115, 13084 (2011).*
[2] P. H. Nguyen, S. M. Park, and G. Stock, Nonequilibrium molecular dynamics simulation of the energy transport through a peptide helix, J. Chem. Phys. 132, 025102 (2010).

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