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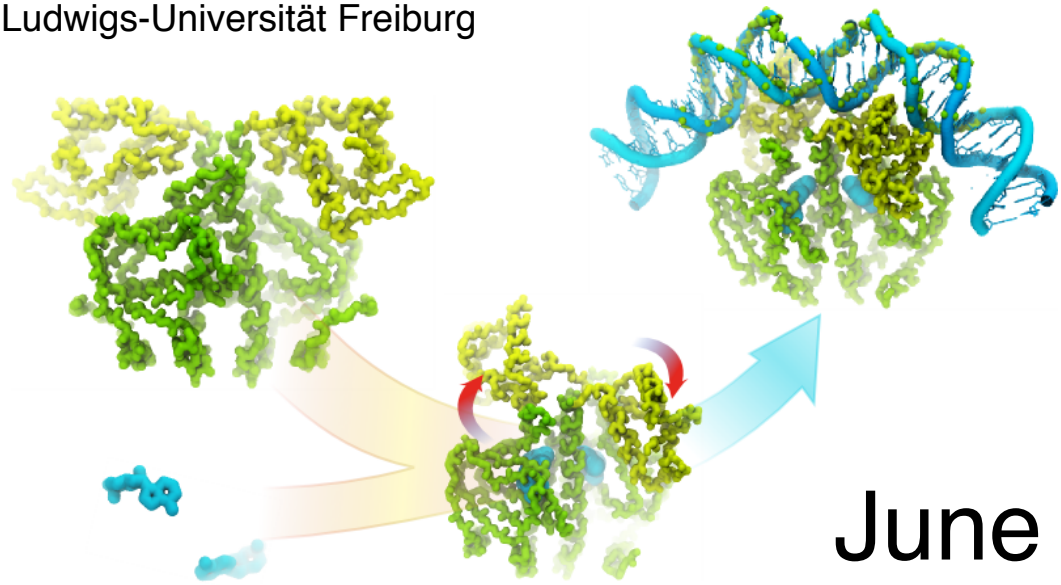

June 20

Towards Understanding Allosteric Dynamics Through Ultrafast IR Spectroscopy

Peter Hamm
University of Zurich

The biological importance of allostery is widely acknowledged and although there are many well-developed models to both understand and predict these interactions, little is known about the mechanism of allosteric transitions at the atomistic level. To study this, we have investigated the protein PDZ2, a single domain protein known to show allosteric properties, with UV-pump IR-probe spectroscopy. To accomplish this we have covalently bound a photo-switchable cross-linker across the allosteric binding site such that upon photo-isomerization it mimics an allosteric conformational transition. The difference FTIR spectra clearly show that there is a reversible change in the protein backbone when switching between cis and trans conformations. The time resolved measurements show that there is a conformational change within the first 20 ps. This signal steadily increases between 10 ns and 100 ns, when the peaks shift by about 10 cm-1, a new peak appears at 1648 cm-1, and the spectra closely resembles the steady state FTIR difference signal. We believe that the first signal reflects those residues closest to the linker, and the later signal reflects a more general relaxation to the perturbation caused by the linker.

Molecular Dynamics Seminars 2012

Seminar Room of Gustav Mie Haus, Ground Floor, 16:15

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