Physikalisches Institut

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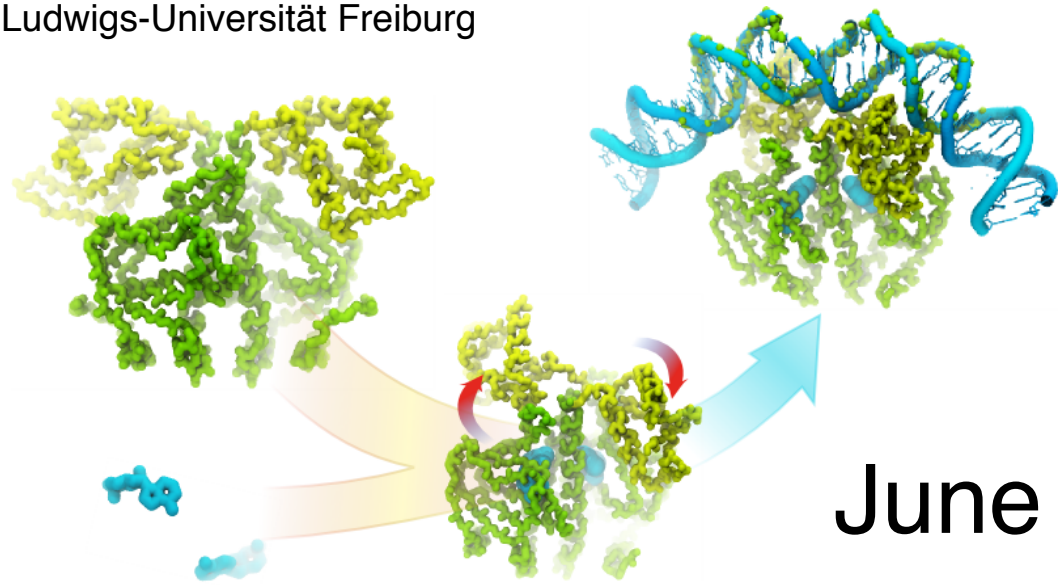

June 13

Biomolecular association on funneled free energy landscapes

Volkhard Helms

Saarland University

Transient, pairwise protein-proteins interactions are crucial parts of bioenergetic and signal transduction pathways. We have studied the association free energy landscape for the Barnase:Barstar complex by Brownian Dynamics simulations. We will use this system to introduce the concept of diffusional protein protein association on conformational energy landscapes. Secondly, unbiased MD simulations were used to study the binding process of a proline-rich peptide to an SH3 domain. In this case, stable complexes were formed within 20 - 130 ns of simulation. Association was found to be governed by the synergistic interplay of long-range electrostatic effects and partial dewetting at contact distances.. Finally, atomistic MD simulations reproducibly recovered the native bound state of the Barnase:Barstar complex. The water in the interfacial gap forms an adhesive hydrogen-bond network between the interfaces stabilizing early intermediates before native contacts are formed. The interfacial gap solvent showed a reduced dielectric shielding up to distances of few nanometers during the diffusive phase. The interfacial gap solvent generates an anisotropic dielectric shielding with a strongly preferred directionality for the electrostatic interactions along the association direction.

Molecular Dynamics Seminars 2012

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

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