



Elitenetzwerk
Bayern



The Dominant Pathways in Rare Conformational and Chemical Reactions

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Abstract:

Classical and ab-initio molecular dynamics simulations represent a standard approach to the theoretical investigation of molecular processes. Unfortunately, the study of rare, thermally activated reactions by these methods is often very challenging, if not impracticable. The main reason is that a large fraction of the computational time is invested to describe the local motion of the system in the meta-stable states. On the other hand, one is mostly interested in the information encoded in the reaction pathways crossing the transition state and connecting the reactant and product states.

In this seminar, we shall present a theoretical and computational method denominated Dominant Reaction Pathways (DRP), which allows to rigorously identify the most statistically significant transition pathways, without investing time in simulating the local thermal motion in the meta-stable configurations,

We will first give a general introduction of the DRP method, and show how it can be used to find the transition state in large conformational spaces. Then, we shall present some applications to the study of the dynamics of protein folding. Finally, we shall discuss how the DRP approach can be extended to the quantum level and applied to identify the most probable pathways of both nuclear and electronic degrees of freedom, in thermally activated chemical reactions.

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