Interplay of Binding, Conformational Change and Reactivity in Biomolecular Systems

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In this talk I will illustrate how molecular simulations can complement experiments in understanding biophysical and biochemical phenomena. The underlying processes cover a broad range of time and length scales rendering a multi-scale treatment mandatory. I will show examples of modelling transitions in complex systems such as enzymatic reactions and will introduce our method for comprehensive sampling of reaction pathways. Furthermore, the impact of small, local changes, such as proton transfers or changes in hydrogen-bonding patterns, on the global function of a biological system will be exemplified. Finally, I will present the role dynamics play in protein-DNA interaction and enzymatic specificity.