Structure, Function, and Dynamics - Insight from Biomolecular Simulations

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At finite, e.g. physiological temperature, molecules are not static entities with a fixed geometry but rather exhibit dynamics, occupying and interchanging between several conformational and configurational states. Often, only a few of those states render the molecule functional, such as the folded form of a protein. And even so often, the transition between states is associated with function such as the switching in a signalling protein, or the chemical reaction catalysed by an enzyme. Both, the intrinsic probability to populate different states as well as the probabilities for transitions between them are influenced by the physical conditions and the molecules' interactions with their environment.

This presentation illustrates how we use molecular simulations to explore the interplay of dynamics, interaction, and reactivity aiming at understanding fundamental chemical and physical processes in biological molecules. The underlying processes cover a broad range of time and length scales rendering a multi-scale treatment mandatory.

Examples will comprise computation of optical spectra and dissecting the relation to conformational transitions. Furthermore, modelling transitions in complex systems such as enzymatic reactions by comprehensive sampling of reaction pathways will be demonstrated. Finally, we will show how small, local changes, such as proton transfers or changes in hydrogen-bonding patterns, can have an impact on the global function of a biological system.