Chemical & Physical Sciences
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NOT JUST PROTEINS: UNRAVELLING THE ROLE OF WATER IN PROTEIN DYNAMICS AND ALLOSTERY

Proteins are considered the machinery of life, performing vital biological functions in the cell. To understand how proteins work and regulate their activity, it is crucial to characterize their dynamics and interactions with water. Water molecules form hydration shells around proteins and hydrogen-bonded networks inside their hydrophobic interiors, influencing their structure, dynamics, and function. Experimental techniques, such as time-resolved X-ray crystallography and nuclear magnetic resonance (NMR) spectroscopy, are used to observe proteins in action with atomistic detail. However, the ensemble-average description of protein dynamics in these experiments requires the parallel development of molecular dynamics approaches, which capture diverse conformational ensembles of proteins and explicit interactions with water molecules. In this thesis, I illustrate how advanced computational techniques, supported by experimental data, reveal the essential role of water in protein dynamics and allostery. These findings not only deepen our understanding of protein behavior but also open potential avenues for protein engineering.