Constant pH Molecular Dynamics

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The development of new methods and models to simulate biological molecules under conditions of varied pH and ionic strength are important tools in advancing our understanding of biological function. In this talk I will provide an overview of our recently developed constant pH molecular dynamics methods, which build on advances in generalized Born theories for intermolecular interactions. Applications focused on characterizing the extreme pKa shifts seen for buried charged residues in Staphylococcal Nuclease will be presented together with problems in which pH changes induce complex conformational changes in protein folding and misfolding.