

### **43a Proteins in Inhomogeneous Environments: Answers from Advanced Monte Carlo Simulations**

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Biological molecules in inhomogeneous environments arise both in nature and in numerous applications. For example, controlling protein adsorption is important in medical implants, biosensors, and protein arrays. Protein stability in confined and crowded environments is also important in fields such as microfluidics and proteomics. Understanding the biophysics involved in such systems will aid in furthering the advancement of the technologies. Single molecule experiments give the ability to measure a number of relevant phenomena, but molecular models are often required to interpret the results and exploit their consequences. Molecular simulations provide a valuable tool for understanding the behavior of biological molecules in inhomogeneous systems at atomic scales. Traditional simulation methods face significant challenges, in part due to the complex energy landscape characteristic to biological molecules. Using density-of-states based methods we are able to overcome several previous limitations. Following a brief introduction to the methods, a number of findings for different systems of interest will be presented. These include a free-energy analysis of the effects of confinement and molecular crowding on protein stability and of the interaction of proteins with different types of surface chemistry and topography.