

## **Probing the electrostatic environment of proteins with constant pH molecular dynamics**

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In this lecture I will describe development and application of the constant pH molecular dynamics methods to calculations of pH-mediated processes in proteins and their assemblies, including viral capsids. pH plays a critical role in the cell in modulating and mediating both physical and chemical processes. I will present results that examine the role of buried charges in proteins and the influence they exert on protein structure and fluctuations. Additionally, I will describe ongoing work that explores the role of electrostatic interactions and their modulation via pH equilibrium in the maturation of viral capsids.