

# Unveiling Proton-coupled Phenomena in Biology and Chemistry at Atomic Resolution

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Many biological processes, such as enzyme catalysis and ATP synthesis, involve conformational dynamics coupled to protonation or deprotonation. Such phenomena can not be studied using traditional molecular dynamics simulations that are based on fixed protonation states. In this talk I will describe the development of a novel technique, called continuous constant pH molecular dynamics (CpHMD), which has opened a door to new insights into ionization-coupled conformational phenomena and de novo prediction of pKa's relevant for biology and chemistry. I will highlight some of the applications to elucidate mechanisms of pH-dependent protein folding, dimerization of spider silk proteins, self-assembly of surfactant micelle and bilayer, as well as electrostatic interactions in the unfolded states.

## References

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