## Recent development and application of continuous constant pH molecular dynamics

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Development of the constant pH molecular dynamics (pHMD) techniques has opened a door to atomically detailed studies of dynamic processes coupled to protonation/deprotonation. Here we discuss the most recent development of the continuous pHMD technique and application studies for gaining novel insights into ionization-coupled conformational phenomena in biology and chemistry. We show that continuous pHMD simulations offer, for the first time, thermodynamic description of coupled protonation and conformational equilibria for proteins. We will also discuss other applications such as pH titration of micelles and pH-dependent phase transitions.