Simulation of pH-dependent Behavior of Liposome

REJWAN ALI, Fordham University & Queensborough Community College of CUNY — Optimized liposome for biomedical delivery applications has been a field of vigorous research for past few decades. While experimental techniques of fluorescence spectroscopy, differential scanning calorimetry and dynamic light scattering report physical suitabilities in several applications of liposomes, molecular dynamics simulation can provide more detailed feature at atomistic level for such biophysical systems. In recent times, experimental results of liposome’s physical properties in different pH environment have widely been reported. The system draws interest for potential applications in several biomedical areas. We will present our molecular simulation results for such system highlighting the effect of pH on hydrogen bonding as well as correlation of dynamics to observed phase behavior.