

Understanding the Role of Large-Scale Protein dynamics in Protein Electrostatics

Dr. Wei Yang
Florida State University (USA)

Protein dynamics is an essential determinant of electrostatic properties. In particular, large-scale protein motions can give rise to unusual electrostatic effects, such as long-range electrostatic coupling, cooperativity and abnormal pKa shifts etc. Due to the timescale limitation, understanding the role of large-scale protein dynamics in protein electrostatics, especially at the atomistic level, has been challenging to molecular dynamics methods. Focusing on energy flow acceleration, the orthogonal space sampling scheme provides a unique framework of quantitatively exploring slow-timescale motion coupled electrostatic effects. The recent method advancement will be presented in this talk.