Effect of Electronic Polarization on Structure and Dynamics of Proteins

John Z.H. Zhang[1,2]

[1]*State Key Laboratory of Precision Spectroscopy, Department of Physics, East China Normal University*

[2]*Department of Chemistry, New York University, New York, NY 1000, USA*

New efficient quantum mechanical method for calculation of protein in solution is developed and employed to generate new force field that features fixed but polarized protein-specific charges (PPC). The PPC provides a realistic description of the polarized electrostatic state of the protein than the widely used amino acid-specific charges. Extensive MD simulations have been performed to study the efficacy of PPC through direct comparisons between results obtained from PPC, the standard AMBER charges and experimental results. The impact of PPC on protein electrostatic interaction, stability of hydrogen bonds, protein-ligand binding and protein dynamics are presented in this talk. The results clearly demonstrate that the correct description of the electronic polarization of protein is crucial and PPC shall have important applications for MD simulation studies of protein structure and dynamics.

References

[1] D.W. Zhang and J.Z.H. Zhang, J. Chem. Phys. **119**, 3599 (2003).
[2] Y. Mei, D.W. Zhang, and J.Z.H. Zhang, J. Phys. Chem. A **109**, 2 (2005).
[3] Y. Mei, C.G. Ji, and J.Z.H. Zhang, J. Chem. Phys. **125**, 094906 (2006).