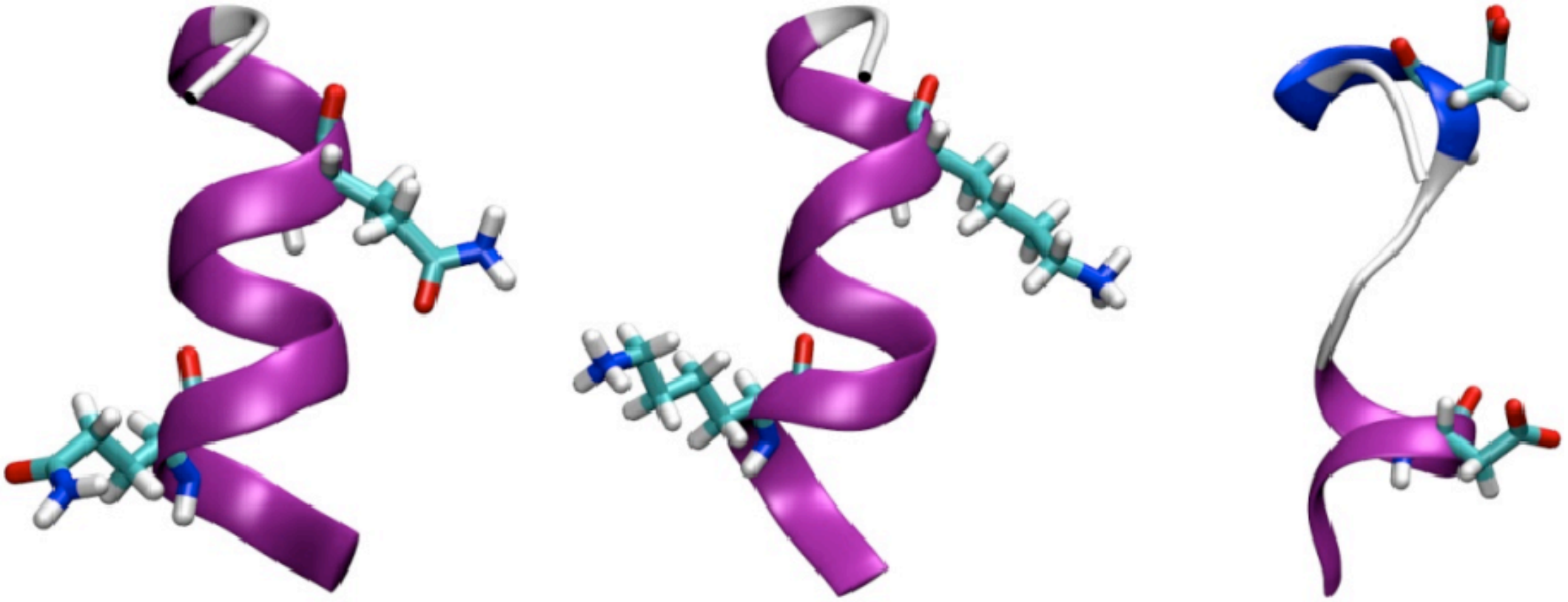
2012年7月6日（星期五）
波谱楼2楼报告厅
上午9：30

Prof. Dawei Zhang
Nanyang Technological University

Dawei Zhang received his B.S. and M.S. degree in chemistry from Nankai University (NKU) in 1993 and 1996 respectively; Ph.D. in Theoretical and Computational Chemistry from New York University (NYU) in 2005; and was a postdoctoral fellow and a research scientist at NYU langone medical center from 2005-2008. He was appointed as an assistant professor of chemistry by Nanyang Technological University (NTU) in 2008.

理论与交叉学术交流系列报告（十）

Protein folding simulations based on charge variation scheme



a: Ac-AA**Q**AAAAA**Q**AAGY-NH_2

b: Ac-AA**K**AAAAA**K**AAGY-NH_2

c: Ac-AA**D**AAAAA**D**AAGY-NH_2

During protein folding, protein undergoes large conformational change. Its electronic structure is very conformation-dependent. Fixed atomic charges may not be always accurate for the whole folding trajectory. Thus, the atomic charges need to vary with the conformation of protein. In this presentation, I will introduce our recent works in which charge variation scheme is employed to study the effects of sequence mutation and the influence of environment on protein folding.