中心系列讲座 ICQM Weekly Seminar Series

"Applying Molecular Dynamics Simulations to Study the Conformations of Biomolecules and Their Dependence on Solvation"

Yiqin Gao高毅勤
College of Chemistry and Molecular Engineering, Peking University

Time: 4:00pm, Mar. 7, 2012 (Wednesday)
时间： 2012年3月7日 （周三）下午4:00
Venue: Room 607, Conference Room A, Science Building 5
地点： 理科五号楼607会议室

Abstract

The application MD simulations to the studies of the structure and dynamics of biomolecules in aqueous solutions is limited by the large computational demand. In this talk we will first discuss our effort in developing enhanced sampling method that allowed us to study complex processes such as protein folding and DNA base-pair flipping. The protein folding simulations allowed us to quantitatively determine the folding free energy landscape of a number of polypeptides. It was found that the folding free energy landscapes of simple beta-hairpins, thus also their folding mechanisms, are sensitive to the amino acid sequence. Both turn stability and hydrophobicity of polypeptides affect strongly their hydrogen bond assembly. We then discuss the molecular mechanisms through which alcohols and inorganic salts affect polypeptide structure formation and hydration. For example, the addition of NaI to the aqueous solution of BBA5 caused its denaturation and significantly weakened hydrogen bonds of the polypeptide. Na2SO3, a "kosmotropes," strengthened the hydrophobic interactions and increased hydrogen bonding of the polypeptide. Finally, if time permits, we will discuss the molecular mechanism through which monohydric methanol and TFE denature BBA5, and polyhydric glycol and glycerol protect the polypeptide structure.

About the Speaker

Professor Gao is a Changjiang Professor of College of Chemistry and Molecular Engineering, Peking University. He received his B.S. in 1993 from Sichuan University and M.S. in 1996 from Institute of Chemistry, Chinese Academy of Sciences and Ph.D. in Chemistry in 2001 from California Institute of Technology in USA under the supervision of Rudolph A. Marcus, a Nobel Prize Laureate in 1992. He was a doctoral Research Fellow in California Institute of Technology and Harvard University from 2001-2004 before joining the faculty of Department of Chemistry, Texas A&M University in 2004.