



中心系列讲座 ICQM Weekly Seminar Series  
**More than one dynamic crossover in  
protein hydration water**



**Giancarlo Franzese**

Universitat de Barcelona

**Time: 4:00pm, March 28, 2012 (Wednesday)**

**时间: 2012年3月28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

Studies of liquid water in its supercooled region have helped us better understand the structure and behavior of water. Bulk water freezes at its homogeneous nucleation temperature (approximately 235 K), but protein hydration water avoids this crystallization because each water molecule binds to a protein. Here, we study the dynamics of the hydrogen bond (HB) network of a percolating layer of water molecules and compare the measurements of a hydrated globular protein with the results of a coarse-grained model that successfully reproduces the properties of hydration water. Using dielectric spectroscopy, we measure the temperature dependence of the relaxation time of proton charge fluctuations. These fluctuations are associated with the dynamics of the HB network of water molecules adsorbed on the protein surface. Using Monte Carlo simulations and mean-field calculations, we study the dynamics and thermodynamics of the model. Both experimental and model analyses are consistent with the interesting possibility of two dynamic crossovers, (i) at approximately 252 K and (ii) at approximately 181 K. Because the experiments agree with the model, we can relate the two crossovers to the presence at ambient pressure of two specific heat maxima. The first is caused by fluctuations in the HB formation, and the second, at a lower temperature, is due to the cooperative reordering of the HB network.

M. G. Mazza, K. Stokely, S. E. Pagnotta, F. Bruni, H. E. Stanley, and G. Franzese PNAS 108, 19873–19878 (2011)

### About the Speaker

Dr. Giancarlo Franzese, leads a research group on Statistical Physics of Complex Matter at the University of Barcelona (UB). He got his PhD in Physics with honors at the University of Naples and was Associate Researcher at the University of Roma Tre, the Boston University, the Second University of Naples and the Center for Statistical Mechanics and Complexity of the “La Sapienza” University of Rome, before moving permanently to Barcelona in 2003. His research uses theoretical calculations and numerical simulations, in many cases in close collaboration with experimental groups. He was cited more than 1470 times (H-index 22), with citations on Science, Nature, PNAS, PRL, receiving interviews on Radio and International Press.