



School of Nano Science

IPM Condensed Matter and  
Statistical Physics Group

## Weekly Seminar

# Probing Complexity in Hydrogen-Bonded Systems with Computational Models

Invited Speaker:

**Dr. Ali Hassanali**

ICTP, Italy

### **Abstract:**

In this talk I will highlight the role of inter-disciplinary computational physical sciences in understanding the complex structural and dynamical properties of hydrogen bonded systems. I will begin by discussing a classical problem in physical chemistry, namely proton transfer in liquid water. Here we elucidate the mechanisms of structural diffusion of the proton through the hydrogen bond network of liquid water using ab initio molecular dynamics simulations. I will then move on to sharing more recent work on understanding the anomalous fluorescence in amyloid proteins which exhibit fluorescence in the absence of aromatic residues. Curiously, we find proton transfer events between the parts of the protein play a critical role in tuning its optical properties. Finally, I will discuss recent work on disentangling the IR spectrum of charged water clusters. In all the systems with hydrogen bonds, quantum effects of the covalent bonds with large zero-point energy has a significant impact on the fluctuations of molecular properties.

Thursday, 23 Ordibehesht 95 (12 May, 2016), 2-3 pm

Farmaniyeh seminar room