



School of Nano Science



IPM Condensed Matter &  
Statistical Physics Group

## Special Seminar

### **Promiscuity in Liquid Water: An Atomistic Perspective**

Invited speaker: Dr. Ali Hassanali

Condensed Matter and Statistical Physics section, ICTP, Italy

#### **Abstract:**

Water molecules love to swing. In this talk, I will highlight some of our recent work, using atomistic simulations, at examining their deviant tendencies by undressing the molecular layers and complexity associated with the origin of density and charge fluctuations in a series of aqueous-related soft-matter systems. In the first part of my talk, I will focus on characterising the properties of the empty space in liquids, highlighting the role of the creation of branched like voids that have an uncanny similarity to the shapes of small polymers. The fluctuations in liquid water look like they are adapted to hosting small charged polymers. These polymers are also decorated with water wires the properties of which, are coupled to their secondary structure. In the second part of my talk, I will discuss attempts to pinpoint the origin of the apparent negative charge of water near hydrophobic interfaces. I will show that asymmetries in the charge transfer along hydrogen bonds due to local coordination defects, can lead to highly non-trivial effects such as swaying the charge of a water molecule in subtle ways to make it either slightly positive or negative. I will conclude with some perspectives on the broader implications of these findings with an emphasis on the fuzziness of the solute-solvent boundary.

**Wednesday, 11 Ordibehesht 1398 (May 1, 2019), 14:00-15:00**

**Seminar Room (classroom A), Farmanieh Building, IPM**