



Vabilo na predavanje / Invitation to the Lecture

Prof. Dr. Ali Hassanali

The Abdus Salam International Centre for Theoretical Physics, Trst, Italija

Torek / Tuesday, 6. 12. 2016 ob / at 13:00

Velika predavalnica Kemijskega inštituta / Lecture Hall at the National
Institute of Chemistry, Hajdrihova 19, Ljubljana

Aqueous Solutions In Silico: Water, Ions, Protons & Proteins

Abstract

Water is one of the most ubiquitous substances in the universe. Despite long study from both experimental and theoretical approaches, phenomena in liquid water and its coupling to other systems continues to be a source of rather rich and interesting physics. In this talk, I will discuss how first principles methods (*ab initio*) play an important role in understanding fundamental properties such as acid-base chemistry and ion diffusion in liquid water. In particular, I will show how these methods elucidate deep insights into the molecular mechanisms associated with the Grotthuss mechanism of proton diffusion in water as well as the anomalous diffusion of water around ions like CsI and NaCl. The importance of nuclear quantum fluctuations and their effect on structural and electronic properties will also be discussed. In the final part of my talk, I will discuss some recent work looking at the coupling of peptide and water hydrogen bond networks in a model protein relevant for neurodegenerative diseases.

