# Ionic Hydration from Born-Oppenheimer Molecular Dynamics Simulations of Clusters

Nuno Galamba
Grupo de Física-Matemática da Universidade de Lisboa, Av. Prof. Gama Pinto 2,
1649-003 Lisboa, Portugal

Ionic hydration plays a fundamental role to many processes in chemistry and biology. Although intensively studied through both experiments and computer simulation techniques there are still many unresolved issues blurring a microscopic-level picture of ionic hydration. The concept of ionic structure makers and breakers and its implication on the stability of macromolecules and molecular assemblies is a prominent example of the later. On this work we give a microscopic-level view of the ionic hydration on finite systems obtained from all-electron Born-Oppenheimer molecular dynamics simulations of aqueous clusters. We discuss the structure and dynamics of water molecules in the hydration shells of specific ions and relate our observations with those portrayed for the ionic hydration shell of bulk aqueous solutions.