

Water surprises from ab-initio molecular dynamics simulations

Roberto Car

Princeton University, Princeton NJ 08544, USA

rcar@princeton.edu

The electronic charge and the corresponding electric field distribution are at the origin of many of the unusual properties of liquid water. First, I will discuss how static and dynamic dielectric properties of water result from the distribution of molecular dipoles and their correlations due to hydrogen bonds. Finally, I will discuss a surprising charging effect that occurs at the interface between water and hydrophobic substances.