Ab-initio simulations of molecular fluids: structural and electronic properties and the influence of a magnetic field

Giulia Galli (*)
Lawrence Livermore National Laboratory, CA, USA.

In this talk recent progress on ab-initio simulations of molecular fluids will be reported. In particular results about water and hydrophobic solutes in water and the influence of a magnetic field on compressed hydrogen will be discussed. Simulations in a magnetic field were carried out with a new method which allows one to retain the computational efficiency of plane-wave like basis sets and fast Fourier transform techniques in supercell calculations in the presence of a uniform, finite field.

(*) Work done in collaboration with Wei Cai, J.Grossman and E. Schwegler.