

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

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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.

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