Position: Postdoctoral fellow

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Curriculum Vitae

Research Interests

The aim of my Ph.D. research was the study of high pressure hydrogen phases, by means of Monte Carlo simulations, both on effective models and from ab initio simulations.

The determination of the physical properties of hydrogen under extreme conditions is of fundamental importance in Astrophysics and Planetary Science to build models describing i.e. brown
dwarfs, stars, giant planets, systems mainly composed by hydrogen. More generally in the field of the Condensed Matter Physics, the interest on high pressure hydrogen was originated by the Wigner and Hungtington prediction on the possible occurrence of a metallization transition in low temperature solids, driven by the pressure.

The experimental compression techniques (static and dynamic) have depicted for hydrogen a phase diagram of unexpected richness. However, the region of the phase diagram in which the most interesting transitions occur is not accessible through experiments. The ab initio simulation techniques are then a fundamental tools to extend our knowledge on hydrogen at extreme pressures.

The most of the simulations are carried out with Born-Oppenheimer (BO) methodologies based on the Density Functional Theory (DFT) evaluation of the electronic ground state at a given nuclear configuration. The accuracy of these simulations is however limited near the metallization transition, due to the well known DFT tendency to favor the metallic versus the insulating states. Recently an alternative approach has been developed, still within the BO approximation: the Coupled Electron-Ion Monte Carlo method (CEIMC), entirely based on MC algorithms, applied both to electrons and nuclei. This method, not suffering of the DFT limitations, may be able to provide accurate results over the entire phase diagram.

Current Research Projects

During my Ph.D. work I applied Monte Carlo methods to investigate the hydrogen properties in three different regions of the phase diagram.

a) Monoatomic hydrogen at ultrahigh pressure (above 10TPa). In this region the thermodynamic properties of hydrogen are well reproduced by an effective one component model, the

Screened Coulomb Plasma model. For this system we first performed a zero temperature study for classical particles, to determine the lattice of lower energy/enthalpy, and then computed the melting temperature in density for classical and quantum particles, by free energy methods and Path Integral MC simulations, and for all the hydrogen isotopes. (*J. Chem. Phys.* **134**, 184505 (2011))

b) Monoatomic hydrogen at 300