Properties of Dense Fluid Hydrogen and Helium and Implications for Giant Gas Planets

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Introduction

The research of dense plasmas has obtained some exciting new impulses from recent discoveries of a large number of extrasolar planets [1, 2, 3]. Most of them are believed to be giant gas planets whose representatives in our solar system are Jupiter and Saturn. Even for the latter ones the inner structure and evolution is not exactly known and still keeps mysteries [4]. This paper reports recent calculations undertaken to obtain the equation of state (EOS) and thus all necessary thermodynamic properties of dense hydrogen-helium mixtures to describe the interior of giant gas planets from first principles.

Method

The plasma under consideration is characterised by partial ionisation, strong correlations and quantum effects. None of them can be considered to be small; an appropriate and reliable technique has to consistently include all of them. Density functional molecular dynamics (DFT-MD) is a technique from first principles that fulfils these requirements [5, 6]. Here, density functional theory (DFT) is used to describe quantum behaviour of the electrons [7] and classical molecular dynamics (MD) is invoked for the ions, which can be describe in this way because of their higher mass. For the connection of both systems, the Born-Oppenheimer (BO) approximation is used. The simulation itself consist of two parts. First, the ground state electronic wave function, and therefore the electronic density, is computed for a fixed ion configuration. From a given electronic density one obtains forces acting on the ions. These are utilised then in the following MD step where Newton's equations are solved for the ions. Then the procedure is repeated. During the calculations an expansion of the electronic wave function into plane waves is used. The number of necessary plane waves and thus the memory needs can be reduced sufficiently

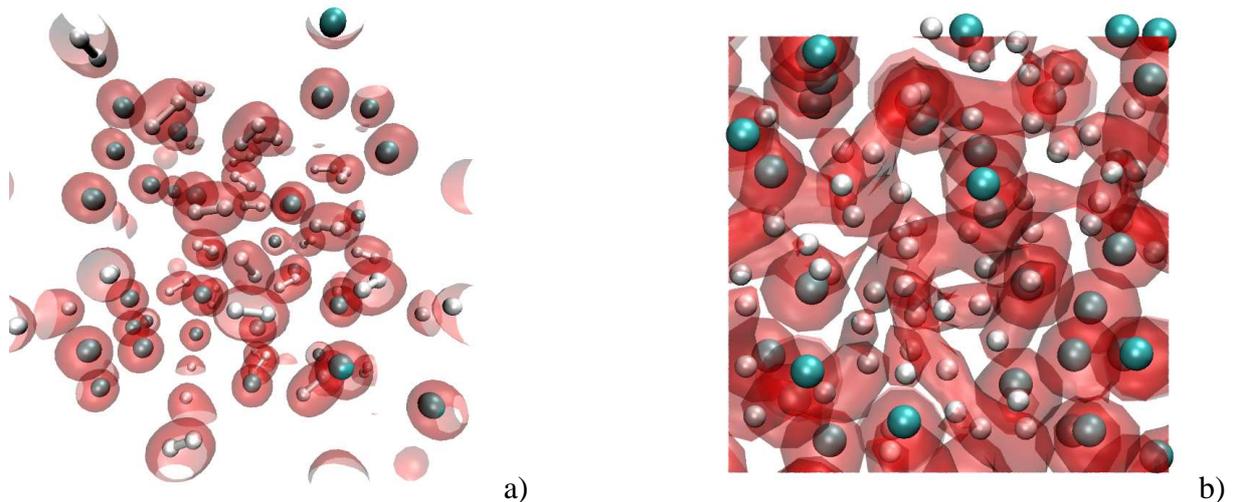a)   b)

Figure 1: View of the simulation cell of a DFT-MD simulation. Hydrogen and helium nuclei are represented by small and large spheres, respectively, and electron density isosurfaces are drawn. In these plots, the mixing ratio is $x = 0.5$, and the temperature is 4000 K. The density corresponds to a) $r_s = 2.4$ (0.3 g/cm^3) at pressure of 8 GPa, and b) $r_s = 0.9$ (5.5 g/cm^3) at pressure of 3800 GPa. These conditions correspond to a molecular phase and to a metallic regime of fluid hydrogen, respectively.

by applying norm conserving pseudopotentials [8]. The only approximation in this method consists in the choice for the exchange-correlation potential. The calculations shown here use the generalised gradient approximation (GGA) which gives very good description of molecules [9]. Naturally, a simulation cannot describe a real many particle system and finite size effects have to be studied and corrections included. Apart from running bigger supercells, this can be accomplished by using k-point grids in the first Brillouin zone [10]. Snapshots of such simulations are presented in fig. 1. Notice that ions are represented by spheres where as for the electrons only isosurfaces of the density can be given because of their quantum character.

Results & Discussion

Together with EOS data, it is possible to obtain information about the ordering of the ions and the energetic structure of the electrons [11, 12, 13]. The calculations reveal for hydrogen a smooth transition from the molecular to the atomic state. The latter state is often referred to as metallic hydrogen due to the fact, that nearly all electrons are free, i.e. the atoms are ionised and the conductivity increases drastically at the transition. Contrary to other methods DFT-MD does not predict a first order phase transition at the molecular-metallic transition which is often referred to as plasma phase transition. In our case, the transition is triggered partly by pressure and partly by temperature, pure pressure dissociation is hard to observe.
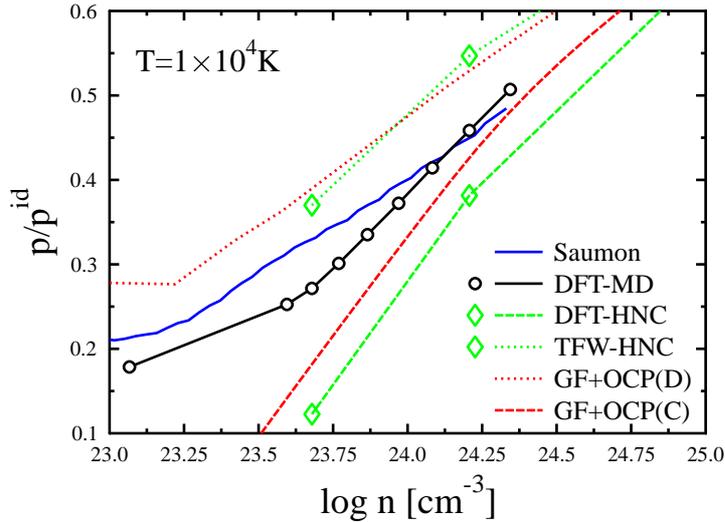
Figure 2: Isotherm of the hydrogen EOS in the metallic regime by various theories. Saumon is a chemical model widely used in astrophysics [17]. DFT-MD is this work, DFT-HNC and TFW-HNC is a combination of DFT and classical integral theory (HNC) by Xu et al. [18]. GF+OCP is a technique using Green's function theory and HNC [19, 20]. (D) denotes the use of the Debye potential (C) the use of the Coulomb potential in the one component system for the ions.

Mixing quantities are important for giant gas planets since they consist of mixtures of hydrogen and helium (and small amounts of heavy Z elements). It is necessary to calculate thermodynamic quantities for mixtures directly and not to rely on mixing schemes like linear mixing. Such schemes can only take into the predefined number of species and fail when dissociation, ionisation or recombination occurs, thus right in the most crucial regions [11]. First principle simulations are capable of treating mixtures directly and will help to answer the question whether hydrogen and helium phase separate inside Jupiter and more importantly inside Saturn [14, 15, 16].

The most mass of a giant gas planet is contained in the inner regions where hydrogen is metallised and possibly helium enriched. Small changes in the EOS can mean significant changes for e.g. the core mass. Fig. 2 provides an overview over the results of several different theories for metallic hydrogen. The differences are quite striking and vary due to the type of description of correlations, quantum effects and screening. The dashed red curve labeled GF+OCP(C) can be considered a lower limit since no screening of the ion interactions is incorporated. On the other hand, the dotted red line should be an upper limit since linear Debye screening is inappropriate under these conditions. Both, Saumon [17] and our results show qualitatively correct behaviour. However, models of giant gas planets using these EOS data will give very different structures.

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