Universität Rostock

Traditio et Innovatio

INSTITUT FÜR PHYSIK

Modeling Brown Dwarfs using *ab initio* equation of state data

Introduction

We present wide-range equations of state (EOS) for hydrogen and helium including accurate data derived from finite-temperature density functional theory molecular dynamics (DFT-MD) simulations for the warm dense matter regime using the VASP package[1], see FIG. 1. This hydrogen/helium Rostock EOS (H/He-REOS) cover a wide range of temperatures and densities. Based on this *ab initio* data set we calculate interior models and mass-radius (MR) relations for Giant Planets and particularly for Brown Dwarfs (BD). We compare our interior models and the MR relations with those derived from the Saumon-Chabrier-van Horn (SCvH) EOS[2].

DFT-MD method

We perform *ab initio* quantum molecular dynamics simulations with a quantum mechanical treatment of the electrons by using finite-temperature density functional theory (DFT) and a classical molecular dynamics simulation (MD) for the ions. EOS data derived from those methods are known to have a high predictive power for high-pressure experiments, i.e. Hugoniot curves for hydrogen[3], see FIG. 2.

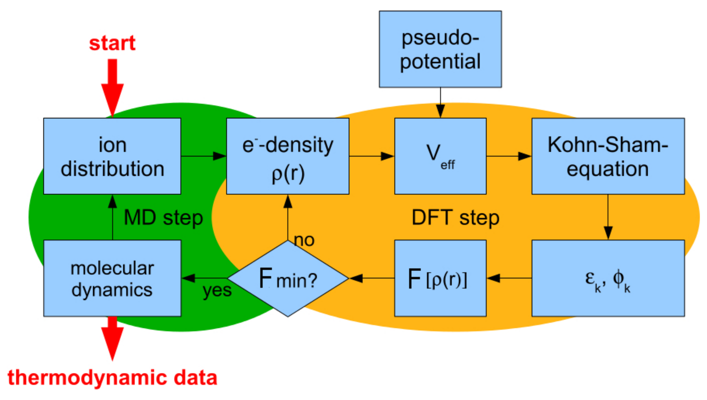

FIGURE 1: Schematic workflow of a DFT-MD simulation as it is implemented in VASP. All our simulations were performed with 256/108 (H/He) particles using the Perdew-Burke-Ernzerhof exchange-correlation functional[4] (PBE) and were evaluated at the Baldereschi mean value point[5]. The Coulomb interactions between the electrons and ions are treated using projector-augmented wave potentials[6,7] with a converged energy cutoff of 1200 eV or the Coulomb potential for high densities with a cutoff of 3-10 keV.

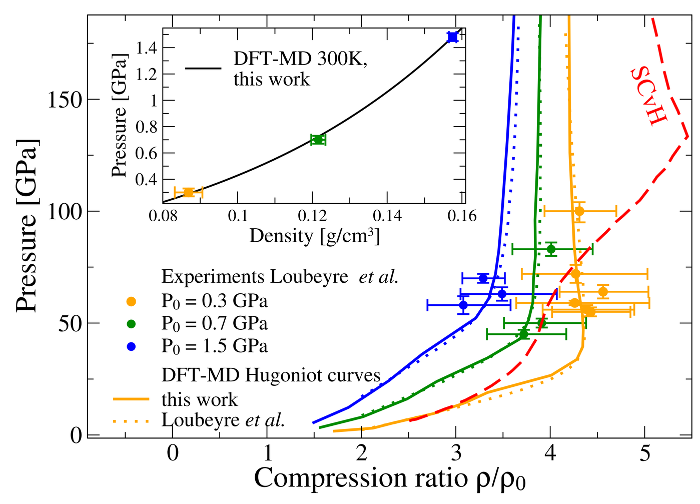

FIGURE 2: Hugoniot curves generated from precompressed hydrogen (T = 297 K) with initial pressures of 0.3 GPa (orange), 0.7 GPa (green) and 1.6 GPa (blue), respectively. Experimental points and theoretical DFT-MD curves (dashed) of Loubeyre *et al.*[8] are compared with our results (solid). Inset: The associated initial precompressed states (same color code as in main frame).

Hydrogen equation of state

Our hydrogen EOS consists of DFT-MD data for the warm dense matter regime and the model EOS of Chabrier and Potekhin[9] for high densities or high temperatures. The dissociated liquid is described within fluid variational theory (FVT/FVT$^+$)[10,11] and the partially ionized matter is characterized by the SCvH-EOS[2]. To ensure thermodynamic consistency and smooth transitions between the parts we had to apply spline interpolation including Path integral Monte Carlo data (PIMC) from Hu *et al.*[12].

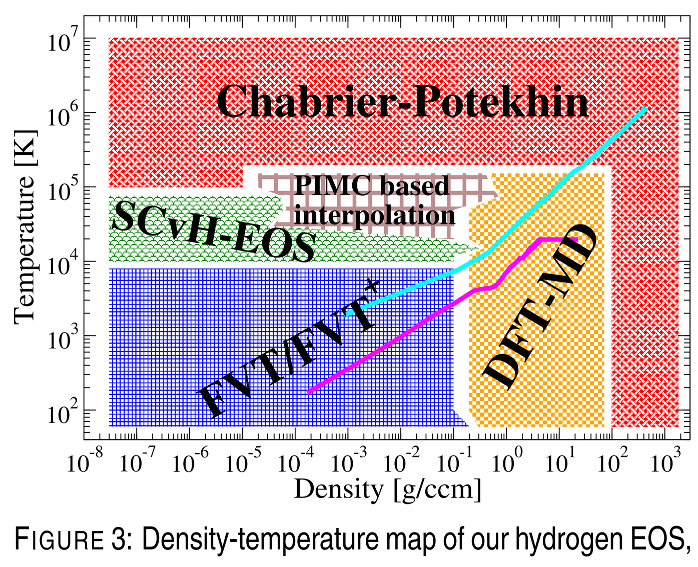

FIGURE 3: Density-temperature map of our hydrogen EOS, see description above, together with interior models for Jupiter (magenta) and the BD Gliese 229b (cyan).

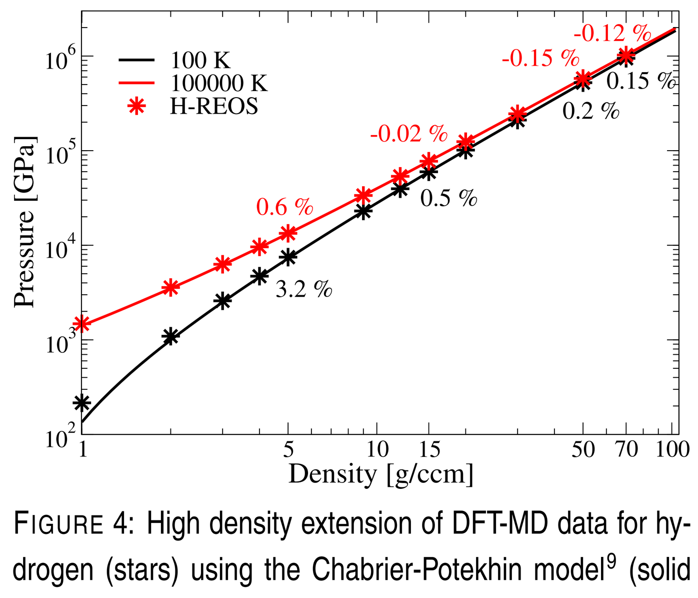

FIGURE 4: High density extension of DFT-MD data for hydrogen (stars) using the Chabrier-Potekhin model[9] (solid curves) with relative deviations for several densities.

Helium equation of state

The helium EOS is composed of DFT-MD data for the warm and hot dense matter regime while for lower densities and highest temperatures we applied the SCvH-EOS where an interpolation between 60 kK and 300 kK was necessary, see FIG. 5. For lower temperatures and low densities we use a virial EOS based on *ab initio* virial coefficients $B_i(T)$ from Bich *et al.*[13] and those of Shaul *et al.*[14] where the pressure $P(\rho,T)$ and the specific internal energy $u(\rho,T)$ are described as follows:

$$P(\rho,T) = P^{\mathrm{id}} + P^{\mathrm{corr}} = \frac{\rho R T}{M}\left[1 + \sum_{i=2}^{\infty} B_i(T)\left(\frac{\rho}{M}\right)^{i-1}\right] \qquad (1)$$

$$u(\rho,T) = u^{\mathrm{id}} + u^{\mathrm{corr}} = u^{\mathrm{id}} - \frac{RT^2}{M}\left[\sum_{i=2}^{\infty} \frac{\mathrm{d}B_i(T)}{\mathrm{d}T}\left(\frac{\rho}{M}\right)^{i-1}\right]. \qquad (2)$$

The ideal parts P^{id} and u^{id} are described by an ideal plasma model.

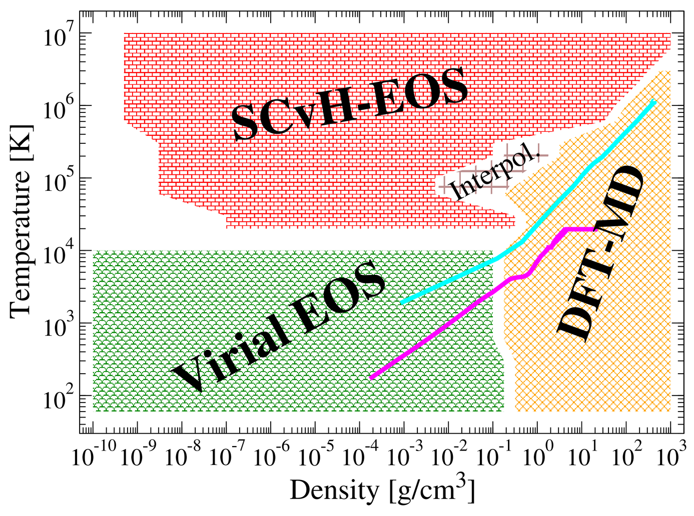

FIGURE 5: Density-temperature map of our helium EOS, see description above, together with interior models for Jupiter (magenta) and the BD Gliese 229b (cyan).

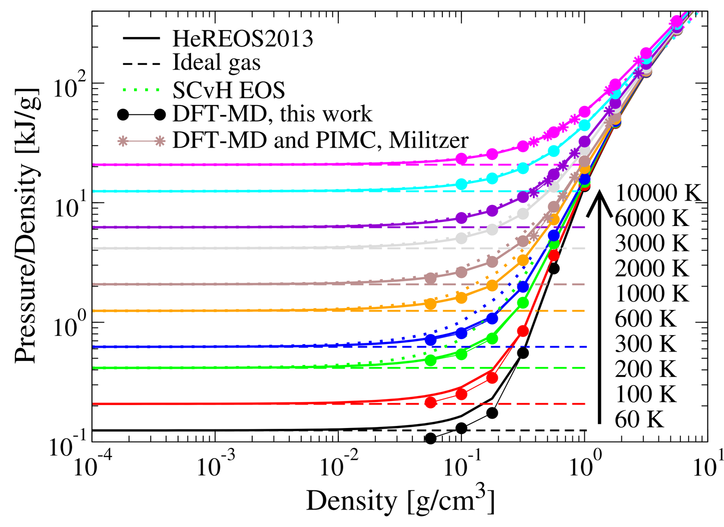

FIGURE 6: Our helium EOS for 60-10000 K in comparison with *ab initio* data from Militzer[15] (stars), the ideal plasma model and the SCvH-EOS[2].

Mass-radius relations and interior profiles

As a first attempt we calculate MR relations and interior models for BDs with an atmosphere as predicted for Gliese 229b by Marley *et al.*[16] yielding to an outer boundary condition of $T(56\mathrm{bar}) = 1880$ K, where the atmospheric temperature profile becomes adiabatic. The estimated mass range of Gliese 229b is very well described by a MR relation with a composition of 71.54% hydrogen, 26.46% helium, and 0.02% metals, see FIG. 7. The metals are represented by the helium EOS scaled by a factor of 4 in density. Assuming a mass of 45 M_{JUP} for Gliese 229b and the same composition as the suited MR relation above, we present interior profiles calculated with the REOS and compare the results with those derived from the SCvH-EOS, see FIG. 8.

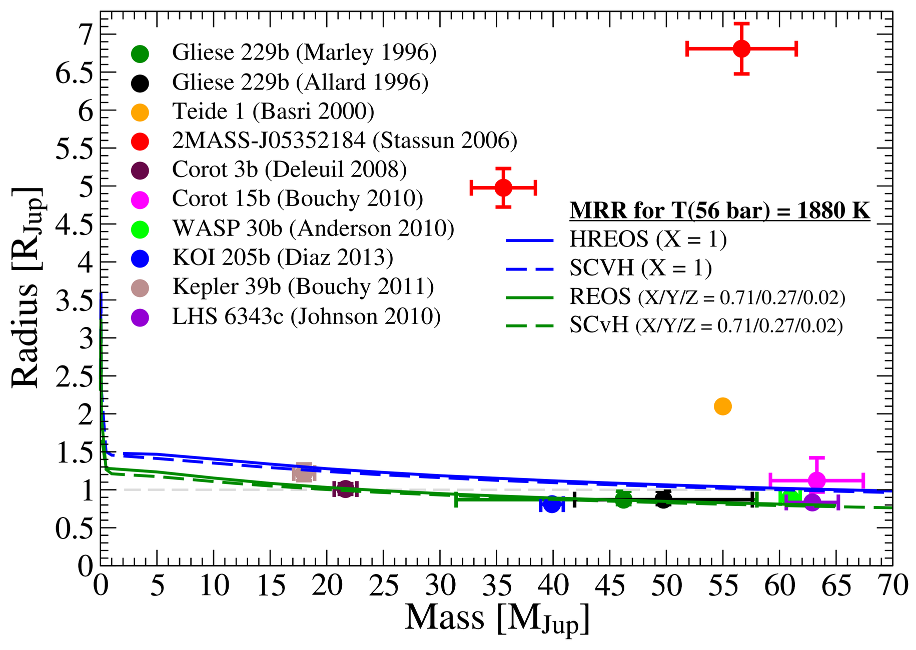

FIGURE 7: MR relations for an outer boundary condition of $T(56\mathrm{bar}) = 1880$ K, see above, calculated with the REOS (solid) and the SCvH-EOS[2] (dashed) for a solar composition (X/Y/Z = 0.7154/0.2646/0.02); green curves) and one of pure hydrogen (X=1; blue curves).

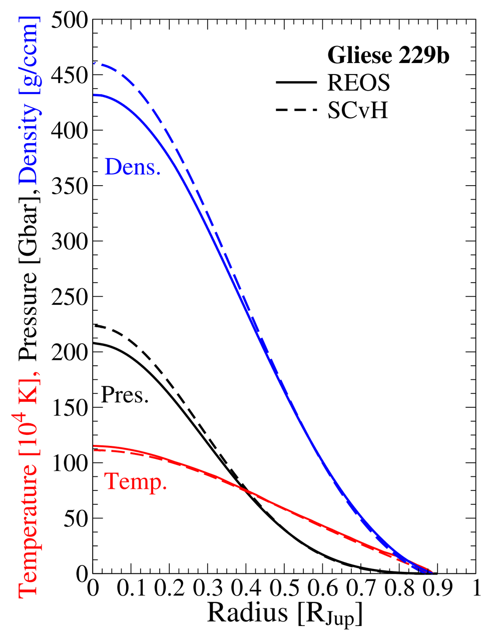

FIGURE 8: Interior profile for Gliese 229b calculated with the REOS (solid) and the SCvH-EOS[2] (dashed). Model assumptions are described above.

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