A NEW AB INITIO EQUATION OF STATE OF HCP-IRON AND ITS APPLICATION TO THE INTERIOR STRUCTURE OF ROCKY SUPER-EARTHS.

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Introduction: More than 600 out of the 3500 exoplanets discovered during the past two decades have sizes between 1 and 1.6 times the Earth's radius or masses less than 10 times the Earth's mass [1] and can potentially be classified as rocky super-Earths. In order to understand the internal and surface dynamics and habitability, the knowledge of their interior structure and composition is necessary. Up to now, observations of rocky super-Earths directly related to the interior structure are limited to mass and radius. From them, inferences on the interior structure can be made if plausible assumptions about the planet's composition are made.

Modeling the interior structure of massive super-Earths requires knowledge of equations of state (EOS) of its constituents. In particular, the EOS of iron at a pressure range significantly above that of the Earth's core – out of reach of current experimental techniques – is of fundamental importance. Standard ab initio calculation methods can be used to compute the equation of state of iron in the pressure range relevant for the core of super-Earths. Here, we calculate the equation of state of hcp-Fe in the pressure range between 0 and 5 TPa to model the interior structure of super-Earths. We use this EOS to discuss the effect of extrapolating "low pressure" equations of state of Fe (validated for the Earth's core) to pressures relevant for super-Earths on the mass-radius relation. We also compute the mass-radius relation for super-Earths by assuming different compositions for the silicate shell and core. Finally, we provide inferences about the interior structure of the rocky super-Earth, Kepler-36b.

EOS of hcp-Fe at extreme pressures: To calculate the EOS of hcp-Fe at T = 0 K in the pressure range 0–5 TPa, Density Functional Theory was used with the Perdew-Burke-Ernzerhof exchange-correlation functional, using the Augmented Plane Waves+local orbitals (APW+lo) method to solve the Kohn-Sham equations [2]. This all-electron approach is particularly suited for crystals with non-standard short bond lengths (high pressure), as no ad-hoc pseudopotentials have to be constructed. In that pressure range, our results can be summarized precisely with a Holzapfel equation [3] (fit residuals <0.15%).

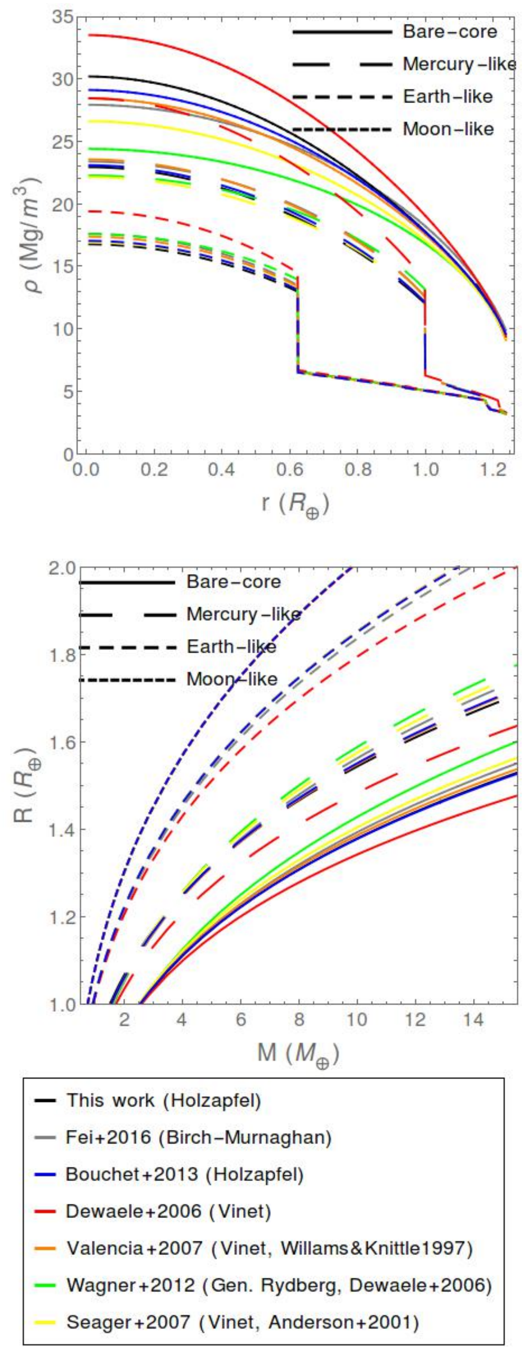

Fig. 1: *Density profiles of super-Earths with R=1.25R⊕ (top) and mass-radius relations (bottom) are compared with each other for our EOS and other published EOSs of iron.*

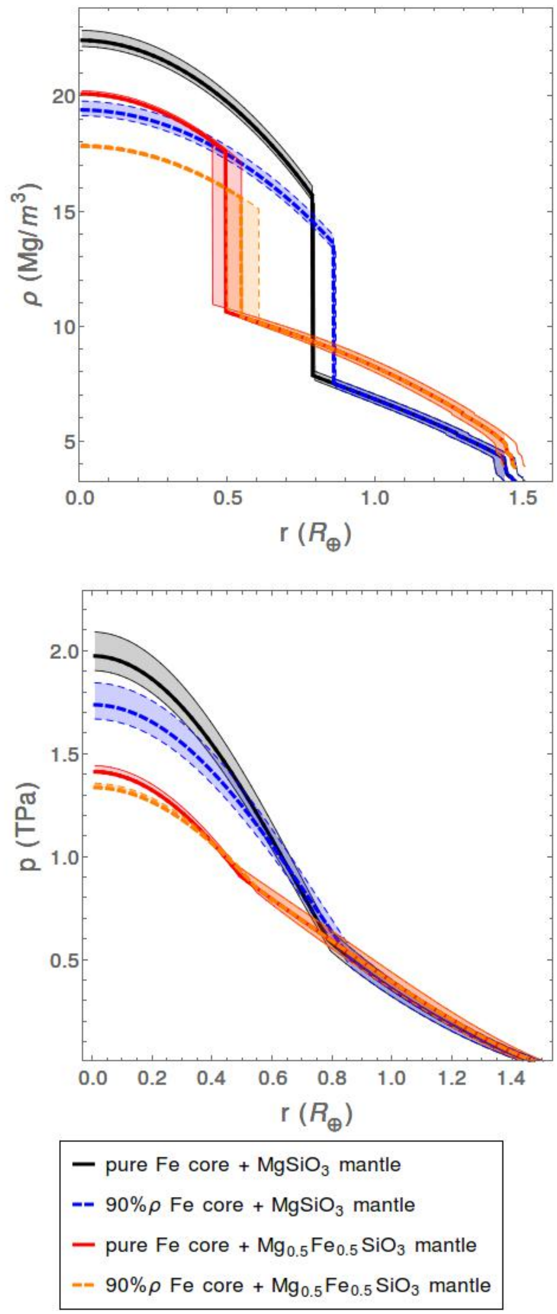

***Fig. 2:** Density and pressure profiles of Kepler-36b assuming different core and mantle compositions. Shaded regions show the uncertainty in its interior structure due to the uncertainty on its mass and radius.*

Effect of EOS of iron on interior structure and mass-radius relations: To study the effect of the EOS of iron on the interior structure we assume an $MgSiO_3$ composition for the mantle and an isentropic temperature profile for the whole planet. The phase diagram of the mantle and the associated thermo-elastic properties are calculated by Gibbs energy minimization with the "EoS" program [4] using the thermodynamic data base assessed by [5]. For the core we use the EOS of hcp-Fe of [6] for pressures below 0.3 TPa and our EOS for pressures up to 5 TPa. We consider the following interior structure models (see Fig. 1): Moon-like, $R_{core}/R_{planet} = 0.2$; Earth-like, $R_{core}/R_{planet} = 0.5$; Mercury-like, $R_{core}/R_{planet} = 0.8$; bare-core, $R_{core}/R_{planet} = 1.0$.

Our results (Fig. 1) show that extrapolations of "low pressure" EOSs of Fe can induce significant differences with respect to our EOS in the mass-radius relation when the core of the exoplanet is larger than an Earth-like core.

Interior structure and composition of Kepler-36b: We compute the interior structure models of Kepler-36b (1.486 ± 0.035 R⊕, $4.45^{+0.33}_{-0.27}$ M⊕, [7]). We assume an isentropic temperature profile within the planet, mantle composition of $Mg_{0.5}Fe_{0.5}SiO_3$ or $MgSiO_3$, and core composition of pure Fe or with a density 90% of that of pure Fe, where the density deficit is due to light elements in the core.

Our results (Fig. 2) show that the inferred core radius depends significantly on the assumed composition of the mantle and to a lesser extent on the core composition. We also find that the core-less model with end-member $FeSiO_3$ composition exceeds the observed mass.

References:

[1] http://exoplanetarchive.ipac.caltech.edu/ [2] Cottenier S. et al. (2011) *EPSL, 312,* 237-242. [3] Bouchet J. et al. (2013) *PRB 87,* 094102. [4] G. Steinle-Neumann & T. Chust (2016), 5th Joint Workshop on High Pressure, Planetary and Plasma Physics. [5] Stixrude L. et al. (2011) *GJI 184,* 1180-1213. [6] Fei Y. et al. (2016) *GRL, 43,* 6837–6843. [7] Carter J. A. et al. (2012) *Science 337,* 556.