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A New Ab Initio Equation of State of hcp-Fe and Its Implication on the Interior Structure and Mass-Radius Relations of Rocky Super-Earths

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Mass-radius relations are used as a first-order estimate to determine the composition and structure of super-Earths (SE) (Mass < 10 M_Earth or 1 R_Earth < Radius < 2 R_Earth). Like for the Earth, it is generally assumed that the core of SEs is mainly made of iron. Since the pressure in their core can be significantly larger, substantial extrapolations of the equation of state (EOS) of iron are required to compute their interior structure. Depending on the mass of the planet this can lead to significant errors. For this reason we develop an EOS of hcp-Fe based on Density Functional Theory (DFT) in the pressure range relevant for large massive SEs and study its effect on the mass-radius relation of rocky-type SEs. Additionally, we quantify the effects of several compositions and thermal states. Our results show that exoplanets computed with extrapolated EOSs of iron can be up to 20% lighter than those computed with our DFT EOS. The thermal effects are about four times smaller but mantle and core composition can influence the planet mass by up to 50%. We also discuss implications of the degeneracy in the mass-radius relation, resulting from compositional variation in the mantle and core, on the interpretation of the interior structure of observed SEs. Finally, as an application, we assess the effects of modeling and observational uncertainties on the inference of the interior structure of Kepler-36b.