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P-V-T equation-of-state of liquid Fe to the TPa regime from *ab-initio* simulations, and what we learn for super-Earth interiors

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The pressure-volume-temperature (*P-V-T*) equation-of-state (EoS) of liquid iron provides important information (reference adiabat, density ρ and higher order thermodynamic parameters) in modelling the internal structure of planetary bodies with Fe-based cores. Relevant *P*-conditions range from a few GPa (Moon, Mercury) through the 100 GPa range (Earth) to several TPa (super-Earths). Experimental data on ρ in the liquid stability field are scarce and a thermodynamic assessment of ρ depends on matching Gibbs energy along the melting line which remains controversial to this day. The alternative determination of a *P-V-T* EoS based on *ab-initio* simulations, on the other hand, suffer from the fact that ρ at ambient *P* is predicted too large by as much as 20% [e.g., 1,2]. Here [2], we have fitted *P-V-T-E-*S_{el} results from *ab-initio* molecular dynamics simulations with a self-consistent thermodynamic EoS formulation [3] and combined it with a correction formalism that accounts for the ρ-mismatch at ambient *P* [4]. As the correction is additive to the Helmholtz potential and shows the correct limiting behavior at high and low ρ, thermodynamic self-consistency of the results is not affected. Using this combination, our EoS reproduces ρ from shock-wave experiments as well as previous models, but shows a significantly improved agreement at ambient *P*, the critical point and the sole ρ measurement in the large-volume press at 4.3 GPa [5]. We explore the performance of our thermodynamic potential and various previously published EoS models for liquid iron [1,6,7] over a wide range of conditions: (i) at ambient pressure as a function of temperature, (ii) along the melting curve of Fe to 40 GPa, relevant for the cores of smaller terrestrial bodies in our solar system, (iii) along isentropes in the Earth's outer core and (iv) for the core of super-Earth Kepler-36b along a previously modelled *T*-profile in the core [8].

The correction term significantly improves the agreement of computed properties with experiments and other thermodynamic models that are based on an assessment of the phase diagram at ambient and moderate *P* [6,7], showing how *ab-initio* molecular dynamics simulations can be used at par with other techniques. For the Earth's core, ρ-profiles from the various models are similar, but higher-order derivatives (acoustic velocity and Grüneisen parameter) show significant differences. For the core model of Kepler-36b [8], differences in ρ from various EoS formulations and implementations [1,2,6,7] are negligible, for core mass they do not exceed 2%, showing robust extrapolation of all models. The robustness of the different formulations of Fe EoS at conditions of the cores of super - Earths is encouraging in the sense that it will allow for a meaningful inversion of planetary structure (e.g., core radius ratio) once relevant astronomical observations become available [9].

References: [1] Ichikawa et al., JGR 119, 240 (2014); [2] Wagle & Steinle-Neumann, JGR (in press); [3] Vlček et al., PRB 85, 184201 (2012); [4] French & Mattsson, JAP 116, 013510 (2014); [5] Tateyama et al., PCM 38, 801 (2011); [6] Dorogokupets et al., Sci. Rep. 7, 41863 (2017); [7] Komabayashi, JGR 119, 4164 (2014); [8] Hakim et al., Icarus 313, 61 (2018); [9] Padovan et al., A&A 620, A178 (2018).

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