Free energies of iron phases at high pressure and temperature: Molecular dynamics study

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The crystal structure of iron, one of the main elements of the Earth's inner core (IC), is unknown at the IC high pressure ($P \approx 3.3$–3.6 Mbar) and temperature ($T \approx 5000$–7000 K). Experimental and theoretical data on the phase diagram of iron at these extreme P–T conditions are contradictory. Applying quasi-ab initio and ab initio molecular dynamics we computed free energies of the body-centered cubic (bcc), hexagonal close-packed (hcp), and liquid phases. The ionic free energies, computed for the embedded-atom model, were corrected for electronic entropy. Such correction brings the melting temperatures of the hcp iron in very good agreement with previous ab initio data. This validates the calculation of the bcc phase, where fully ab initio treatment is not technically possible due to large sizes required for convergence. The resulting phase diagram shows stabilization of the bcc phase prior to melting in the pressure range of the IC [1]. The research was conducted within the framework of the HSE University Basic Research Program.

[1] Belonoshko A B, Fu J and Smirnov G 2021 *Phys. Rev. B* **104** 104103