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Phase diagram of pure iron in Earth's core from deep learning

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Iron is considered to be the main component of the Earth's core. Substantial efforts have been made to understand its phase diagram and physical properties at extreme conditions. However, it remains debated about how the atoms in solid iron are arranged at Earth's core conditions, where possible candidates include hexagonal close-packed (hcp), body-centred cubic (bcc), and face-centred cubic (fcc) structures. As crystal structure and physical properties are closely related, there is also a significant uncertainty in the properties of Earth's core, such as elasticity, heat conductivity, and density, making the accurate interpretation of seismic observations difficult. Here we aim to study the phase stability of solid iron at Earth's core conditions. For this, a deep-learning interatomic potential was developed with *ab initio* accuracy but is more cost-effective. To further check the performance of such potential, we examine the elastic and plastic behaviour of hcp iron and the effects of structural defects at inner core conditions [1]. We then compute the Gibbs free energy of the bcc, fcc, hcp and liquid phases by performing large-scale molecular dynamics simulations. The calculated free energy allows for determining the phase stability of solid iron in Earth's core.

[1] Li, Z., & Scandolo, S. (2022). Elasticity and viscosity of hcp iron at Earth's inner core conditions from machine learning-based large-scale atomistic simulations. *Geophysical Research Letters*, *49*, e2022GL101161.