

Impact of magnetism on Fe phase diagram under extreme conditions

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Iron is a major component of the cores of the Earth and inhabited exoplanets. Its phase diagram at extreme pressures (P) and temperatures (T) is the subject of extensive debate. While recent experiments provide evidence for the stability of the body-centered cubic (bcc) phase, several theoretical studies point to the stability (even though marginal) of the hexagonal close-packed phase (hcp). None of those studies considered the itinerant magnetism of iron at extreme conditions. We compute the high-pressure phase diagram of Fe using density functional theory-based molecular dynamics (DFT MD) in which the paramagnetic nature of Fe is treated within the model of thermally induced longitudinal spin fluctuations (LSF). The LSF DFT MD with 16 valence electrons favors bcc phase stability. Two-phase large-scale simulations with quantum accurate machine learning potentials provide us with both melting and hcp-bcc phase boundaries. The computed phase diagram agrees with most of the experimental data and solves most of the numerous controversies. We conclude that the account for magnetism results in the new physics of iron under extreme conditions and brings the theory in agreement with experiment and seismic data. We expect that the approach we use can be applied to other metals where itinerant magnetism is important.

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The crystal structure of iron, the major component of the Earth's inner core (IC), has been the subject of ongoing discussion in a number of recent and not-so-recent papers, both experimental [1–12] and theoretical [13–30]. The extreme pressure (P) (3.3–3.6 Mbar) and temperature (T) (5000–7000 K) conditions of the IC make the experiments difficult, even though some unique experiments are conducted at pressures up to 10 Mbar [10]. Considering experimental difficulties, theory becomes a valuable asset in the interpretation of experimental data. Recently, it has been shown that the experimental spectrum collected for iron at the pressure of about 5.5 Mbar at temperatures close to the melting point contains peaks that can be explained by the stabilization of the body-centered cubic phase [31]. Earlier, the 11-coordinated

phase of iron, which is the high-PT bcc phase of iron, was observed in yet another experiment [11]. Notwithstanding that some experiments did not observe the bcc phase in the PT range close to the Fe melting curve at high pressure, we have to conclude that the stability of the bcc phase is likely. A positive signal weighs more than the absence of a signal. Several theoretical studies, based on the standard DFT approach, support the stability of the hcp phase in the PT region below the melting curve. However, the properties of the Earth's inner core are in nearly perfect agreement with the properties of the bcc phase and in sharp contrast with the properties of the hcp phase. One such property is the shear modulus [28,32]. Although most of the DFT studies have certain problems, their consistency regarding the bcc instability suggests that the disagreement with the experiment is rooted in neglecting some physics and that the standard DFT does not correctly describe the physics of iron at extreme PT conditions.

As has been demonstrated in Ref. [30], the missing magnetic effects in standard DFT simulations at the extreme PT conditions are longitudinal spin fluctuations (LSF), which exist in the paramagnetic state [33]. Although local magnetic moments are finite in the disordered local moment (DLM) presentation of the paramagnetic state in bcc Fe at ambient

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pressure above the Curie temperature in DFT calculations, they vanish either at temperatures above 6000 K (just due to trivial one-electron excitations within the Mermin DFT generalization to finite temperatures) or at low temperatures but extremely high pressure above 200 GPa. This behavior is, however, an artifact of the lack of LSF in standard DFT calculations. In fact, local magnetic moments of Fe become finite and relatively large even when both temperature and pressure correspond to the Earth's core conditions, provided that one accounts for a longitudinal spin degree of freedom in the statistical thermodynamics consideration [30].

As will be shown here, the account of LSF significantly affects the relative stability of the bcc phase at the high P–T conditions of planetary cores. This happens because the free energy difference between bcc and hcp phases is of the order of a few meV [16], hence even small corrections due to magnetism could radically change the calculated phase diagram. To correctly assess the effect of magnetism on the Fe phase diagram, it is necessary to compare the phase diagrams calculated with and without magnetism. Particularly critical is the calculation of melting curves. The phase with the highest melting temperature is the stable submelting phase. We use *ab initio* molecular dynamics (AIMD) and machine learning (ML) force field to compute phase boundaries. A detailed description of the methods we use for calculations is provided in Supplemental Material [34] (see also Refs. [35–65] therein).

First, we use the two-phase approach in nonmagnetic AIMD calculations to obtain the reference melting temperature of the hcp phase at 360 GPa, without relying on experimental data or other computed data. Although this value was calculated several times in the literature, the distinctive features of our approach are large simulation cells (512 hcp and 512 liquid atoms with a common interface at the beginning of the simulations) and the finite electronic temperature (the Fermi-Dirac smearing parameter is equal to 0.61 eV). We observe that at $T = 6950$ K and $P = 360$ GPa, the initial hcp liquid transforms into the hcp phase with stacking fault defects, while at $T = 7050$ K and $P = 360$ GPa, the same cell melts. Thus, the melting temperature of hcp iron in the nonmagnetic approximation with the PAW-16 pseudopotential in the VASP package is 7000 ± 50 at 360 GPa. The melting temperature obtained from fully *ab initio* MD runs serves as the basis for further validation of the generated machine learning potentials. We use these AIMD trajectories to generate two separate ML potentials. The results show excellent agreement between the AIMD and ML-MD calculations—both ML force fields predict freezing of the hcp structure at 6950 K and melting at 7050 K as expected. Thus, small differences in forces do not lead to different melting temperatures. We might expect a similar accuracy for *bcc*-liquid two-phase simulations, though we do not have a reference melting temperature from fully *ab initio* MD runs.

Therefore, we extend our methodology to obtain the melting temperature at 120, 360, and 500 GPa with three different pseudopotentials available in VASP. These temperatures are summarized in Table I. Using the nonmagnetic approximation, we find that the bcc phase is thermodynamically stable, i.e., has a higher melting point than the hcp phase, at 360 GPa with PAW-8 and PAW-14 pseudopotentials. However, this result could not be used as an argument for the stability of the

TABLE I. Melting temperatures of bcc and hcp phases from nonmagnetic ML-MD calculations. Typical errors are about 10 K.

Pseudopotential	Structure	Melting temperature, K		
		120 GPa	360 GPa	500 GPa
PAW-8	bcc		6375	7275
	hcp	4387	6275	7325
PAW-14	bcc		7262	8425
	hcp	4312	7075	8587
PAW-16	bcc		6962	7875
	hcp	4287	6990	7975

bcc phase: PAW-14 approximation fails to describe the interatomic forces or the high-pressure cold curves and the PAW-8 model systematically underestimates interatomic forces. A detailed discussion of the pseudopotentials' accuracy is available in the Supplemental Material. We also could not calculate the melting temperature of the bcc phase at 120 GPa, since the bcc-liquid system quickly transforms into the hcp phase below the melting line.

At the same time, the melting temperature of the hcp phase depends on the pseudopotential. A comparison of different *ab initio* points near the melting line is shown in Fig. 1. Similarly to Ref. [24], the PAW-8 model gives the lowest melting temperature, while the PAW-14 predicts the highest

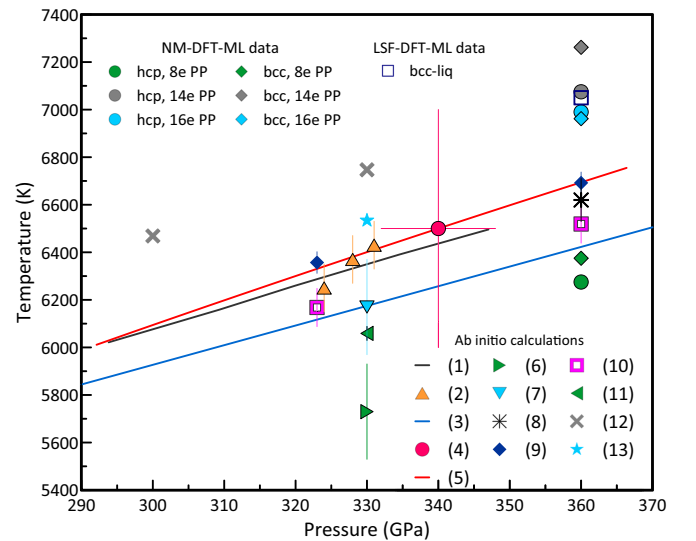


FIG. 1. *Ab initio* melting curves and points of hcp phase: (1) free energy calculations [66]; (2) direct coexistence simulations [67]; (3) free energy calculations [68]; (4) two-phase simulations from Ref. [21] (bcc melting curve almost coincides with the hcp curve); (5) Simon fit from Ref. [69] based on the data from Ref. [70]; (6) free energy calculations using PAW-8 pseudopotential in VASP [17]; (7) free energy calculations using PAW-16 pseudopotential in VASP [17]; (8) solid-liquid coexistence method [71]; (9) free energy calculations [16]; and (11)–(13) free energy calculations using PAW-8, PAW-14, and PAW-16 correspondingly in VASP [24]. *Ab initio* melting points of bcc phase: (10) free energy calculations [16]. Our magnetic and nonmagnetic hcp and bcc melting points (solid green, gray, and blue circles and diamonds) are also shown for comparison.

melting temperature. However, the difference is quite large—at 500 GPa the difference in T_m between PAW-8 and PAW-16 is about 1000 K. From our observation, the melting line at high temperatures is quite sensitive to the smearing parameter of electrons. Since the authors of Ref. [24] did not provide specific details about the choice of this parameter, we assume that this is the main source of discrepancy between our works.

Now, being informed of the phase relations in nonmagnetic Fe, we will consider the impact of the high-temperature magnetic excitations, namely LSF, which is the central part of our study. As has been mentioned above, they are not accounted for in the standard DFT. More elaborate electronic structure calculations based on the dynamical field approximation (DMFT) [72,73] or time-dependent DFT [74] take into account LSF. However, they are impractical for large-scale AIMD simulations, which are of prime importance to accurately evaluate the free energy of different Fe phases at the extreme PT conditions. Therefore, we use here a DFT-based statistical ansatz, within which they can be accounted for in the paramagnetic state using a magnetic configuration of spins approximating the DLM state within a supercell and the LSF magnetic entropy, added to the local Kohn-Sham potential of each iron atom [30]. The magnetic entropy in the DFT self-consistent calculations gives rise to finite magnetic moments and contributes to the *ab initio* free energy (see Supplemental Material for the details). The LSF model is sufficiently simple to keep AIMD simulations and subsequent training of ML potentials affordable. Recently, a similar but more elaborated LSF-DFT approach was used in calculations of bcc Fe at the Earth core conditions [75]. However, it is computationally too demanding for large supercell AIMD calculations.

Such LSF-DFT-based ML potentials correctly reproduce the stability of the hcp lattice at low temperatures and high pressures. At the same time, these potentials predict the stability of the bcc phase near the melting curve. The melting temperature of the bcc phase in this case practically coincides with the melting temperature of the hcp phase in nonmagnetic calculations. At 120 and 360 GPa, we calculate the temperature of the hcp–bcc phase transition. Such calculations are difficult due to the possibility of long-time coexistence of solid phases close to the P–T range of the transition. The upper estimate of the temperature of such a transition is defined as the stability limit of the hcp phase, above which we observe a spontaneous transition of the hcp phase into the stable bcc phase. Similarly, the lower estimate of the transition temperature is determined by the stability limit of the bcc phase. Between these values, the kinetics of the phase transition does not allow us to observe a direct hcp–bcc transformation within the reasonable computation time.

The stability of the bcc phase at high pressures means that we should observe the bcc–fcc coexistence line. Our approximation cannot be used for a quantitative description of this phase transition (see Supplemental Material for the discussion). However, we could estimate the fcc–bcc transition temperature even without the fcc phase in the training set. We get $T_{\text{fcc-bcc}} = 2500$ K at 50 GPa, which corresponds to the lower estimates of the fcc melting. The resulting P–T phase diagram that presents the experimental data and our LSF DFT magnetic melting points is shown in Fig. 2.

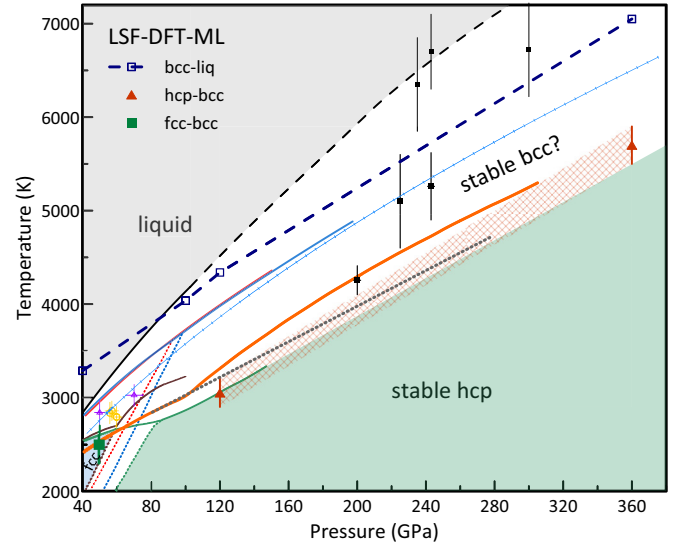


FIG. 2. Pressure-temperature phase diagram of iron. Filled areas show the lower estimate of liquid and solid stability regions from the experimental data. Open blue squares and dashed curves show the melting line of the bcc phase from our calculations including the LSF term. Red triangles and crossed pattern illustrate the bcc-hcp boundary. Green square gives the fcc-bcc coexistence. Experimental data are also shown for comparison. Melting curve from static measurements: solid black line (Williams *et al.* [7]); solid green line (Boehler *et al.* [5] and Aquilanti *et al.* [4]); solid brown line (Shen *et al.* [76]); solid red line (Anzellini *et al.* [3]); purple triangles (Jackson *et al.* [77]); yellow circles (Zhang *et al.* [78]), solid orange line (Sinmyo *et al.* [79]); solid blue line (Hou *et al.* [80]). Melting curve from dynamic measurements: dashed black line (Williams *et al.* [7]), solid blue line with tick marks (Kraus *et al.* [10]), black filled squares (Refs. [1,8,81,82]). Gray dotted line gives the hcp–bcc coexistence from Ref. [9]. Brown, red, blue, and green curves show the isostructural hcp–fcc transition, correspondingly (Shen *et al.* [76], Anzellini *et al.* [3], Hou *et al.* [80], Boehler *et al.* [5]).

For the nonmagnetic calculations, theoretical melting temperatures of hcp Fe (Fig. 1) at the pressure of 360 GPa are within about 500 K for the 16 valence electrons PP. This is much smaller than the difference (more than 1000 K) between the experimental melting curves already at the pressure of 150 GPa (Fig. 2). Since the melting curves diverge on pressure increase, the difference would become larger at the pressure of 360 GPa. This means that the theory allows us to discriminate between experimental melting curves. Furthermore, we trust simulations with the highest number of valence electrons (16) rather than the lowest one (8). Also, we expect simulations with the largest cell size to be more reliable, since long-wave phonons are excluded in small cells, which leads to the underestimation of the melting temperature. Finally, we consider two-phase simulations (Figs. S5, S6, S7) to be more reliable than free energy calculations because of mutual error cancellation in the former. This approach has also been supported by other researchers (see, e.g., [16,65]), and its robustness has been demonstrated in several papers [83,84]. As a result, we get the melting point of hcp Fe (when no magnetism is taken into account) to be about 7000 K at the pressure of 360 GPa, which is somewhat higher than previous simulations (Table I

and Fig. 1). To summarize, all the results are presented for calculations with large cells (making hcp Fe more stable than in small cells), with 16 valence electrons, and with the help of the two-phase method, which allows us to achieve high precision of predictions.

The central result obtained in this study when magnetism is considered is quite remarkable (Fig. 2). Normally, two-phase simulations are used to determine the melting temperature of the solid phase in contact with the liquid phase. However, in this study, the liquid part of the two-phase computational cell facilitates the solid-solid phase transition and provides an unambiguous conclusion about the relative stability of the hcp and bcc phases. The simulations of the hcp+liquid system result in the homogeneous hcp cell if the temperature is below the critical temperature and in the bcc structure if the temperature is above the critical temperature. Getting the solid phase that was not initially present in the two-phase system is rather rare for computational studies.

Let us discuss how the calculated hcp-bcc phase boundary compares with the available experimental data. Brown and McQueen [1] reported a solid-solid phase transition at the pressure of 200 GPa and the temperature between 4100 and 4400 K (the large uncertainty was due to the unknown heat capacity). Recently, Singh *et al.* [85] reported the bcc peak in the x-ray spectrum obtained during shock compression of iron at the pressure of 210 GPa and the temperature of 4350 K. These two points are identical within mutual error bars. It is also within error bars from the locus of the hcp-bcc transition determined in the diamond-anvil cell with laser heating experiment and reported by Hrubak *et al.* [9]. Note that Hrubak *et al.* [9] collected the bcc spectra *in situ* experiments. Furthermore, these P-T conditions are very close to the points reported by Sinmyo *et al.* [79] and Boehler [5]. Finally, at this pressure and higher, Ping *et al.* [11] report 11-coordinated iron—and such coordination is the property of the bcc phase [15,31]. Both papers by Sinmyo *et al.* [79] and Boehler [5] interpreted their data as the observation of melting. Note that these interpretations are in conflict with the experimental data by Anzellini *et al.* [3], who reported melting at much higher temperatures yet reported a rapid crystallization where Sinmyo *et al.* and Boehler reported melting. While Boehler's interpretation is based on visual observations of sample changes, Sinmyo *et al.* report a plateau on the voltage-temperature plot. Such a plateau is due to the latent heat of a phase transition. Sinmyo *et al.* interpreted this phase transition as melting. However, there is no reason to believe that it was indeed melting and not a solid-solid (for example, hcp-bcc) phase transition. To summarize, in the vicinity of the P-T point at about 200 GPa and 4000 K we have three experiments reporting spectroscopic data consistent with the bcc stabilization, and three experiments reporting a phase transition (without spectroscopy data). Out of the latter three experiments, two interpret their data as melting, and one interprets the transition as a solid-solid transition. To be consistent with the data of Anzellini *et al.* [3], we have to interpret the 'melting' experiments without any supporting spectroscopy data as the manifestation of the solid-solid transition.

We now have to conclude that when itinerant magnetism is considered, the hcp-bcc transition computed in this study is a perfect fit to the experimental data (Fig. 2). The highest

P-T conditions obtained in a diamond-anvil cell with laser heating are reported by Hirose *et al.* [6]. They are 356 GPa and 5450 K. This is pretty much exactly the conditions at the point 360 GPa and 5500 K, which is the end-point of the computed in this study hcp-bcc transition (Fig. 2). Therefore, we are also in very good agreement with that experiment. Note that Hirose *et al.* could not go to higher temperatures at the pressure of 356 GPa because the strong contamination of the iron sample sets in. This is indirect evidence of the hcp-bcc transition because the bcc phase is superionic and that likely causes strong contamination of iron in the Hirose *et al.* [6] experiment when the hcp-bcc phase boundary is crossed.

Of course, when experimental datasets are mutually incompatible (e.g., Refs. [3,9,79]), we cannot get agreement with all of them. Generally, two datasets are considered as evidence of the hcp stability in the inner core, one from Ref. [12] and another from Ref. [3]. As for the former, even though the pressure conditions were very high (almost up to 3 Mbar), the temperatures were comparably low, below the computed hcp-bcc transition. Therefore, our theoretical data is in perfect agreement with the Ohtani *et al.* [12] dataset, where only the hcp phase was observed. Regarding the Anzellini *et al.* [3] experiment, we note that they observe fast recrystallization nearly exactly where we see the phase transition from hcp to bcc (Fig. 2). At a higher temperature, experimentalists do not report any bcc peaks, but they do not report liquid peaks either. Rather, in support of melting, they point to the appearance of a diffuse signal (yet the solid peaks do not disappear). We note that the bcc phase is superionic, and the abundant diffusion in bcc (no such diffusion occurs in hcp) in principle might produce the diffuse signal. Note that such a diffuse signal might have confused a large group of researchers [10] who observed the submelting bcc phase of iron but mistakenly interpreted it as the liquid diffuse peak [31].

We do not review in detail the experimental inconsistencies of the fcc melting line due to the limitations of our method in this region of the phase diagram. However, we could speculate that the bcc phase is also stable below 100 GPa, and some experimentalists see not melting but the fcc-bcc transition. In that case, the results of such experiments could be affected by the kinetics of such transition, as was discussed for graphite melting [86].

The bcc-liquid phase boundary is not affected by magnetism because of a similar impact on both the bcc and liquid phases. At the pressure of 360 GPa, iron melts at about 7000 K. However, it melts not from the hcp phase but from the bcc phase. Note, that we cannot even compute the hcp phase melting temperature anymore—the hcp spontaneously transforms to bcc if simulated for a sufficiently long time (Fig. S8).

One might ask why the comparatively small changes in the free energy due to magnetism lead to such drastic changes in the phase diagram of iron. Sun *et al.* [17] demonstrated that a few meV change in the free energy of an iron phase leads to a 100 to 200 degrees change in the melting temperature. Accounting for magnetism leads to an order of 20 meV free energy change between hcp and bcc phases in favor of bcc (and liquid). In terms of melting temperatures, we are talking about thousands of degrees of melting temperature change. This is quite dramatic. The proximity of melting temperatures

of non-magnetic hcp and bcc phases is extreme—the difference between them is within 100 K. This is why the account for magnetism leads to a completely different topology of the iron phase diagram that allows us to explain the experimental data. Whether the account of magnetism is critical when computing the phase diagrams of other metals is hard to tell, but it is clear that this subject is in need of investigation.

We have demonstrated that the account for magnetism brings the phase diagram of iron in agreement with experimental data at high pressure and temperature. While the model of iron considered in this study is perhaps not perfect, the ability of the model to resolve a number of controversies is remarkable. Fitting of ML potentials to the MD data on energies and forces during the simulation of large cells is crucial for obtaining robust results. ML potentials should be used to compute data within a range of pressures and temperatures around the point where the potentials have been trained using LSF-DFT MD data, otherwise the magnetic and electronic entropies are not reproduced correctly. The two-phase method for computing phase boundaries is universal and should be used consistently in the case when one of the solid phases involved is superionic and the use of a harmonic solid as a standard state leads to uncertain errors in calculations of the free energy.

Although the account of magnetism in first-principles calculations is vital, it leads to time-consuming computations, and this study required significant computational resources. The energy changes due to magnetism are small, and it might be tempting to use nonmagnetic DFT MD runs to compute the properties of the bcc phase for small cells. We would like to warn that giving in to such temptation might be dangerous. The bcc phase is in part stabilized by the collective superionic motion of atoms [15], Fitting ML potentials to MD data

collected for small cells may produce misleading results since configurations relevant for superionic motion might not be adequately accounted for in small cells.

The phase diagram of iron computed in this study brings seismic data on Earth's core and the theory of iron into agreement. While certain questions, mainly on the experimental side, still remain open, we hope they will be resolved by careful experiments with full control of the P–T conditions and the structure of a sample along with sufficient time for maintaining the sample at these conditions, so that kinetic problems could be ruled out. Our study opens an avenue for studying iron in its stable structure under the conditions of the Earth's inner core and the conditions in the cores of exoplanets. This, in turn, will facilitate the educated search for inhabited planets.

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Data availability. Results of our simulations are available from authors on a reasonable request.

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