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Impact of magnetism account on computation of iron phase diagram

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Iron (Fe) is a major component of the Earth and inhabited exoplanets cores, yet its phase diagram at extreme pressures (P) and temperatures (T) is a subject of extensive debate. Since the solid core is at the temperature close to melting it is of ultimate importance to know the structure of the sub--melting phase. Such knowledge enables understanding of the planet evolution from the beginning to the current state and predicting the future. While recent experiments provide the 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. Here, we computed the melting curves using the density functional theory based molecular dynamics (DFT MD) with and without thermally induced longitudinal spin fluctuations (LSF). The non-magnetic DFT MD simulations result in stability of the *hcp* phase as the submelting phase with 8 and 16 valence electrons while the *bcc* phase stabilizes for the case of 14 valence electrons. The LSF DFT MD with 16 valence electrons favors the *bcc* phase stability. Therefore, we conclude that the account of magnetism results in the new physics of iron at extreme conditions and brings the theory in agreement with experiment as well as seismic data on the Earth Inner Core.