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Effect of vacancy formation in solid iron under high pressure JIN-CHUN LI, DONG-BO ZHANG, Beijing Computational Science Res Ctr, TAO SUN, University of Chinese Academy of Sciences — Solid iron has been widely used in material engineering, and it is proposed as the fundamental component of the Earth's core, so magnetic and mechanical properties of iron at high pressure have attracted extensively experimental and theoretical studies. In this work, we perform systematic calculations to investigate the lattice constants, enthalpy, magnetic moment, elastic properties of perfect crystalline solid iron for a wide range of pressures by using first-principles. Then, in order to study the effect of point defect in the solid iron in extreme conditions, the mono-vacancy is involved in stability, magnetic and elastic properties of iron. Furthermore, different sized supercells within mono-vacancy model are applied to research pressure influence on vacancy concentration.

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