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High-pressure behavior of iron and iron-alloys

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As the most stable element in the periodic table and a final fusion product of stars, iron is ubiquitous in the universe, and its presence likely leads to the formation of cores in planetary bodies that form from refractory oxides, similar to the terrestrial bodies in our solar system, termed super-Earths. Physical and chemical properties of iron at high pressure are therefore of great interest in the study of planetary interiors, beyond the Earth and our solar system. At the same time, iron has played a critical role in the development of approximations to the exchange and correlation potential in Kohn-Sham density functional theory (KS-DFT). The failure to properly describe the ground-state of iron (ferromagnetic bcc) in the local density approximation provided an early impetus to the development of generalized gradient formulations. The magnetic structure of the high-temperature phase fcc led to early non-collinear magnetic formulations of the charge density. At pressures of the Earth's core (~300 GPa, with a relative compression of ~0.6 with respect to the ambient pressure volume), hybridization effects for 3d and 4s electrons (typically considered valence at ambient conditions) with 3s and 3p states (core) makes choices on the treatment of electronic bands a tricky business. At higher pressure that prevail in the interior (and therefore hypothetical cores) of super-Earths (exceeding TPa), choices on the treatment of electronic states become even more complex. Here I review high-pressure results using KS-DFT for iron and dilute iron alloys that are of importance in a planetary context, and discuss apparent and potential limitations. Properties discussed range rom pure compression behavior to atomic and electronic transport properties.

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