Intermediate-spin ferrous iron in the Earth’s lower mantle?\(^1\) HAN HSU, Department of Physics, National Central University, Jhongli City, Taoyuan 32001, Taiwan, RENATA WENTZCOVITCH, Department of Chemical Engineering and Materials Science, Minnesota Supercomputing Institute, University of Minnesota, Twin Cities — Using density functional theory + self-consistent Hubbard U (DFT+Usc) calculations, we investigate intermediate-spin (IS) ferrous iron (Fe\(^{2+}\)) in major lower-mantle minerals, ferropericlase (Fp) and magnesium silicate (MgSiO\(_3\)) perovskite (Pv). In both minerals, two distinct types of IS Fe\(^{2+}\) are found. In Fp, while both types of IS Fe\(^{2+}\) are configured \(t^5_2 \cdot e^1_4\), one has a \(d_{z^2}\) electron and the other has a \(d_{x^2-y^2}\) electron, referred to as the IS\((z^2)\) and IS\((x^2-y^2)\) state, respectively. The IS\((z^2)\) state has an exceptionally high QS (\(\geq 5.5\) mm/s); the IS\((x^2-y^2)\) state has a quite low QS (\(<0.5\) mm/s). Also, the IS\((z^2)\) state has a stronger on-site Coulomb interaction and much higher energy. In Pv, while Fe\(^{2+}\) substitutes Mg in the dodecahedral site, it is effectively under a distorted octahedral crystal field, and the two IS states can be characterized by their filled \(e^\_g\)-like orbitals as well. These two IS Fe\(^{2+}\), in contrast to those in Fp, are energetically competitive, and they both have a small QS (\(<1.6\) mm/s). Our calculations show that all IS Fe\(^{2+}\) in lower-mantle minerals are unfavorable, and their QSs are all inconsistent with experiments. Therefore, IS Fe\(^{2+}\) is highly unlikely in the Earth’s lower mantle.

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