Abstract Submitted
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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 $t_{2g}^5\ e_g^1$, one has a d_{z2} electron and the other has a d_{x2-y2} 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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