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First-principles study of spin-state crossovers and hyperfine interactions of ferric iron in magnesium silicate perovskite[1] HAN HSU, University of Minnesota, PETER BLAHA, TU Vienna, MATTEO COCOCCIONI, RENATA WENTZCOVITCH, University of Minnesota — The spin-state crossover in iron-bearing $MgSiO_3$ perovskite, the most abundant mineral in the Earth, may significantly affect the properties of Earth's lower mantle. However, details of this phenomenon have been very unclear, owing to the complicated nature of this mineral, mainly the coexistence of ferrous and ferric iron. Using the density functional theory plus Hubbard U (DFT+U) methods, we investigated the spin states and hyperfine interactions of ferric iron in this mineral. We show that a crossover from high-spin to low-spin state occurs within the lower-mantle pressure range, and it is accompanied by a noticeable volume reduction and an increase in iron nuclear quadrupole splitting (QS). These results are consistent with recent x-ray diffraction and Mössbauer spectroscopy measurements [K. Catalli *et al.*, Earth Planet. Sci. Lett. **289**, 68 (2010)].

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