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Spin states and hyperfine interactions of iron in (Mg,Fe)SiO_3 perovskite under pressure[1] PETER BLAHA, TU Vienna, HAN HSU, KOICHIRO UMEMOTO, RENATA WENTZCOVITCH, University of Minnesota — We have found several metastable equilibrium sites for substitutional iron in (Mg,Fe)SiO_3 with the guidance of first-principles phonon calculations. In the relevant energy range, there are two distinct sites for high-spin (HS), one for low-spin (LS), and one for intermediate-spin (IS) iron. The two competing HS sites have different iron nucleus quadrupole splittings (QS) due to their different d-orbital occupancies. At low pressure, the HS site with QS of 2.3 mm/s is more stable, while the HS site with QS of 3.3 mm/s is more favorable at higher pressure. The crossover from low-QS to high-QS site occurs between 4 and 24 GPa, depending on the exchange-correlation functional and on the inclusion of Hubbard U. Our calculation supports the notion that the transition observed in recent Mössbauer spectra corresponds to an atomic site change rather than a spin-state crossover.

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Han Hsu
University of Minnesota

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