

Abstract Submitted
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First-principles investigation of the spin state of ferrous iron in MgSiO_3 under pressure¹ YONGGANG YU, CEMS, University of Minnesota, RYAN REQUIST, Friedrich Alexandre University Erlangen 91058, Germany, KOICHIRO UMEMOTO, RENATA WENTZCOVITCH, MSI and CEMS, University of Minnesota — We present a density functional study of the pressure induced spin transition in ferrous iron in MgSiO_3 perovskite and post-perovskite. We address the influence of iron concentration and configuration (structural and magnetic), as well as technical issues such as the nature of the exchange correlation (XC) functional (LDA versus PBE-GGA) on the spin transition pressure. Supercells containing up to 160 atoms were adopted to tackle these issues. We show that there are preferred configurations for high-spin and low-spin iron and that the spin transition pressure depends strongly on iron concentration and XC functionals. We also address the possibility of a structural change accompanying the spin transition.

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