

Abstract Submitted
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Pressure induced iron spin state changes in MgGeO₃ Perovskite and Post-perovskite¹ KANCHAN SARKAR, GAURAV SHUKLA, MEHMET TOPSAKAL, RENATA WENTZCOVITCH, University of Minnesota Twin cities — MgGeO₃-perovskite is a low pressure analog of MgSiO₃-perovskite, the main Earth forming phase, and is used to shed light on several phenomena that occur in MgSiO₃, particularly the post-perovskite transition. As such, experimental investigations of spin state changes in Fe-bearing MgGeO₃ might help to clarify some aspects of this phenomenon in MgSiO₃. Using DFT+U calculations, we have investigated pressure induced spin state changes in Fe²⁺ and Fe³⁺ in MgGeO₃ perovskite and post-perovskite and their effect on the post-perovskite transition. We uncover a direct relationship between average Fe-O bond-lengths and spin transition pressures in all cases. The effect of iron on the post-perovskite transitions in these phases can also be related to the average Fe-O bond lengths.

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Gaurav Shukla
University of Minnesota Twin cities

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