

High-Spin to Low-Spin Transition in Magnesiowustite: Seismic Signature

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High resolution X-ray spectroscopy has recently demonstrated that iron in the major lower mantle (LM) minerals undergo a high-to-low spin transition at LM pressures. Previous failures of standard DFT and LDA+U approaches to describe this phenomenon have hindered its investigation and consequences of fundamental importance to geophysics, such as heat transport in Earth's mantle.

Here, using the latest rotationally invariant first principles formulation of LDA+U with optimized effective U, we report the first successful study of this transition in low solute concentration $\text{Mg}(1-x)\text{Fe}x\text{O}$, magnesiumwustite. This is believed to be the second most abundant phase of Earth's LM. We also investigate the elastic signature of this transition. We find large and temperature sensitive contrast in elasticity across the spin transition in iron.

This encouraging result appears to open for exploration a new class of problems of enormous significance to deep Earth geophysics.

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