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High-to-low spin transition in iron in Magnesiowüstite: elastic properties[1] CESAR R.S. DA SILVA, Minnesota Supercomputing Institute, University of Minnesota, TAKU TSUCHIYA, Geodynamics Research Center, Ehime University, Japan, RENATA M. WENTZCOVITCH, Department of Chemical Engineering and Materials Science, Minnesota Supercomputing Institute, University of Minnesota, STEFANO DE GIRONCOLI, SISSA and DEMOCRITOS National Simulation Center, Trieste, Italy — The high-to-low spin transition in iron in Magnesiowüstite (Mw), $Mg_{(1-x)}Fe_x$,O, is accompanied by considerable volume reduction. This changes the elastic properties of Mw across this transition. Using an LDA+U method with consistently calculated Hubbard U, we investigate the elastic signature of this transition. We find temperature sensitive changes in elasticity across this transition. In Earth's lower mantle, this transition should occur continuously and leave behind an unnoticeable sign.

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Cesar R.S. da Silva
Minnesota Supercomputing Institute, University of Minnesota

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