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Elasticity of ferropericlase at lower mantle conditions RENATA WENTZCOVITCH, Department of Chemical Engineering and Materials Science, Minnesota Supercomputer Institute, University of Minnesota, ZHONGQING WU[1], Laboratory of Seismology and Physics of Earth's Interior, School of Earth and Space Sciences, University of Science and Technology of China, Hefei, JOAO FRANCISCO JUSTO, 3 Escola Politécnica, Universidade de São Paulo, CP 61548, CEP 05424-970, São Paulo, SP, Brazil — The discovery of spin-state changes (crossovers) in ferropericlase (Fp) and in silicate perovskite (Pv) under pressure has raised new questions about Earth's mantle properties. Despite extensive experimental work on the elasticity of Fp throughout the crossover, inconsistencies reported in the literature are still not explained. We introduce here a theoretical framework for thermoelasticity across spin-state changes, apply it to Fp by combining it with predictive first principles DFT+U calculations, and contrast results with available data on samples with various iron concentrations. We explain why the shear modulus of Fp should not soften throughout the spin crossover under hydrostatic conditions and show the importance of constraining well the elastic properties of minerals at lower mantle conditions and likely compositions without extrapolations.

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