Abstract Submitted
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Pressure-induced magneto-structural transition in iron via a modified solid-state nudged elastic band method[1] NIKOLAI A. ZARKEVICH, DUANE D. JOHNSON[2], Ames Laboratory, U.S. Department of Energy at Iowa State University, Ames, Iowa 50011-3020 — Materials under pressure may exhibit critical electronic and structural transitions that affect equation of states, as known for superconductors and the magneto-structural transformations of iron with both geophysical and planetary implications. While experiments often use constant-pressure (diamond-anvil cell, DAC) measurements, many theoretical results address a constant-volume transitions, which avoid issues with magnetic collapse but cannot be directly compared to experiment. We establish a modified solid-state nudge elastic band (MSS-NEB) method to handle magnetic systems that may exhibit moment (and volume) collapse during transformation. We apply it to the pressure-induced transformation in iron between the low-pressure body-centered cubic (bcc) and the high-pressure hexagonal close-packed (hcp) phases, find the bcc-hcp equilibrium coexistence pressure and a transitional pathway, and compare to shock and DAC experiments.

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