

Abstract Submitted
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Fe K pre-edge of Fe₂O₃ at High Pressure¹ SHIBING WANG, Department of Applied Physics, Stanford University, WENDY MAO, Department of GES, Stanford University, Photon Science, SLAC National Accelerator Laboratory, YONG CAI, Brookhaven National Laboratory, NOZOMU HIRAOKA, HIROFUMI ISHII, National Synchrotron Radiation Research Center, Taiwan, YANG DING, YUMING XIAO, PAUL CHOW, HO-KWANG MAO, JINFU SHU, Geophysical Laboratory, Carnegie Institution of Washington, CHICHANG KAO, Brookhaven National Laboratory — Hematite (α -Fe₂O₃), as an archetypal 3d transition metal oxide and important earth mineral, undergoes a series of electronic transitions and structural changes at high pressure. At ambient conditions, Fe₂O₃ adopts the α -Al₂O₃ structure and is an antiferromagnetic Mott insulator, with five 3d electrons in the high-spin state. Upon increasing pressure, it transforms from a high-spin state to a low-spin state in the 40-70 GPa range. Here we report experimental results for the Fe K-edge spectra of Fe₂O₃ collected in-situ at high pressure using synchrotron x-ray absorption spectroscopy in partial fluorescence yield geometry. The pre-edge features give explicit information about the crystal field splitting energy (CFSE) of octahedrally coordinated Fe³⁺ in Fe₂O₃ as a function of pressure, mapping the electronic structure (high-spin to low-spin) transition. The K- α emission spectra at high pressure are also presented.

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Shibing Wang
Department of Applied Physics, Stanford University

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