

Abstract Submitted  
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**Theoretical X-ray Spectroscopy for Strongly Correlated Materials at High Pressure**<sup>1</sup> ADAM P. SORINI, CHENG-CHIEN CHEN, SHIBING WANG, WENDY L. MAO, THOMAS P. DEVEREAUX, Stanford Institute for Materials and Energy Science, CHI-CHANG KAO, SSRL, SLAC National Accelerator Laboratory — We present theoretical x-ray spectra for correlated d- and f-electron materials under extreme conditions. We use exact-diagonalization to study small clusters of atoms including ligand charge-transfer and atomic-multiplet effects. These techniques allow us to extract information from spectroscopic measurements regarding phase transitions in strongly correlated materials as a function of pressure. We show recent results for hematite (Fe<sub>2</sub>O<sub>3</sub>) which undergoes a variety of phase transitions (structural, spin, metal/insulator) near 50 GPa, which have been observed using hard x-ray quadrupolar absorption. We also apply our models to the correlated f-electron “volume collapse” systems which show complex behavior under pressure.

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