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Simulation of the X-ray Emission Spectrum from Early Lanthanides[1] WEI-TING CHIU, University of California, Davis, CHUNJING JIA, BRIAN MORITZ, TOM DEVEREAUX, SIMES, SLAC National Accelerator Laboratory and Stanford University, MAGNUS LIPP, Condensed Matter and Materials Division, LLNL, DEVON MORTENSEN, GERALD SEIDLER, University of Washington, RICHARD SCALETTAR, University of California, Davis — For decades it has been known that certain Lanthanide metals, such as cerium and praseodymium, exhibit a volume collapse transition at a critical pressure. The volume change correlates with charge transfer from 4f orbitals to higher energy conduction bands due small differences in energy. To date, high pressure X-ray emission measurements have enabled the determination of the bare 4f moment of Lanthanide metals.[2] In particular at the L_{γ_1} emission line, the intensity of a satellite peak captures the behavior of the 4f electrons across the volume collapse transition. Here we use exact diagonalization for an atomic model of the Lanthanides, including orbital site energies and core-, valence-, and conduction-band multiplet interactions to simulate the x-ray emission spectrum. The multiple interactions are derived from atomic structure calculations, augmented by effective 4f-to-conduction-band hybridization term. The Kondo screening effect from the conduction electrons at high pressure changes the 4f occupation, resulting in a change of the satellite peak intensity, which well reproduces the experimental findings in the early Lanthanide metals.

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[2]M. J. Lipp *et al.*, PRL **109,** 195705(2012).

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