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EXAFS Spectroscopy of Structurally Tunable Charge Density Wave Materials[1] NATHAN TURNER, Washington State Univeristy, SARAH KIM, Washington State University, MATTHEW MARCUS, SIRINE FAKRA, Lawrence Berkeley Laboratory, JAMES BROZIK, SUSAN DEXHEIMER, Washington State Univeristy — We present EXAFS spectra and modeling of a series of quasi-one-dimensional mixed-valence platinum-halide linear chain materials. The materials exhibit a Peierls distortion, with alternating Pt-halide bond lengths, and fractional charge states on alternating Pt ions in the chain, giving rise to a charge density wave ground state. Varying the halide controls the strength of the charge density wave and the Peierls distortion. Oriented Pt LIII edge fluorescence and transmission EXAFS spectra were collected for each halide species for x-ray polarizations parallel and perpendicular to the chain axis. Modeling was carried out using FEFF9, allowing determination of the photoelectron threshold energies and mean-square relative displacement disorder parameters in addition to verifying bond lengths previously determined by x-ray diffraction. We find distinct photoelectron threshold values for the two inequivalent Pt ions in each of the mixed-valence chains, and find that the difference in threshold values varies systematically with the amplitude of the charge density wave. The disorder parameters correlate with the Peierls distortion and with the mass of the halide ion, reflecting thermal disorder from population of low-frequency chain-axis vibrational modes.

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