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Charge Density Wave Disproportionation in Pd(III)-containing PdTeI PATRICK COTTINGHAM, JOHN SHECKELTON, DAVID MILLER, JAMES NEILSON, TYREL MCQUEEN, Johns Hopkins University — Exotic electronic properties in strongly correlated materials often emerge from the interplay of structure and charge. In most Pd^{3+}-containing materials, Pd^{3+} statically disproportionates into Pd^{2+} (d^8) and Pd^{4+} (d^6) with square planar and octahedral geometries, respectively. However, high-resolution diffraction data acquired for PdTeI indicate exclusively octahedral coordination of the Pd species within this compound. Temperature-dependent electrical resistivity measurements of this material performed in our lab show a hysteresis between $T_{CDW1} \sim 120$ K and $T_{CDW2} \sim 50$ K, indicative of a first-order phase transition. The most likely origin of this anomaly is the formation of a CDW involving partial, dynamic charge disproportionation of Pd^{3+}. In addition, low-temperature diffraction data show a broadening of Bragg peaks on cooling which is indicative of strain or of disorder concomitant with disproportion. In this presentation the temperature dependencies of the magnetic susceptibility, heat capacity, and electronic properties of PdTeI will be discussed in the context of CDW formation.

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