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Electronic and magnetic properties of the chain compounds $\text{K}_3\text{T}_2\text{O}_4$ (T=Ni, Pd, Pt) KLAUS KOEPERNIK, IFW, Dresden, DEEPA KASINATHAN, WALTER SCHNELLE, HELGE ROSNER, MPI CPfS, Dresden — Recent susceptibility measurements on the chain compound $\text{K}_3\text{Pd}_2\text{O}_4$ were interpreted in terms of localized spin 1/2 Pd moments on one of the two crystallographically different Pd sites, only [*R.V. Panin et al., J. Solid St. Chem.* **180**, 1566 (2007)]. The main exchange interaction was reported to be antiferromagnetic from the negative Curie-Weiss temperature $\Theta = -80\text{K}$. Earlier measurements for the isostructural and isovalent Ni and Pt compounds suggest an antiferromagnetic coupling for T=Ni whereas it is ferromagnetic for T=Pt. [*H. Zentgraf et al., Z. Anorg. allg. Chem.*, **462**, 92 (1980)] Here, we report an electronic structure study focusing on the interplay of covalency, spin-orbit coupling and correlation to describe the behavior of this compound family. The inclusion of strong Coulomb repulsion at the transition-metal sites is necessary to obtain the correct insulating ground state observed in recent measurements for the Pd system. The origin of the different magnetic behavior will be discussed.

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