Abstract Submitted
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Bonding, Backbonding and Spin-Polarized Molecular Orbitals: Basis for Magnetism and Semiconducting Transport in V[TCNE]$_{x\sim2}$[1] JEFFREY KORTRIGHT, Lawrence Berkeley National Laboratory, DEREK LINCOLN, RUTH SHIMA EDELSTEIN, ARTHUR EPSTEIN, The Ohio State University — V[TCNE]$_{x\sim2}$ films exhibit magnetic order up to 400 K, magneto-resistance, and photo-induced magnetism. Yet the spin-polarized interactions between the TM and molecular species underlying these properties have remained elusive, in part because of its structural disorder. Using element-specific x-ray absorption spectroscopy (XAS) and magnetic circular dichroism (MCD) at the V L edges, and the C and N K edges we have gained new insight into these mechanisms [1]. We find evidence for covalent bonding between the V e_g and TCNE σ MO states, and a weaker interaction between V t_{2g} and TCNE π MO states, consistent with a generalized bonding/backbonding model with V octahedrally coordinated by N in σ-bridging positions between TCNE radical anions. C and N XAS and MCD reveal spin-polarized splitting of the former LUMO of neutral TCNE, indicating that a direct exchange interaction underlies these properties. This indicates an active role of TCNE$^{\bullet-}$ in the magnetic properties of extended V[TCNE]$_{x\sim2}$ and related systems, which is distinctly different from superexchange models generally used to describe magnetic Prussian blue analogs. [1] Phys. Rev. Lett. **100**, 257204 (2008).

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Jeffrey Kortright
Lawrence Berkeley National Laboratory

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