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Understanding the Gap in Polyoxovanadate Molecular-Based Magnets A. BARBOUR, R.D. LUTTRELL, J. CHOI, J.L. MUSFELDT, University of Tennessee, D. ZIPSE, N.S. DALAL, Florida State University, D.W. BOUKHVALOV, Russian Academy of Sciences Ural Division, V.V. DOBROVITSKI, Ames Laboratory, M.I. KATSNELSON, Radboud University, A.I. LICHTENSTEIN, Universität Hamburg, B.N. HARMON, P. KÖGERLER, Ames Laboratory — We report a joint experimental and theoretical investigation of the transport gap, optical properties, and electronic structure of two chemically similar, inhomogeneously mixed-valent polyoxovanadate molecule-based magnets. We attribute the substantial gap in $[\text{NH}(\text{Et})_3]_4[\text{V}_8^{\text{IV}}\text{V}_4^{\text{V}}\text{As}_8\text{O}_{40}(\text{H}_2\text{O})]\cdot\text{H}_2\text{O}$ to weak p - d hybridization and a large on-site Coulomb repulsion ($U = 5$ eV). The reduced gap in $[\text{NH}(\text{Et})_3]_3[\text{V}_6^{\text{IV}}\text{V}_6^{\text{V}}\text{As}_8\text{O}_{40}(\text{HCO}_2)]\cdot 2\text{H}_2\text{O}$ is associated with a smaller value of U , at least from a molecular point of view, although the transport properties also reflect subtle organization of the molecular structure and the difference between direct and indirect intermolecular charge transfer. A detailed analysis of the vibrational response supports the important role of local molecular distortion and hydrogen bonding in the intramolecular and intermolecular charge transport in $[\text{NH}(\text{Et})_3]_4[\text{V}_8^{\text{IV}}\text{V}_4^{\text{V}}\text{As}_8\text{O}_{40}(\text{H}_2\text{O})]\cdot\text{H}_2\text{O}$. This work is supported by PRF and the U.S. Department of Energy.

Andi Barbour
University of Tennessee

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