

Abstract Submitted
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Molecular Model for Chevrel Phase Superconductivity¹ JIA CHEN, Department of Applied Physics, Columbia University, ANDREW MILLIS, Department of Physics, Columbia University, DAVID REICHMAN, Department of Chemistry, Columbia University — Inspired by the search for emergent properties in molecular assemblies, we studied superconductivity in chevrel phase compounds, which are built on Mo_6X_8 ($X = \text{S}, \text{Se}, \text{Te}$) molecular clusters. We used density functional and density functional perturbation theory to calculate the coupling between partially filled molecular orbitals and vibrational modes, thereby identifying the $E \otimes e$ Jahn-Teller interaction as a crucial coupling. Many-body (Eliashberg and dynamical mean field based) methods are used build a theory for superconductivity. Insights from this work that can be used to guide discovery of additional superconductors will be discussed.

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