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Electronic structure of CuTeO₄ and its relationship to cuprates¹ MICHAEL NORMAN, ANTIA BOTANA, Materials Science Division, Argonne National Laboratory — Based on first principles calculations, the electronic structure of CuTeO₄ is discussed in the context of superconducting cuprates. Despite some significant crystallographic differences, we find that CuTeO₄ is similar to these cuprates, exhibiting a quasi two dimensional electronic structure that involves hybridized Cud and O-p states in the vicinity of the Fermi level, along with an antiferromagnetic insulating ground state. Hole doping this material by substituting Te⁶⁺ with Sb⁵⁺ would be of significant interest.

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Michael Norman Materials Science Division, Argonne National Laboratory

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