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Electronic Structure of Cubic Copper Monoxide P.M. GRANT, W. SIEMONS, G. KOSTER, R.H. HAMMOND, T.H. GEBALLE, Stanford University — We report the calculation of the band structure and optical properties of the rocksalt form of copper monoxide. Although this particular crystal structure does not exist in bulk form for CuO, at least two groups, including ourselves, have succeeded in growing by "forced epitaxy," several atomic layers of cubic CuO on rocksalt proxy substrates such as MgO and STO. For our computation, we employed the DFT/LDA+U method known to give valid results for rocksalt NiO and FeO. Our results show cubic CuO, like these two materials, to be an antiferromagnetic Mott-Hubbard insulator whose band gap is primarily determined by charge transfer between filled O 2p bands and empty Cu 4s states, with localization of the Cu 3d hole by on-site coulomb repulsion frustrating what otherwise would be metallic behavior. We compare our results with NiO, FeO and the natural form of CuO found in the monoclinic mineral tenorite.

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