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Electronic Properties of Rocksalt Copper Monoxide PAUL MICHAEL GRANT, W2AGZ Technologies — Rocksalt copper monoxide, although not yet synthetically realized in bulk form, can be studied computationally as a proxy for the family of layered HTSC copper oxides. We report results for a series of tetragonal CuO rocksalt structures with c/a lattice parameter ratios ranging from 1.0 to 1.5, employing the plane-wave pseudopotential method with exchange/correlation LDA+U. As expected, we obtain a metallic state for U = 0 at all values of c/a given that the nominal valence electron configuration for Cu in copper monoxides is $3d^9$ yielding a partially occupied conduction band. However, completely unexpected was our finding similar metallic properties in rocksalt CuO for all physically plausible values of U (up to 10 eV) and c/a between 1.0 to approximately 1.2. Only for c/a > 1.2 do our calculations reveal the opening of a Mott-Hubbard charge-transfer gap. We interpret our results[1] as supporting the original motivations of Bednorz and Mueller that high temperature superconductivity in the layered copper oxide perovskites may begin with their tendency to exhibit Jahn-Teller strong electron-phonon coupling[2].

[1]P. M. Grant, J. Phys: CS **129** (2008) 01242.
[2]J. G. Bednorz and K. A. Mueller, Rev. Mod. Phys. **60** (1988) 585.

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