TITLE:

A Density-Functional Study of the Electronic and Magnetic Properties of Tetragonal Copper Monoxide as a Proxy for High Temperature Superconductivity

ABSTRACT:

Of all the 3d transition metal oxides, from manganese and elements up to copper, only the latter monoxide does not naturally crystallize in face-centered cubic rocksalt symmetry. It has been shown such is likely a result of the extreme Jahn-Teller degeneracies that would result within the ensuing CuO bonds, which in Nature is relieved by the monoclinic distortion seen in the mineral tenorite [1]. However, it has been found possible to "force epitaxially" grow 4-5 layers of fcc tetragonal CuO on suitable perovskite substrates [2]. A "c/a-axis" elongation of roughly 1.3 – 1.4 stabilizes the ground state as reported in [1]. What is paramount is that fcc tetragonal CuO contains the essential feature of all high temperature superconducting copper oxide perovskites without the complicating inclusion of "3rd elements," and thus provides a simple "proxy" to understand the origin of high-Tc. We report using density-functional-theory towards this end. We add charge to the relevant Cu-O bond states, compensated by background "jellium" to simulate doping. We introduce an empirical screening of coulomb repulsion and present our results in the phase diagram context of the "Great Quantum Conundrum [3]." [1] P. M. Grant, *Journal of Physics: Conference Series* **129**, 012042 (2008) doi:10.1088/1742-6596/1/0124042
[2] W. Siemons, *Physical Review B* **79**, 195122 (2009) doi:10.1103/PhysRevB.79.195122
[3] P. M. Grant, "The Great Quantum Conundrum," *Nature* **476**, 37 (2011)