

Abstract Submitted
for the CAL13 Meeting of
The American Physical Society

**A DFT Study of Tetragonal Rocksalt Copper Monoxide: A Proxy
Structure for Understanding HTSC in the Copper Oxide Perovskites**

PAUL GRANT, W2AGZ Technologies — Copper monoxide does not naturally crystallize in face-centered cubic rocksalt symmetry. It has been shown such may result from Jahn-Teller degeneracies which are relieved by distortion into monoclinic tenorite. It has been found possible to “force epitaxially” grow 4-5 layers of fcc tetragonal CuO on suitable perovskite substrates. A “c/a-axis” elongation of roughly 1.3 – 1.4 stabilizes the ground state. 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-T_c. 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, suggesting electron-phonon coupling underlies HTSC, in the phase diagram context of the “Great Quantum Conundrum (Nature, 2011).”

Paul Grant
W2AGZ Technologies

Date submitted: 02 Aug 2013

Electronic form version 1.4