Abstract Submitted
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A DFT study of rocksalt proxy copper monochalcogenide structures – Implications for possible high-Tc superconductivity P.M. GRANT, W2AGZ Technologies, R.H. HAMMOND, Stanford University, W2AGZ TECHNOLOGIES/GLAM, STANFORD UNIVERSITY COLLABORATION — We report findings derived from a series of DFT calculations on the structural stability and paramagnetic ground states of four idealized copper monochalcogenide (CuO, CuS, CuSe, CuTe) rocksalt structures. Note that none of these target compounds occur naturally, but can possibly be fabricated using "forced epitaxy" MBE methods, as has been done to grow CuO tetragonal rocksalt films 5-6 monolayers thick.[1,2] Therefore, we treat all examples we report herein as proxies intended to explore candidate implications for possible future high-T_C materials. In particular, we find, as might be expected from the long accepted Van Vleck-Anderson-Hubbard formalism describing antiferromagnetic insulators, the Neel temperature scales upward roughly as the width of the spin-carrying bands near or adjacent to the Fermi level or energy gap. We conclude such trend might result in higher superconducting transition temperatures should this be mediated by carrier-spin excitation/fluctuation driven pairing scaled by T_N. Finally, we briefly discuss synthetic paths to realizing actual embodiments of our proxy exercises.

[1]W. Siemons, et al., PRB 79, 195122 (2009), DOI: 10.1103/PhysRevB.79.195122.
[2]P. M. Grant, J. of Physics: CS 129, 012042 (2008), DOI: 10.1088/1742-6596/129/1/012042

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