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Session Y47: Theory of Strongly Correlated Superconductivity

8:00 AM–11:00 AM, Friday, March 7, 2014
Room: Mile High Ballroom 4F

Sponsoring Unit: DCMP
Chair: Brian Moritz, SLAC National Accelerator Laboratory

Abstract: Y47.00008 : A DFT study of rocksalt proxy copper monochalcogenide structures -- Implications for possible high-Tc superconductivity

9:24 AM–9:36 AM

Preview Abstract

MathJax ***On*** | *Off* ← *Abstract* →

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