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A DFT study of electron-phonon coupling in proxy rocksalt CuX (X = S, Se, Te) structures and its relationship to possible manifestation of superconductivity PAUL GRANT, W2AGZ Technologies, ROBERT HAMMOND, Stanford University — We have previously reported our computational studies on idealized copper monochalcogenide rocksalt structures, both cubic and tetragonal, focusing on their possible antiferromagnetic properties as determined within a Van Vleck-Mott-Anderson-Hubbard framework [1]. For all values of Hubbard U in the range 0-7 eV, only copper monoxide exhibits a Mott-Hubbard electronic structure [2-3], the remainder (S, Se, Te) yielding metallic states characterized by nesting Fermi surfaces arising from Jahn-Teller degenerate s-p overlap. These results suggest exploring possible manifestation of superconductivity via electron-phonon mediated Cooper pairing. We will disclose our results to date applying the Eliashberg-McMillan-Allen-Dynes strong coupling framework to the DFT –derived electronic and vibrational states of CuS, CuSe and CuTe.

[1] P. M. Grant and R. H. Hammond, BAPS 59, Y47.00008 (2014).
[2] W. Siemons, et al., PRB 79, 195122 (2009), DOI: 10.1103/PhysRevB.79.195122.
[3] P. M. Grant, J. of Physics: CS 129, 012042 (2008), DOI: 10.1088/1742-6596/129/1/012042.

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