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.