A DFT study of electron-phonon coupling in proxy rocksalt CuX (X = S, Se, Te) structures and its relationship to possible manifestation of superconductivity

P. M. Grant
R. H. Hammond

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.