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Can simple hydrocarbon molecular solids superconduct? A theoretical investigation of superconductivity in K_3Picene XUHUI LUO, UIC & NIST, SERDAR OGUT, UIC, TANER YILDIRIM, UPenn & NIST — Unlike many well established high temperature (T_c) superconductors such as cuprates, M_3C_{60}, MgB_2 and iron-pnictides, the possibility of superconductivity in molecular hydrocarbon solids remains a controversial issue. This topic became active again by a recent study reporting superconductivity up to $T_c \sim 17$ K in potassium doped Picene [1], a wide-bandgap semiconducting solid hydrocarbon. However, there is no theoretical study about possible mechanism of superconductivity. In this talk, we present a detailed first-principles study of the electron-phonon (el-ph) coupling in doped organic molecular solids. Due to large system size, the calculation of el-ph coupling using the standard linear response theory is not feasible. Hence, we have developed a finite-displacement method where both the phonon energies and el-ph coupling can be easily calculated for large systems. We have tested our code for well-established superconductors such as K_3C_{60} and MgB_2. As a comparison, we have also studied the el-ph coupling in alkali-doped Pentacene, a similar well-studied hydrocarbon in which no superconductivity has been observed. We discuss the effect of charge transfer as well as pressure on $T_c$for solid Picene and make predictions for future possible experiments.
[1] Mitsuhashi et al. Nature, 464, p. 76 (March, 2010).

Xuhui Luo
UIC & NIST

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