Downfolding electron-phonon Hamiltonians from ab-initio calculations: application to K_3 picene

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In this work[1], we propose an electron-phonon parameterization which reproduces the geometry and harmonic frequencies of a real system, by taking structural parameters either from experiment or density functional theory. With respect to standard electron-phonon models, it adds a "double-counting" correction, which takes into account the lattice deformation as the system is dressed by low-energy electron-phonon processes. We show the importance of this correction by studying potassium-doped picene (K_3 picene), recently claimed to be superconductor with T_c of up to 18 K. The Hamiltonian parameters are derived from ab-initio density functional theory, and the lattice model is solved by dynamical mean-field theory. Our calculations include the effects of electron-electron interactions and local electron-phonon couplings. Even with the inclusion of a strongly coupled molecular phonon, the Hubbard repulsion prevails and the system is an insulator with a small Mott gap of $\approx$0.2 eV. This work founds the basis of more reliable low-energy electron-phonon models and calls for a reinvestigation of the theoretical results obtained so far from ab-initio parametrizations of systems with strong electron-electron and electron-phonon couplings.

[1] G. Giovannetti, M. Casula, Ph. Werner, F. Mauri, and M. Capone, to appear soon in PRB, arXiv: 1406.4108 (2014).