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Ab initio studies of low dimensional organic systems

We study a number of charge transfer (CT) salts in the framework of ab initio density functional theory and determine the parameters of the effective Hubbard Hamiltonian describing the low energy excitations. For the $K^-(BEDT\text{-}TTF)_2 X$ (X= $Cu_2(CN)_3$, $Cu(SCN)_2$, $Cu[N(CN)_2]Br$, $Cu[N(CN)_2]Cl$) family of CT salts, we find that the widely used semiempirical parameters should be significantly revised in the direction of less frustrated, more anisotropic triangular lattices. We also investigate the lattice underlying the $K^-(BEDT\text{-}TTF)_2 Hg(SCN)Cl_2$ compound. We investigate the electronic structure of the possible spin liquid system $EtMe_3Sb[Pd(dmit)_2]_2$ ($Et=C_2H_5$, $Me=CH_3$). The ß''-$(BEDT\text{-}TTF)_2 SF_5 CHFCF_2 SO_3$ charge transfer salt is interesting due to a transition from metal to insulator as function of pressure; the small degree of dimerization in the ß''-phase leads to a complex frustrated square lattice with many inequivalent hopping pathways. The $(BEDT\text{-}TTF)_2 Ag(CF_3)_4$ (TCE) has recently been shown to crystallize in a structure in which a'-phase and K^-phase BEDT-TTF layers alternate. Possibly, the increased two-dimensionality of this compound enhances its superconducting properties..

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