Modeling multi-orbital molecular conductors

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We theoretically study molecular conductors in which multiple molecular orbitals (MO) are involved. In metal complex molecules described as $M(L)_2$, where a metal atom $M$ is bonded between two ligand units $L$, the energy gap between frontier MO becomes small, and then in the crystal, energy bands originated from different MO can overlap. We have proposed a scheme of constructing tight-binding models for such multi-MO systems, $M$(tmdt)$_2$ [1] and $X$[Pd(dmit)$_2$]$_2$ [2], based on first-principles band calculations; namely, to choose the basis functions as linear combinations of MO, which are more localized in space, called fragment-MO. This scheme enables us to systematically understand electronic structures of different materials, as well as to investigate effects of electron-electron Coulomb interaction in a natural way. Mean-field studies give a variety of phases including, in addition to conventional ordering seen in single-orbital systems, spin/charge ordering where the multiple MO degree of freedom is involved.