

Electronic structures of metallic and superconducting metal dithiolene complexes

Reizo Kato

Condensed Molecular Materials Laboratory, RIKEN, 2-1, Hirosawa, Wako-shi, Saitama 351-0198, Japan,

Metal dithiolene complexes have provided a variety of molecular conductors. Among them, anion radical salts of metal-dmit complexes $M(\text{dmit})_2$ (dmit = 1,3-dithiole-2-thione-4,5-dithiolate; $M=\text{Ni}, \text{Pd}$) are of special interest. The electronic state depends on the central metal ion and the counter cation.

The Pd salts provide a strongly correlated two-dimensional system with a quasi triangular lattice formed by $[\text{Pd}(\text{dmit})_2]_2^-$ dimers. An important aspect of the Pd salts is a HOMO-LUMO interplay which comes from strong dimerization and a small HOMO-LUMO energy splitting. Most of them are Mott insulators at ambient pressure. The localized electrons exhibit frustrated paramagnetism. At low temperatures, the spin frustration is removed by various transitions, including antiferromagnetic ordering, (intra- and inter-dimer) charge ordering, and valence bond ordering (spin gap formation). The Mott insulating state can be suppressed by the application of hydrostatic or uni-axial pressure, which provides metallic behavior accompanied by superconductivity.

