Materials science of single-component pure organic metals

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Exotic electronic properties of molecular conductors originate from low dimensionality of their band structures, reflecting anisotropic orientation of π -orbitals. Charge-transfer complexes have given many fantastic electronic systems including superconductors [1], but single-component conductors are relatively small in number as yet [2, 3], especially pure organic metals excluding metal ions. The reason is that there exist no clear criteria for overcoming the Mott-Hubbard gap in the single-component system without supports of d-orbitals.

Tetrathiafulvalene-extended dicarboxylate (TED) is the first single-component pure organic metal, which exhibits metallic conduction at ambient pressure (Fig. 1) [4]. The conductivity of single crystals exceeds 2000 S/cm at room temperature with characteristic temperature dependence of resistivity with $\rho \propto T^3$ [5]. Crystal and electronic structure reveal that TED is a two-dimensional metal system and give a new insight into metallization mechanism in pure organic molecules. Moreover, the electronic behavior, thermopower and existence of polymorph single crystals highlight its unique materials science, which has not been observed in other molecular conductors.



Fig. 1. Molecular structure of TED (left) and DFT band structure (right)

References

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