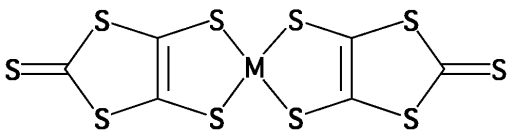
Manipulation of π electrons in molecular crystals

Reizo KATO
Condensed Molecular Materials Laboratory, RIKEN

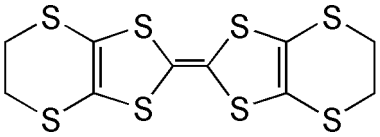
Abstract

Properties of condensed matter are governed by behavior of electrons. Diversity in electron behavior derives from characters of atomic orbitals (s, p, d, f....) or bonding orbitals (σ, π, δ...) where electrons are accommodated. Among them, π electrons are of special interest, as shown in polyacetylene (one-dimensional pπ system) and in graphene (two-dimensional pπ system). Our interest is conducting or localized (but potential itinerant) π electrons in molecular crystals (molecular conductors). It should be emphasized that electronic structures (energy bands) of molecular conductors are remarkably simple and clear. In general, transfer integrals between frontier molecular orbitals govern the essential electronic structure and are sensitive to molecular arrangement and orientation in crystals, because component molecules belong to the conjugated π system with highly anisotropic molecular shapes. A variety of chemical modifications enable fine tuning of electronic properties. Notably, chemical modification in the insulating part, as well as in the conducting part, can control electronic properties, because the insulating part can affect molecular arrangement and orientation in the conducting part. The number of π carriers (electrons or holes), band filling, can be controlled by doping procedures. Especially, electrostatic doping (ESD) is a useful method where undesirable effects of disorder can be avoided.

I will demonstrate manipulation of π electrons in molecular conductors by chemical and physical methods; 1) An introduction of supramolecular interaction (halogen bond) and 2) ESD into thin single crystals of organic Mott insulators using the field-effect transistor configuration.



$M(dmit)_2$



BEDT-TTF

References:

K. Hazama, S. Uji, Y. Takahide, M. Kimata, H. Satsukawa, A. Harada, T. Terashima, Y. Kosaka, H. M. Yamamoto, and R. Kato, Phys. Rev. B, **83**, 165129:1-165129:9 (2011).

Y. Kawasugi, H. M. Yamamoto, N. Tajima, T. Fukunaga, K. Tsukagoshi, and R. Kato, Phys. Rev. B, **84**, 125129:1-125129:9 (2011).