Single- component Molecular Metals

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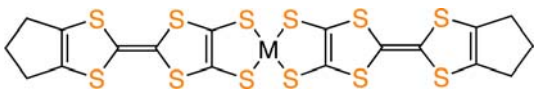
The realization of a molecular metal based on single-component molecules had been one of the important target in the field of molecular conductors. In contrast to typical inorganic metals composed of single elements, such as sodium and copper, all of the examples of molecular metals had consisted of more than two components. In 2001, we have prepared the first example of the crystal of a neutral transition metal complex with extended-TTF ligands, $[Ni(tmdt)_2]$ (tmdt = trimethylenetetrathiafulvalenedithiolate) exhibiting metallic behavior down to very low temperature [1, 2]. $[Ni(tmdt)_2]$ crystal has a simple triclinic structure and the unit cell contains only one molecule (Figure 1). A direct experimental evidence for the three-dimensional electron and hole Fermi surfaces in $[Ni(tmdt)_2]$ was obtained by detecting the quantum oscillations in magnetization at very high magnetic field (or de Haas-van Alphen (dHvA) effect) [3].

Unlike the neutral bis(dithiolato)nickel complex, the neutral bis(dithiolato)gold complex has an odd number of electrons, which makes a gold complex very attractive. The crystal structure of $[Au(tmdt)_2]$ is isostructure to that of $[Ni(tmdt)_2]$. The ESR and magnetic susceptibility measurements revealed that $[Au(tmdt)_2]$ has the antiferromagnetic phase transition around 110 K [4]. The first principle band structure calculation by S. Ishibashi and K. Terakura suggested the disappearance of a part of the Fermi surfaces of $[Au(tmdt)_2]$ below the phase transition temperature [5]. $[Au(tmdt)_2]$ is the noble molecular conductor exhibiting magnetic transition above 100 K where the same π electrons bear electrical conductivity and magnetic order. Here, the variety of crystal structures and their physical properties of single-component molecular conductors with different central metal atoms (Cu, Zn, Co) will also be presented.



$[M(tmdt)_2]$ (M = Ni, Au)

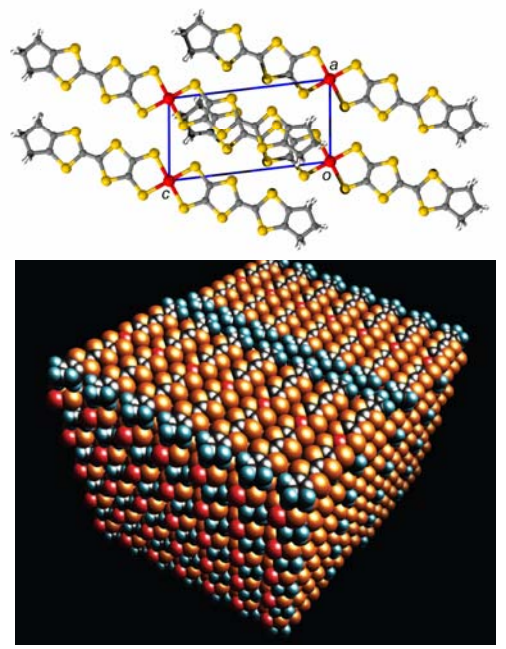


Figure 1: Crystal structure of $[M(tmdt)_2]$ (M = Ni, Au)

[1] A. Kobayashi, et al.,*Chem. Rev.*, **104** (2004) 5243.
[2] H. Tanaka et al., *Science*, **129** (2001) 285.
[3] H. Tanaka et al., *J. Am. Chem. Soc*. **126** (2004) 100518.
[4] B. Zhou et al., *J. Am. Chem. Soc*. **128** (2006) 3872.
[5] S. Ishibashi et al., *J. Phys. Soc. Jpn*. **74** (2005) 776.