

**Electronic Structure of Au(tmdt)₂ Crystal
with Low-Photon Energy Ultraviolet Photoelectron Spectroscopy
(tmdt, trimethylenetetrafulvalenedithiolate)**

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Recently, Kobayashi *et al.* synthesized a single-component molecular conductor Au(tmdt)₂ (tmdt, trimethylenetetrafulvalenedithiolate). The metallic character of the electronic structure, however, has been elucidated by a theoretical calculation^[1], because of the difficulty in the sample preparation suitable for ultraviolet photoelectron spectroscopy (UPS) measurement. The difficulty may come from poor solubility and thermal stability and small size of the Au(tmdt)₂ crystals. In this study, we have successfully detected the electronic structure of the Au(tmdt)₂ crystal with low-photon energy Xe I (8.437 eV) UPS. Photoelectrons excited by Xe I resonance line have a long mean-free-path. This advantage makes it possible to detect photoelectrons from the bulks covered by impurity molecules.

The sample is prepared by fractioned the small Au(tmdt)₂ crystals onto the Grafoil (Union Carbide) substrate in the air. Figure 1 shows the Xe I UPS spectrum of Au(tmdt)₂ at 297 K. In the difference spectrum (b), we find a clear structure A, which can be divided into two Gaussian components. The onset of the component A₁ at lower binding energy merges into the Fermi level (E_F). The electronic structure is corresponding well to the calculation. The components A₁ and A₂ can be ascribed to SOMO and HOMO-1, respectively. These results indicate that most of our sample may not have metallic character, but molecular aggregates. We will discuss phase transition of Au(tmdt)₂ including the result of the temperature dependence.

[1] S.Ishibashi *et al.*, J.Phys.Soc.Jpn. **74** (2005) 84.

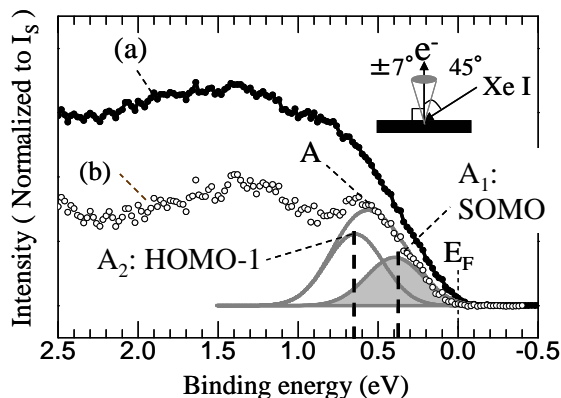


Fig.1 Angle integrated XeI UPS (normal emission) of the Au(tmdt)₂ sample (a) at 297 K. The difference between spectrum (a) and Grafoil substrate is shown as (b).