(8) Materials & Nanoscience:

2229 - Multi-band molecular conductors

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Abstract Body:
Molecular conductors have been characterized by simple and clear electronic structures where a conduction band originates from one of frontier molecular orbitals (HOMO or LUMO) and the tight-binding band picture works quite well. Recently, however, an increasing number of molecular conductors have been reported to exhibit more than two bands near the Fermi level and the multi-band interactions provide unique physical properties. We are investigating multi-band molecular conductors with four-probe resistivity measurements under high-quality hydrostatic pressure using a diamond anvil cell (DAC) technique developed by us and the first principles DFT calculations. We will introduce the following two types of multi-band molecular conductors based on metal complexes;
(1) Single-component molecular conductors that possibly have the Dirac cone structure.
(2) π-d molecular conductor where the HOMO band, as well as the hybridization of LUMO and Cu d orbital, contributes to a metallic state in the high pressure region.