単一成分分子性導体の多軌道モデルと磁気状態

Multi-orbital model and magnetism in single-component molecular conductors

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Electronic states in the isostructural family of single-component molecular conductors $M(tmdt)_2$ (M=Ni, Au, Cu) [1] are studied theoretically, by considering effective multi-orbital Hubbard models. The transfer integrals and relative orbital energies, based on a "fragment" description for the molecular orbitals near the Fermi level, are determined by numerical fitting to the first-principles (ab initio) band structures, which show systematic variation among the three compounds [2,3,4]. Not only the bonding and the antibonding pπ orbitals from the embedded TTF skeleton of the ligands, but also the p-d mixed orbitals centered at the M (metal atom) site contribute to the electronic band structure near the Fermi level: pdπ orbital for $Ni(tmdt)_2$, and pdσ orbital for $Au(tmdt)_2$ and $Cu(tmdt)_2$.

By further taking account of the Coulomb interaction (i.e. Hubbard models), we study effects of electron correlation within mean-field approximation for the Au and Cu compounds, where magnetic transitions are found but with very different characters; $Au(tmdt)_2$ is metallic and the transition temperature is 110 K, while $Cu(tmdt)_2$ is insulating and the transition temperature is 12 K. In the presentation, we will discuss the origin of such difference based on ground state phase diagrams, where different types of magnetic ordering are found to be stabilized.

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