

Coexistence of Magnetism and Conductivity in Bis(ethylenedi sel eno) Tetrathiafulvalene (BEST) with Octahedral Anions Hexacyanoferrate (III) and Nitroprusside

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Abstract: Using an accurate density-function method, we explore the coexistence of the magnetism and conductivity in bis(ethylenedi sel ena)-tetrathiafulvalene (BEST) with the paramagnetic hexacyanoferrate(III) $[\text{Fe}(\text{CN})_6]^{3-}$ or the photochromic nitroprusside anion $[\text{Fe}(\text{CN})_5\text{NO}]^{2-}$. The total and partial densities of states, and the atomic spin magnetic moments are calculated and discussed. It is found that the up- and down-spin total densities of states (DOS) are continuous in the vicinity of the Fermi level, there is overlap between the HOMO and LUMO in the up-spin subbands and the down-spin subbands, which reveals that these types of compounds have conductive properties. From the total and partial densities of states and atomic spin magnetic moments, it is shown that the spin magnetic moments of $(\text{BEST})_4[\text{Fe}(\text{CN})_6]$ is mainly assembled at the iron atom and the cyanogen radical, and the spontaneous magnetic moments for $(\text{BEST})_2[\text{Fe}(\text{CN})_5\text{NO}]$ come from iron atom, cyanogen and nitric oxide radical. To our best knowledge, it is the first theoretical study on the coexistence of the magnetism and conductivity of these compounds.

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Key words: magnetic properties, conductive properties, first-principles method

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