DFT+U vs. many-body model approach for a model of metalorganic switch

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We consider a metalorganic system with valence tautomeric properties[1] as a molecular switch. The molecule includes a delocalized spin of the organic subunit coupled with the localized spin centered on copper atom with its co-ligands and may appear in the several spin and charge states[2].

We use the results of the DFT calculations to compute the parameters of a many-body model of the system. To obtain the correct hierarchy of magnetic states a multi-orbital two-center Hamiltonian is proposed. The model is subsequently studied within an effective field approach and the exact diagonalization method. On this basis we indicate the limitations of the effective field description and stress the importance of accurate treatment of the Coulomb correlations for a detailed explanation of the switching behaviour.

References:

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