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ab initio Study of Electronic Structure and Magnetic Properties of a Novel Two-Dimensional Copper(II)-Radical Complex $[Cu(NTTmPy)_2(N_3)_2]_n$

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Abstract: The full-potential linearized augmented plane wave (FPLAPW) method with the generalized gradient approximations (GGA) is applied to study the compound $[Cu(NTTmPy)_2(N_3)_2]_n$ (NITmPy=2-(3'-Pyridy1)-4, 4, 5, 5-tetramethylimidazolin-1-oxy1-3-oxide). The total density of states (DOS) and the partial density of states (pDOS) are calculated to explain the electronic and the magnetic properties of $[Cu(NTTmPy)_2(N_3)_2]_n$. It is found that $[Cu(NTTmPy)_2(N_3)_2]_n$ is stable in the ferromagnetic state and the magnetic moment of the molecule mainly comes from the Cu atoms (0.518 μ_B) with partial contribution from N, O atoms of nitronyl nitroxide radicals. There exist orbital hybridization between 3d orbital of Cu and p orbitals of N(1) (from pyridyl rings of the NITmPy ligands) and N(4) (from azido group) and the weak direct exchange interactions between Cu and O atoms of nitronyl nitroxides. In addition, the bridging carbon atom (C(6)) carries a significant negative spin density (-0.019μ_B). The sign alternation of the magnetic moment along the pyridyl ring is obtained, which agrees with experiments.

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