First-Principles Study of the Ferromagnetic and Semiconductor Properties of [Mn(4,4′-bipy)(N3)2]n

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Based on density functional theory, the full potential linearized augmented plane wave (FPLAPW) method is applied to study the electro nic structure and the magnetic properties of the compound [Mn(4,40-bipy)(N3)2]n. The density of states, the spin magnetic moment and th e electronic band structure are calculated. The results indicate that the compound has ferromagnetic and semiconductor properties. It is foun d that there is hybridization

between the d orbital of the central Mn atom and the p orbital of the N atom, and that there exists a spin delocalization from the Mn ato m towards the N atoms of the EE-azide groups. Through the EE-azide bridges, the spin delocalization makes the neighboring Mn atoms havin g a dominant ferromagnetic interaction. The magnetic moment 5.0 μB per molecule mainly comes from Mn ion with little contribution from t he EE-azide groups.

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