

Magnetic behavior of chromium ions in various molecular structures

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We investigate, using density functional theory, chromium ions embedded within heteronuclear molecular ring Cr_8Cd and pentameric coordination polymer Cu_3Cr_2 .

We present electronic and magnetic properties, including the magnetic moments and the spin charge density maps for various spin configurations. Furthermore, the exchange coupling parameters between transitional metals ions are extracted and the results are compared with magnetic measurements.

In the ground state, the magnetic moments are highly localized on Cr positions whereas those of Cu are rather delocalized. For the systems in question, the simulation results are qualitatively in agreement with empirical results.

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