DFT STUDY ON A CHAIN MODEL OF THE CHROMIUM-BASED MOLECULAR MAGNETS

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9.7 cm

We present a density functional theory (DFT) study of the electronic and magnetic properties of the chromium-based molecular rings. The all-electron linearized augmented plane wave method (LAPW) implemented in the Wien2k package [1] is used to calculate the electronic states, exchange coupling parameters and magnetic anisotropy of a infinite chain model system of Cr_8. We demonstrate how the chain model mimics with good approximation the electronic and magnetic properties of the original Cr_8 molecule [2], and offers an unique opportunity, in virtue of the reduced computational effort, for carrying out extensive investigations of molecules belonging to the Cr-based molecular rings family [3].

[1] P. Blaha, K. Schwarz, G. Madsen, D. Kvasnicka, and J. Luitz, WIEN2K, An Augmented Plane Wave + Local Orbitals Program for Calculating Crystal Properties (see www.wien2k.at for details).
[2] V. Bellini, A. Olivieri and F. Manghi, Phys. Rev. B **73**, 184431 (2006).
[3] D. M. Tomecka, V. Bellini, F. Troiani, F. Manghi, G. Kamieniarz, and M. Affronte (to be submitted).

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