The low and high spin ground states in molecules containing $[Mn_3^{II}Mn^{III}]$ and $[Mn_2^{II}Mn_2^{III}]$ metallic cores

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We present the experimental and theoretical results for two recently synthesized [1] tetranuclear magnetic clusters containing $[Mn_3^{II}Mn^{III}]$ (**1**) and $[Mn_2^{II}Mn_2^{III}]$ (**2**) metallic cores. From the theoretical point of view, we have analyzed the magnetic susceptibility and magnetization of both compounds in terms of the Heisenberg spin model using exact diagonalization technique. We have achieved quantitative agreement between theory and experiment for **2** and semi-quantitative for **1**. Moreover, the model predictions for **1** are supported by DFT calculations, using the PBE functional. Analyzing the energy structure of both compounds, we have found that the topology of interactions in **1** molecule is particularly suitable for synthesis of molecules with the ground state $S = 1/2$ and the interactions between Mn^{II} ions are crucial to get the lowest energy gap higher than that observed in the chromium-based molecules.

References:

[1] M. Sobocińska et al., Dalton Trans. **45** (2016) 7303