Simulations of molecular nanomagnets with various metallic cores and topologies

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We present the results of simulations of a class of molecular nanomagnets with ring, centered ring and dimer topologies. We demonstrate [1,2] that anisotropic Heisenberg model describes quantitatively magnetic properties of a family of the doped Cr_8 molecular rings revealed by the variety of experimental techniques. Interestingly, the nearest neighbor coupling parameters between the localized spins are all transferable across its members. We show that the broken symmetry approach within density functional theory, based on suitable functionals, provides a reliable tool [2,3] to extract magnetic exchange coupling parameters in all rings considered.

The molecular complex containing the bimetallic core Ni_6Cr [3], representing the centered ring geometry as well as its analogue geometrically frustrated are also simulated using the phenomenological and DFT approach. Consequently, the magnetic properties observed are quantitatively explained. In the isotropic limit of the model and the spin frustration switched on, the sequence of the ground states determined by the total spin S is obtained in agreement with the fundamental Lieb-Mattis theorem. Curiously enough, the temperature dependence of the susceptibility product χT with characteristic minimum and maximum is revealed not only as a signature of competition between the ferro- and antiferro-magnetic interaction but also as a symptom of the spin frustration phenomenon.

We have pioneered the application of the Heisenberg-type model to rare-earth dimers [4]. To that end, a new family of 3d-4f coordination polymers has been synthesized in search for new single-molecule magnet materials containing highly anisotropic lanthanides. Their magnetic properties have been explained quantitatively by comprehensive phenomenological modeling.

References:

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