Nanocomposites and nanomaterials

Impact of surface fluctuations on temperature transition of spin-crossover compounds

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Spin crossover (SCO) systems are relatively rare class of transition metal complexes that display molecular magnetic bistability and interconverted reversibility upon external stimuli. Under normal conditions, these complexes can exhibit spin crossover, that is, the entropy-driven thermal transition from a diamagnetic low-spin (LS) state, to a paramagnetic high-spin (HS) state.

The current theoretical study addresses to the role of surface-environment effects of spin crossover nanocrystals in the occurrence of phase transition in the material. The important issue is to understand the interplay of cooperativity of the system and the fluctuations of its environment. Phenomenologically, the interactions in molecular spin crossover nanoparticles can be modelled in a simplest way by the Ising-like Hamiltonian

$$\mathrm{H} = -h_0 \sum_i s_i - \sum_i^s h_i(t) s_i - \sum_{\langle ij \rangle}^b J_{ij}^b s_i s_j - \sum_{\langle ij \rangle}^s J_{ij}^s s_i s_j - \sum_{\langle ij \rangle}^{b-s} J_{ij}^{b-s} s_i s_j \qquad (1)$$

Here s_i is a fictitious spin (pseudospin) operator which has two eigenvalues ±1, corresponding to the HS and LS states of respective $i-s$ molecule, $\langle ij \rangle$ denotes the summation over all nearest-neighboring spin pairs. The Ising-like Hamiltonian describes the elastic interaction between spin states via the near neighbor coupling of two-level units. The intersites short-range coupling constants J_{ij}^{α} measured in energy units, are parameters of the theory, where $\alpha = b, s, b-s$ correspond to occupied pairs of bulk sites, surface sites and bulk-surface sites.

In the results of our investigation it was found out that the shapes of the loops and the loop area depend on the values of surface intermolecular interaction as well as on the strength of ligand field fluctuations of spin crossover particle. The interplay between the surface random ligand field variation and the cooperativity explains the enhancement of the width of the thermal hysteresis loop.

1. *Gudyma Iu., Maksymov A.* Surface-environment effects in spin crossover solids // Appl. Surf. Sci.-2017.-**407**.-P.93-98.