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The hysteretic behavior of noise perturbed spin-crossover nanocrystals

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In this work we studied the microscopic aspects of spin transition in Ising-like spin-crossover (SC) model with fluctuating parameters. The nature of fluctuations is presupposed to be thermal. Their description together with the theoretical background of SC compounds is given in [1]. The Ising-like SC model with only short-range interactions in general form is described by the following Hamiltonian:

$$H = -J\sum_{\langle ij\rangle} s_i s_j - h\sum_i s_i \,, \qquad (1)$$

where $s_{i,j}$ is pseudospin scalar variable taking the value ± 1 corresponding to low-spin (LS) (-1) and high-spin (HS) $(+1)$ state respectively; J is the ferromagnetic interaction constant; $h = \Delta - kT\ln g$ is external effective field depending on energy gap between LS and HS state Δ, temperature T (here $k = 1$ and is Boltzmann constant) and degeneracy ratio between HS and LS state g. We presuppose that contact with environment lead to fluctuation of potential barrier height which now must be characterized by the following equation $\Delta(t) = \Delta_c + \xi(t)$, where $\xi(t)$ describes the fluctuations. In general this term may be white or colored which implies the specific correlation function. We found the transition temperature curves showing hysteresis for SC system with colored and white space-time correlated fluctuation. But for more accurate description of cooperative phenomena the difference in structural properties for LS and HS state must be taken into account. Due to atom-ligand distance changes the interaction parameter J is different depending on the state of interacting molecules. For two interacting molecules there are three different value of J: (i) when the both molecules are in LS state (J is minimal), (ii) when they are in HS state (J is maximal), and (iii) when one molecule is in LS ant other in HS state (J takes intermediary values). These features also contribute to hysteretic behavior of spin-crossover system.

1. *Iu. Gudyma, C. Enachescu, A. Maksymov* Kinetics of nonequilibrium transition in spin-crossover compounds // Nanocomposites, Nanophotonics, Nanobiotechnology, and Applications - Springer-Verlag, New York, 2014.