## Nanocomposites and nanomaterials

# Effects of pressure on phase transitions in spin-crossover molecular nanocrystal

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A class of spin crossover (SC) molecular complexes is formed by $3d^4$ -$3d^7$ transition metal ions in a quasi-octahedral coordination environment for appropriate values of the ligand field. In the SC compounds, a metal ion can be in either a low-spin (LS) or high-spin (HS) state, depending on the strength of the ligand field. It was also clarified that in spin-crossover solids the spin transition is accompanied by a molecular volume changes due to internal structural rearrangements (metal–donor atom bond length increase) in solids. In general, the coupling between the spin transition and molecular volume changes is a very complex phenomenon [1].

Thermal and pressure induced behaviour of SC nanosystem, has been modelled in the framework of Ising-like model on a simple regular cubic lattice. In our lattice-spin model, energies of intra-site transition, inter-ions interaction and elastic self-energy of lattice have been considered. Taking into account strain effects because of molecular distortion as perturbation, the model was obtained for this lattice. The coupling between magnetic and structural degrees of freedom is one of the sources of the first-order magnetic phase transitions. From analytical derivations and Monte Carlo simulations the temperature-induced spin transition curves for various values of volume increasing were obtained. By detailed analysis of critical temperatures during cooling and heating processes the state diagram has been built. The spin-crossover system can have three types of behaviour of molecular fraction in the HS state that is driven by pressure: hysteresis behaviour, behaviour with second-order transition and behaviour without a phase transition.

The pressure action on spin-crossover solids demonstrates the possibility to ‘fine tune’ the crystal field strength and thereby induces a controlled thermal spin transition in a paramagnetic compound. The application of pressure turns out to be equivalent to creating ‘chemical pressure’, also called image pressure, by isostructural diluting the Fe(II) SCO compound with a transition metal of different ionic radius. The displacement of transition temperature to higher values has a great potential for the practical applications of these effects at room temperatures.

*1. Gudyma Iu.V., Ivashko V.V.* Spin-crossover molecular solids beyond rigid crystal approximation // Nanoscale Res. Let. – 2016. – **11**. – 196 (8pages).