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Ising-Like Model of Nanosize Spin-Crossover Molecular Crystals

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Abstract

The properties of spin-crossover nanoparticles were investigated within a framework of Ising-like model. By involving the Monte Carlo simulation tools, a thermal transition of spin-crossover solids with local random fields of various statistical characteristics and without stochastic origins has been analyzed. In three-dimensional spin-crossover crystal, the presence of fluctuations may provoke the hysteresis for the system with gradual non-hysteretic transition in contrary to the one that undergoes the first-order phase transition, in which the fluctuations play destructive role on system cooperativity vanishing the hysteresis loop. The changes of transition temperatures characterizing the systems bistable properties for 3D lattices with ferromagnetic and antiferromagnetic couplings of surface's molecules and their dependence on its size and fluctuation strength were obtained. Also, the regions with hysteretic and non-hysteretic behavior have been found.