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ABSTRACT BOOK

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AND NANOMATERIALS”**

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Abstract book

Monte Carlo simulation of bond-random spin-crossover compounds

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Spin-crossover (SCO) complexes are the transition metal coordination compounds with the electronic configuration ranging between $3d^4$ and $3d^7$ (manganese, iron, chromium, and cobalt) in (pseudo)octahedral surroundings. The variation of some external stimuli causes the reversible phase transition from low spin (LS) diamagnetic state to high spin (HS) paramagnetic state in SCO materials. The SCO is one of the best examples of molecular electronic bistability [1].

Intermolecular interactions are mediated by small molecular distortions that lead to some randomness of bonds. This leads to a treating intermolecular interaction as random bond [2]. Our model is a random-bond version of the well-known pseudo-spin model of spin-crossover solids, and is similar to the Edwards-Anderson model with the external field.

The Ising-like model of spin-crossover solid compounds with random bonds has been studied by intensive numerical Monte Carlo simulation. A numerical solution to the problem is found and analyzed. The six typical cases of the temperature behavior of spin-crossover compounds for random intermolecular bonds have been studied.

Random distribution of intermolecular coupling results in the peculiarity of cooperative behavior, such as narrowing hysteresis loops or their vanishing or a more complex quasi-spin glass state. Our investigations could be helpful in the understanding of various patterns in real SCO systems.

The successful implementation of the described approach for providing a facile way to include random intermolecular interactions paves the way for future research about the role of such interactions within SCO compounds.

1. Gudyma Iu., Maksymov A., Enachescu C. Phase transition in spin-crossover compounds in the breathing crystal field model / *Phys. Rev. B* – 2014. – **89**, 224412.

2. Gudyma Iu., Yarema V. Bond-random model of spin-crossover compounds: similarities and differences from spin glasses // *Applied Nanoscience*. – 2022. – **12**, P. 747–753.

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