Spin-crossover molecular hexagonal nanocrystal

Gudyma Iu.V.*, *Yarema S.V.

Physical Technical and Computer Sciences Institute of Yuriy Fedkovych Chernivtsi National University, Kotsyubynsky 2, 58012, Chernivtsi, Ukraine. E-mail: yugudyma@gmail.com

Spin-crossover (SCO) complexes are transition metal coordination compounds that undergo reversible phase transitions between low spin (LS) diamagnetic and high spin (HS) paramagnetic states upon exposure to external stimuli. Such molecular spin-crossover can occur for certain first series transition metal ions with $3d^4$–$3d^7$ electronic configurations, and these materials are attractive due to their unique electronic bistability that holds promise for various technological applications [1].

The present study investigates the spin-crossover transition in a hexagonal lattice of finite size consisting of a grid of SCO molecules. The lattice is a standard model for the study of spin-crossover phenomena, and the finite size simulates more realistic experimental conditions. The work addresses to the role of the type of lattice and its finite size in the occurrence of phase transition in the spin-crossover nanocrystal. We used the Metropolis algorithm of Monte Carlo simulations to calculate the system's magnetization for various grid sizes and intermolecular interaction strengths.

Our findings indicate a transition from LS to HS states and vice versa for some grid sizes and intermolecular interaction strengths. We observed the dependence of the transition on the interaction strength by varying this parameter. Additionally, the transition behavior is influenced by the size of the finite lattice, as shown by our simulations.

In conclusion, our Monte Carlo simulations of a hexagonal lattice of finite size have allowed us to observe the transition of different kind from LS to HS states for various grid sizes and interaction forces. These results shed light on the cooperative behavior of intermolecular interactions in SCO systems and suggest potential avenues for further research in this area.

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. On the role of random bond in spin-crossover compounds// Applied Nanoscience (2022).