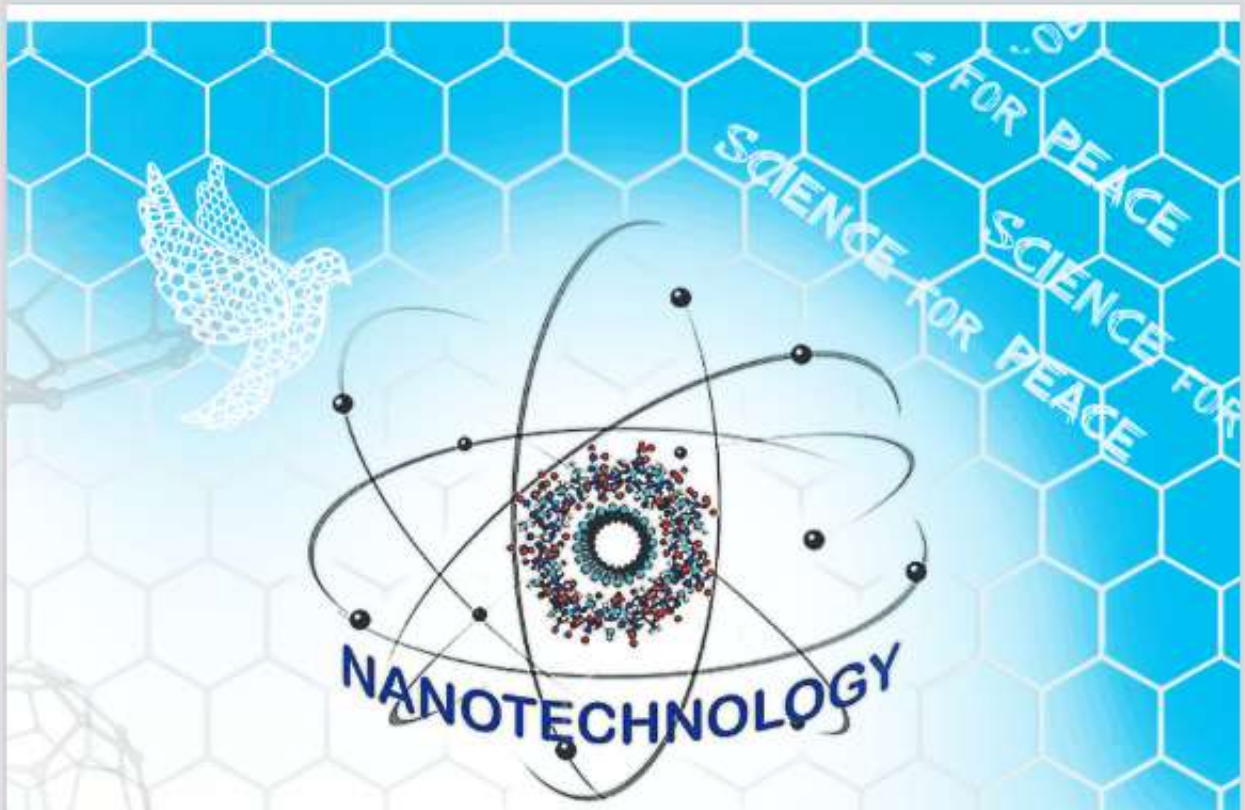

ABSTRACT BOOK

International research
and practice conference:

NANOTECHNOLOGY AND NANOMATERIALS (NANO-2022)

25-27 August 2022
Lviv, Ukraine

INTERNATIONAL RESEARCH AND PRACTICE CONFERENCE "NANOTECHNOLOGY AND NANOMATERIALS"

(The NANO-2022 Conference is dedicated to the International Year of Basic Sciences for Sustainable Development)

25-27 of August 2022

Lviv, UKRAINE

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 3d4 and 3d7 (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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Науковe видання

The International research and practice conference
"Nanotechnology and nanomaterials"
(NANO-2022)

Book of abstracts is published in authors' edition without modifying by the Organizing Committee

Head of Organizing Committee:
Dr. *Olena Fesenko*, Institute of Physics of the NAS of Ukraine
Design and layout: *Volodymyr Havlo.*

Technical support in the course of the International conference (NANO-2022). Junior Researchers of the Institute of Physics of the NAS of Ukraine A.D. Yaremkevych (media assistance) and Y.S. Kifiuk (sound equipment and photo report), Leading Engineers of the Institute of Physics of the NAS of Ukraine Maksym Rallev (informational and transportation support), O.P. Budnyk (registration of participants and excursions), Pavlo Golub (registration of participants and general questions), Vitaliy Tkachenko (registration support), A.V. Klochek (registration of participants and general question), T.V. Tsebrienko (registration support).

Підписано до друку 04.05.2022. Формат 60x84/$_{16}$.
Папір офсетний. Друк офсетний. Умовн. друк. арк. 3,48.
Наклад 300 прим.Зам. № 46190.

ТзОВ "Галицька видавнича спілка"
вул. Тугана-Барановського, 24, м. Львів, 79005,
тел.: (032) 276-37-99
Свідоцтво суб'єкта видавничої справи ДК № 7408 від 27.07.2021 р.

Друк: ТзОВ "РВФ "Поліграф-сервіс"
вул. Грабовського 11/13, м. Львів, 79008
тел.: (067) 673-85-75
Свідоцтво про внесення суб'єкта видавничої справи до державного реєстру видавців, виготовників і розповсюджувачів видавничої продукції серія ДК № 3900 від 14.10.2010