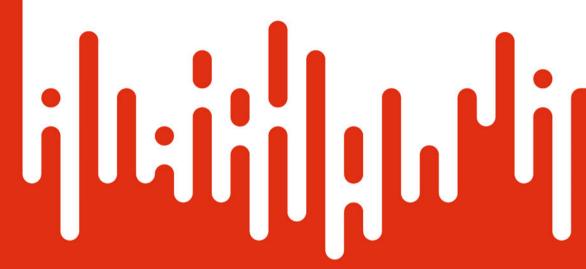
Rachid Masrour



Electronic, Magnetic, and Thermoelectric Properties of Spinel Ferrite Systems

A Monte Carlo Study, Mean-Field Theory, High-Temperature Series Expansions, and Ab-Initio Calculations



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Rachid Masrour Laboratory of Solid Physics Faculty of Sciences Dhar El Mahraz Sidi Mohamed Ben Abdellah University Fez. Morocco

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General Introduction

AB₂O₄ spinel oxides comprising two transition metal elements (i.e., A and B) and oxygens exhibit interesting and varying structural, electrical, and magnetic properties. Among them, NiCo₂O₄ has an inverse spinel structure in which half of Co ions occupy tetrahedral sites (A-sites), whereas the other half of Co ions and all Ni ions occupy octahedral sites (B-sites) [1, 2]. In recent years, Ferrimagnetic Nanoparticles (FMNPs) have witnessed extensive nanoscience growth due to their unique magnetic properties of nanoparticles (Fe₃O₄, Fe₂O₃) and synthesis methods [3]. Fe₂O₃ exhibits solid magnetic characteristics due to its high magnetization saturation (M_s), 92 emu/g of material at ambient temperature, and high curie temperature (T_c) of 577 °C [4]. Antiferromagnetic (AFM) spintronics is an emerging field aiming to manipulate and control spins for future data storage applications [5–7]. Such interest is owing to the promising features hosted by AFM materials, including non-stray fields, high exchange interaction, manipulation of the spin wave at the terahertz frequencies, and efficiency in transport mechanisms compared to Ferromagnetic (FM) counterparts [8–10]. The ferrimagnetic systems are well adapted to study magnetic properties of a certain type of magnetic materials which are solicited for the aforementioned technological applications as well as academic researches [11, 12]. Theoretically, several studies on mixed-spin systems have been carried out to investigate their magnetic properties by using different numerical techniques of statistical physics, including renormalization group technique [13, 14], mean-field approximation [15, 16], effective-field theory [17, 18], Monte Carlo simulations [19, 20], or exact recursion relations on various structures such as square [22], honeycomb [23], Bethe-Heitler production of dileptons with high invariant mass [24], cubic lattices, and hexagonal core-shell structure [26, 27]. The novel dynamic behaviors in a ferrimagnetic Gd_x(FeCo)_{1-x} nanosphere model with different Gd compositions ranging from x = 0 to 0.44 at finite 0–1200 K temperatures using stochastic atomistic numerical calculations [28]. Stanciu et al. experimentally observed the temperature dependence of dynamic modes in amorphous GdFeCo using an all-optical pumpprobe technique; the Ferromagnetic Resonance (FMR) frequency rapidly increased when the temperature approached the angular momentum compensation point. Also,

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Kim et al. experimentally determined that domain wall mobility in a GdFeCo ferrimagnet is enhanced at the angular momentum compensation temperature. Zhu et al. proposed a robust means of determining the angular momentum compensation point in ferrimagnets based on the Curie-Weiss theory. Yamamoto et al. [32, 33] employed Density Matrix Renormalization Group Technique (DMRG) and Quantum Monte Carlo (OMC) method to calculate the thermodynamic properties of the Heisenberg ferrimagnetic mixed-spin chain. By using the DMRG and Spin-Wave Theory (SWT), Langari studied the phase diagram of XXZ anisotropic ferrimagetic spin-(1/2, 1) chain under the presence of a transverse magnetic field. Chen [35, 36] investigated the excited states and thermodynamic properties of the Heisenberg ferrimagnetic spin chain by using Dyson–Maleev Mean-Field (DMMF) theory and Bond Operator (BO) method. The Double Perovskite Oxides (DPO) with general formula A₂BB'O₆ (where A is alkaline or rare earth metal and the cation B(B') having 3(4/5)d states are taken from two different transition metals) have attained much interest due to their unusual and marvelous physical properties such as colossal magnetoresistance [37, 38], multiferrocity [39], thermo-electricity [40], structure stability [41], magnetodielectricity [42], giant anisotropic magneto-caloric effect, etc. [43]. The density functional theory, Monte Carlo simulations, Green function, and high-temperature series expansions were applied for a series of spinel systems [44–47].

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About the Author



Prof. Rachid Masrour from Morocco, actually, is Research Professor in the Faculty of Sciences Dhar El Mahraz at Sidi Mohamed Ben Abdellah University, Fez, Morocco. He completed his Ph.D. in March 2006 at same University. His research interests lie in the area of Condensed Matter Physics, Material Sciences, Material for energy, Magnetism,.... He has 322 articles published in Web of Science and 10 book chapters published in international journal and 2 books (https://www.bookpi.org/bookstore/pro duct/new-frontiers-in-physical-science-research/) with h-index 32. He participated in more 100 Moroccan and international conferences. He's a Referee of a several articles and also Editorial Board Members in different international journals. He has a lot of collaboration with laboratories from abroad. He has been honored with International Association of Advanced Materials Young Scientist Medal in recognition for their contribution to "Magnetism, Electromagnetism and Spintronics" and delivered a lecture in the Advanced Materials World Congress October 11–14, 2022. One of the world's most cited top scientists in material physics (top 2 %, Stanford University Ranking, US, 2020). He won the prize for best oral presentation Award for MCGPD-2021, by Indian Association for Crystal Growth & Indian Science; Technology Association International Organization for Crystal Growth, July 5-8, 2021. The prizes are awarded during the closing ceremony of the congress; and Outstanding Scientist Award (VDGOOD PROFES-SIONAL ASSOCIATION, 15-02-2020, India). It was among the most critical in 2020 by Elsevier. Has been

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admitted as a fellow of IAAM (International Association for Advanced Materials, Stockholm, Sweden) in recognition of their contribution to the Li-ion battery as well as the right to use the "FIAAM" designation letters in 2023.