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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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General Introduction

AB_2O_4 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, $NiCo_2O_4$ 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 (Fe_3O_4 , Fe_2O_3) and synthesis methods [3]. Fe_2O_3 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 pump–probe technique; the Ferromagnetic Resonance (FMR) frequency rapidly increased when the temperature approached the angular momentum compensation point. Also,

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 (QMC) 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 ferrimagnetic 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 $A_2BB'O_6$ (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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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.