1.

Record Nr.	UNINA9910746286403321
Autore	Masrour Rachid
Titolo	Electronic, magnetic, and thermoelectric properties of Spinel Ferrite systems : a Monte Carlo study, mean-field theory, high-temperature series expansions, and ab-initio calculations / / Rachid Masrour
Pubbl/distr/stampa	Cham : , : Springer International Publishing AG, , 2023 ©2023
ISBN	3-031-40613-3
Edizione	[1st ed.]
Descrizione fisica	1 online resource (xiv, 128 pages) : illustrations
Collana	SpringerBriefs in Materials Series
Disciplina	620.1697
Soggetti	Metals - Magnetic properties
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di contenuto	Intro -- General Introduction -- References -- Contents -- About the Author -- 1 Exchange Interaction Types in Magnetic Materials -- 1.1 Magnetic Interactions -- 1.2 Magnetic Dipole Interaction -- 1.3 Direct Exchange Interaction -- 1.4 Indirect Exchange Interaction -- 1.5 Super-Exchange Interaction -- 1.6 Ruderman-Kittel-Kasuya-Yosida Exchange Interaction -- 1.7 Double Exchange Interaction -- 1.8 Spin Models -- 1.8.1 Ising Model -- 1.8.2 Potts Model -- 1.8.3 Continuous Spin Model -- 1.8.4 N-Component Vector Models -- 1.8.5 The Spherical Model -- 1.8.6 Model of D'Edwards Anderson -- 1.8.7 Model of Sherrington and Kirkpatrick -- 1.9 Boundary Conditions -- 1.9.1 Periodic Boundary Conditions -- 1.9.2 Periodic Boundary Conditions Screw -- 1.9.3 Anti-periodic Boundary Conditions -- 1.9.4 Free Edge Boundary Conditions -- 1.10 Calculation of the Values of the Exchange Integrals by Mean Filed Theory -- 1.11 High-Temperature Series Expansions -- 1.12 Critical Exponents and Scaling Laws -- References -- 2 Computational Methods: Ab Initio Calculations and Monte Carlo Simulations -- 2.1 Density Functional Theory -- 2.1.1 Born-Oppenheimer Approximation -- 2.1.2 The Hartree and Hartree-Fock Approximations -- 2.1.3 Thomas-Fermi Model -- 2.1.4 Theorems of Hohenberg and Kohn (H.K) -- 2.1.5 Kohn-Sham Formulation -- 2.1.6 Functional Exchange and Correlation -- 2.1.7 Pseudo-Potentials -- 2.2 Monte Carlo Simulations -- 2.3 Simulation Algorithms -- 2.4

Conclusion -- References -- 3 Magnetic Properties of (Fe23+) [Fe3+M2+]O42- (M = Co, Cu, Ni and Fe) Inverse Ferrite Spinels: A Monte Carlo Study -- 3.1 Introduction -- 3.2 Ising Model -- 3.3 Monte Carlo Simulations -- 3.4 Results and Discussion -- 3.5 Conclusions -- References -- 4 Thermoelectric and Spin-Lattice Coupling in a MnCr2S4 Ferrimagnetic Spinel -- 4.1 Introduction -- 4.2 Ab Initio Calculations.

4.3 Monte Carlo Study -- 4.4 Results and Discussion -- 4.5 Conclusion -- References -- 5 Magnetic Properties of LiMn1.5Ni0.5O4 Spinel: Ab Initio Calculations and Monte Carlo Simulation -- 5.1 Introduction -- 5.2 Ab Initio Calculation -- 5.3 Monte Carlo Simulation -- 5.4 Results and Discussion -- 5.5 Conclusion -- References -- 6 Magnetic Properties of Inverse Spinel Fe3O4 Nano-Layer: A Monte Carlo Study -- 6.1 Introduction -- 6.2 Ising Model and Monte Carlo Simulations -- 6.3 Results and Discussion -- 6.4 Conclusion -- References -- 7 Electronic and Magnetic Structures of Fe3O4 Ferrimagnetic: Ab Initio Calculations, Mean-Field Theory, and Series Expansion Calculations -- 7.1 Introduction -- 7.2 Electronic Structure Calculations -- 7.3 Theories and Models -- 7.4 Results and Discussion -- 7.5 Conclusions -- References -- 8 Magnetic Properties of Mixed Ni-Cu Spinel Ferrites Calculated Using Mean-Field Approach -- 8.1 Introduction -- 8.2 Methodology -- 8.3 High-Temperature Series Expansions -- 8.4 Results and Discussion -- 8.5 Conclusions -- References -- 9 Effect of Cobalt on NiCr2O4: Calculation of Critical Temperature and Exchange Interactions -- 9.1 Introduction -- 9.2 Theories -- 9.2.1 Green's Functions Theory -- 9.2.2 Mean Field Theory -- 9.3 Results and Discussion -- 9.4 Conclusion -- References -- 10 Studying the Effect of Zn Substitution on NiFe2O4 Spinel Systems -- 10.1 Introduction -- 10.2 Theories -- 10.3 Results and Discussion -- 10.4 Conclusion -- References -- General Conclusion.

| Sommario/riassunto | This book explores magnetic properties and critical temperatures in inverse ferrite Fe(MFe)O spinels (e.g., Fe, Co, Ni). It calculates transition and Curie Weiss temperatures, providing insights into their thermodynamic behavior. Using the full potential linearized augmented plane wave (FP-LAPW) method, it investigates electrical and magnetic structures of spinel chromite, revealing magnetic moments in MnCrS. Seebeck coefficient and electrical conductivity are also calculated. Advanced techniques like Monte Carlo, DFT+U, and FLAPW analyze magnetic characteristics of LiMn.Ni.O and electronic/magnetic structures of FeO. High-temperature series expansions calculate Neel temperature and critical exponents, while GFT determines thermal magnetization and susceptibility. The analysis exposes exchange interactions' effects on magnetic order and introduces asymmetric phases in ferrimagnetic spinel systems. This book serves as an invaluable resource for researchers, academics, and enthusiasts seeking a comprehensive understanding of magnetic properties and critical phenomena within diverse spinel materials |