

Theory of x-ray absorption spectroscopy for ferrites

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Olle Eriksson^{1,5} and Patrik Thunström^{1,*}¹Department of Physics and Astronomy, Uppsala University, Box 516, Uppsala SE-751 20, Sweden²Université de Strasbourg, IPCMS, CNRS-UNISTRA UMR 7504, 67034 Strasbourg, France³Oreosphere AB, Torshamningsgatan 30B, 164 40 Kista, Stockholm, Sweden⁴School of Computational Sciences, Korea Institute for Advanced Study, Seoul 02455, South Korea⁵Wallenberg Initiative Materials Science, Uppsala University, Box 516, Uppsala SE-751 20, Sweden (Received 4 July 2023; revised 15 February 2024; accepted 20 February 2024; published 14 March 2024)

The theoretical calculation of the interaction of electromagnetic radiation with matter remains a challenging problem for contemporary *ab initio* electronic structure methods, in particular, for x-ray spectroscopies. This is not only due to the strong interaction between the core hole and the photoexcited electron, but also due to the elusive multiplet effects that arise from the Coulomb interaction among the valence electrons. In this work we report a method based on density functional theory in conjunction with multiplet ligand-field theory to investigate various core-level spectroscopies, in particular, x-ray absorption spectroscopy (XAS) and x-ray magnetic circular dichroism (XMCD). The developed computational scheme is applied to the $L_{2,3}$ XAS and XMCD edges of magnetite (Fe_3O_4) as well as cobalt ferrite (CoFe_2O_4) and nickel ferrite (NiFe_2O_4). The results are in overall good agreement with experimental observations, both regarding the XAS $L_{2,3}$ branching ratio, the peak positions, as well as the relative intensities. The agreement between theory and experiment is equally good for XAS and the XMCD spectra, for all studied systems. The results are analyzed in terms of σ_{ij} and t_{2ij} orbital contribution, and the robustness of the spectra with regard to the uncertainties of the Slater parameters is investigated. The analysis also highlights the strong effect of the $2p$ - $3d$ interaction in x-ray spectroscopy.

DOI: 10.1103/PhysRevB.109.115126

I. INTRODUCTION

Core-level spectroscopy is one of the most powerful techniques for probing the electronic structure of strongly correlated electron systems, as the interaction between x-rays and matter gives element-specific insights into the magnetic and electronic properties of materials, as well as their structural and chemical properties. In particular, the development of synchrotron radiation facilities and recently, x-ray free-electron lasers, have made the analysis efficient and the resolution very high in energy, and in specific cases, in time [1]. This increase in the experimental resolution has made it possible to detect fine features and structures in the x-ray spectra [2,3]. This development of experimental tools and techniques calls for a novel theoretical approach to compute x-ray absorption spectra, most notably, for systems with complex or correlated electronic structures, like magnetites as well as cobalt and nickel ferrites. In this work we focus specifically on these materials and on insights for the theoretical description of x-ray absorption spectroscopy (XAS) and x-ray magnetic circular dichroism (XMCD).

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For the theoretical modeling of core-level and x-ray absorption spectroscopy, there have been two main distinct methodologies that are primarily used today. The first one is based on density functional theory (DFT) and the Kubo formula [4], while the second focuses on multiconfiguration effects [5]. Both methodologies are well reviewed in the literature (see, for example, Refs. [6,7]). The DFT-based methods are essentially parameter-free and provide, as a main advantage, a description of magnetism, structural properties, and chemical bonding in general. These methods are designed for the ground-state properties of materials, and hence their description of the excited states probed with x-ray spectroscopy is very limited. This is due to an incomplete treatment of electronic correlations, in particular, the multiconfigurational effects. Overall, these methods work best for widely dispersive electron systems. In contrast, atomic multiplet theory is essentially intended for a better description of the multiconfigurational effects originating from on-site electron-electron interaction [8]. For practical computational efficiency, the multiplet theory is often implemented for an isolated ion and thus neglects hybridization effects. It is therefore not surprising that this implementation of the theory has been found to work best for localized electronic states, e.g., the $4f$ orbitals of rare-earth elements. However, effects like crystal-field splitting and orbital hybridization can be treated by adding suitable model terms to the Hamiltonian of the system. The resulting theory is often referred to as the multiplet ligand-field theory (MLFT) [8]. This theory is very powerful in reproducing experimental spectra when the

Theory Apps Of Ferrites

Thomas Griffiths



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Theory and Application of Ferrites Ronald F. Soohoo, 1960 Theory of ferrites Their science and technology Properties of matter in the solid state Dielectric properties of ferrites Magnetic properties of ferrites The permeability tensor Eddy current hysteresis and residual losses in ferrites Measurements of ferrite properties Propagation of electromagnetic waves in infinite anisotropic media Propagation of electromagnetic waves through anisotropic waveguides Application of ferrites below microwave frequencies Longitudinal field devices Transversely magnetized ferrite devices Dielectric loading and tapered field devices Field displacement devices Cutoff phenomena in magnetized ferrites Nonlinear ferrite devices System application of ferrite devices Mathematical formulae Derivation of the perturbation relations Transcendental equation involving the propagation constant Discussion of gaussian and mks practical units Some design problems of microwave ferrite devices *Theory and Applications of Ferrites at Microwave Frequencies* Perry Hatch Vartanian (Jr.), 1956 *Spinel Ferrite Materials* Gagan Kumar Bhargava, Pankaj Sharma, Sagar E Shirsath, Sanjeev Kumar, Sumit Bhardwaj, 2024-11-30 *Spinel Ferrite Materials Fundamentals Progress and Applications* provides a systematic and comprehensive review of the latest research in ferrite materials to assist students researchers and practitioners The book focuses on the synthesis methodology the structural electrical and magnetic properties and various applications of spinel ferrites The book pays particular attention to synthesis techniques and subsequent applications in biomedicine microwave absorption nanoelectronics wastewater treatment sensing and photocatalysis Provides a systematic efficient and comprehensive review of ferrite nanoparticles Investigates the structural electrical and magnetic characteristics of spinel ferrite nanoparticles Describes the advanced techniques required for the synthesis of spinel ferrite materials *National Bureau of Standards Miscellaneous Publication*, 1965 *NBS Special Publication*, 1965 **Slow Waves in Ferrite Media, and Their Interaction with Electron Streams** Jerome Spector, 1961 **Multifunctional Inorganic Nanomaterials for Energy Applications** H.P. Nagaswarupa, Mika E.T. Sillanpää, H.C. Ananda Murthy, Ramachandra Naik, 2024-06-19 *Multifunctional Inorganic Nanomaterials for Energy Applications* provides deep insight into the role of multifunctional nanomaterials in the field of energy and power generation applications It mainly focuses on the synthesis fabrication design development and optimization of novel functional inorganic nanomaterials for energy storage and saving devices It also covers studies of inorganic electrode materials for supercapacitors membranes for batteries and fuel cells and materials for display systems and energy generation Features Explores computational and experimental methods of preparing inorganic nanomaterials and their multifunctional applications Includes synthesis and performance analysis of various functional nanomaterials for energy storage and saving applications Reviews current research directions and latest developments in the field of energy materials Discusses importance of computational techniques in designing novel nanomaterials Highlights importance of multifunctional applications of nanomaterials in the energy sector This book is aimed at graduate students and researchers in materials

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in Chapter 10 there are described different ferrite devices created on the bases of the above indicated phenomena and obtaining wide application in SHF technology This chapter ends with the consideration of the problems of theory and design of linear ferrite SHF devices

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