

Magnetism out of disorder in a $J = 0$ compound Ba_2YIrO_6

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We systematically investigate the magnetic properties and local structure of Ba_2YIrO_6 to demonstrate that Y and Ir lattice defects in the form of antiphase boundary or clusters of antisite disorder affect the magnetism observed in this d^4 compound. We compare the magnetic properties and atomic imaging of (1) a slow cooled crystal, (2) a crystal quenched from 900°C after growth, and (3) a crystal grown using a faster cooling rate than the slow cooled one. Atomic imaging by scanning transmission electron microscopy (STEM) shows that quenching from 900°C introduces antiphase boundary to the crystals, and a faster cooling rate during crystal growth leads to clusters of Y and Ir antisite disorder. STEM study suggests the antiphase boundary region is Ir-rich with a composition of $\text{Ba}_2(\text{Y}_{1-x}\text{Ir}_x)\text{IrO}_6$. The magnetic measurements show that Ba_2YIrO_6 crystals with clusters of antisite defects have a larger effective moment and a larger saturation moment than the slow-cooled crystals. Quenched crystals with Ir-rich antiphase boundary shows a slightly suppressed saturation moment than the slow cooled crystals, and this seems to suggest that antiphase boundary is detrimental to the moment formation. Our DFT calculations suggest magnetic condensation is unlikely as the energy to be gained from superexchange is small compared to the spin-orbit gap. However, once Y is replaced by Ir in the antisite disordered region, the picture of local non-magnetic singlets breaks down and magnetism can be induced. This is because of (a) enhanced interactions due to increased overlap of orbitals between sites, and, (b) increased number of orbitals mediating the interactions. Our work highlights the importance of lattice defects in understanding the experimentally observed magnetism in Ba_2YIrO_6 and other $J = 0$ systems.

I. INTRODUCTION

The magnetic properties of octahedrally coordinated Re^{3+} , Ru^{4+} , Os^{4+} , and Ir^{5+} with a d^4 electronic configuration were first studied around 1960s.¹ The large crystal electric field prefers the low spin configuration for these 4d/5d transition metal compounds. The strong spin orbit coupling and the hybridization between transition metal d -orbital and oxygen p -orbital further complicate the magnetic behavior by reducing the magnetic moment or the orbital angular momentum, respectively. In the presence of a strong spin-orbit coupling, a temperature independent magnetic susceptibility is expected.

Both 4d and 5d transition metal ions in the d^4 (ie. $t_{2g}^4e_g^0$) configuration are expected to be non-magnetic in both the weakly and strongly correlated limits. In the weakly correlated picture, t_{2g} shells are split into a fully filled $j = 3/2$ shell and an empty $j = 1/2$ shell due to strong spin-orbit coupling. Spin-orbit coupling then opens up a bandgap between the $j = 3/2$ and $j = 1/2$ bands leading to a non-magnetic insulating ground state. In the strongly correlated picture, the first two Hund's rules require each d^4 site to be in a total $S = 1$ and total $L = 1$. Strong spin-orbit coupling then yields a local $J = 0$ state on every ion. Again the ground state is non-magnetic.

Interest in d^4 magnetism was revived after a report of long range magnetic order in Sr_2YIrO_6 ² and the proposal of a condensation mechanism for magnetism in d^4 Mott insulators.³ It was predicted that the hopping of electrons between neighboring sites would lead to an exchange interaction that could compete with the onsite spin-orbital singlet and generate a local moment.² The anomalous magnetic moments observed in $A_2\text{YIrO}_6$ ($A=\text{Sr}$, and Ba) double perovskites and the fragile magnetism in $R_2\text{Os}_2\text{O}_7$ (R =rare earth) have been the subject of intense theoretical and experimental investigations.^{2–15} A fundamental question still remains: what is the root cause of the anomalous magnetism in these $5d^4$ compounds?

There are two prominent explanations which have been applied to these $5d^4$ materials. The first explanation is quenching of the orbital degrees of freedom through octahedral distortions. Uniaxial distortions (ie. $\delta(\mathbf{L} \cdot \hat{n})^2$) split the t_{2g} orbitals into an orbital singlet and an orbital doublet. When the orbital doublet is lower in energy, the doublet is filled and the singlet is empty, and the conclusion is still a non-magnetic ground state. However if the orbital singlet is lower in energy, it is occupied by two electrons while the other two electrons occupy the doublet. This half filled orbital doublet then has a total spin $S = 1$ leading to a magnetic ground state. Cao et. al.² proposed this distortion mechanism was the cause of the

Magnetism In Disorder

**Claudine Lacroix, Philippe
Mendels, Frédéric Mila**



Magnetism In Disorder:

Magnetism In Disorder T.J. Hicks, Amorphous Magnetism Takahito Kaneyoshi, 2018-01-18 This book presents some of the methods used in the theory of amorphous magnetism from a single standpoint that amorphous magnets have a topologically disordered structure of the type given by the dense random packing of hard spheres The primary aim is to show systematically the present theoretical apparatus in a form which would allow the reader to use it in investigations of still unsolved problems Even within these limits the theory of amorphous magnetism is now a very large subject This book is not designed to review all the developments in this rapidly developing area It is primarily intended for the novice in this field rather than the specialist *Aspects Of Modern Magnetism - Lecture Notes Of The Eighth Chinese International Summer School Of Physics* F C Pu, Y J Wang, Chang-he Shang, 1996-05-04 This book a collection of works by leading figures in the field is devoted to the latest developments of modern magnetism including micromagnetism nanomagnetic materials magnetic multilayers macroscopic quantum magnetism rare earth intermetallic compounds giant magnetoresistance and their applications Some new concepts and theories are also included for a better understanding of these novel phenomena This book can be used as an advanced text book on magnetism and materials science for graduate students in physics and materials science departments It is also useful as a research reference for condensed matter physicists and materials scientists Introduction to Frustrated Magnetism Claudine Lacroix, Philippe Mendels, Frédéric Mila, 2011-01-12 The field of highly frustrated magnetism has developed considerably and expanded over the last 15 years Issuing from canonical geometric frustration of interactions it now extends over other aspects with many degrees of freedom such as magneto elastic couplings orbital degrees of freedom dilution effects and electron doping Its is thus shown here that the concept of frustration impacts on many other fields in physics than magnetism This book represents a state of the art review aimed at a broad audience with tutorial chapters and more topical ones encompassing solid state chemistry experimental and theoretical physics *Spintronics Handbook, Second Edition: Spin Transport and Magnetism* Evgeny Y. Tsymbal, Igor Žutić, 2019-05-20 The second edition offers an update on the single most comprehensive survey of the two intertwined fields of spintronics and magnetism covering the diverse array of materials and structures including silicon organic semiconductors carbon nanotubes graphene and engineered nanostructures It focuses on seminal pioneering work together with the latest in cutting edge advances notably extended discussion of two dimensional materials beyond graphene topological insulators skyrmions and molecular spintronics The main sections cover physical phenomena spin dependent tunneling control of spin and magnetism in semiconductors and spin based applications **Handbook of Spin Transport and Magnetism** Evgeny Y. Tsymbal, Igor Zutic, 2016-04-19 In the past several decades the research on spin transport and magnetism has led to remarkable scientific and technological breakthroughs including Albert Fert and Peter Grunberg s Nobel Prize winning discovery of giant magnetoresistance GMR in magnetic metallic multilayers Handbook of Spin Transport and Magnetism

provides a comprehensive balance between theory and experiment. *Theory of Itinerant Electron Magnetism* Jürgen Kübler, 2017-03-23 This book in the broadest sense is an application of quantum mechanics and statistical mechanics to the field of magnetism. Under certain well described circumstances an immensely large number of electrons moving in the solid state of matter will collectively produce permanent magnetism. Permanent magnets are of fundamental interest and magnetic materials are also of great practical importance as they provide a large field of technological applications. The physical details describing the many electron problem of magnetism are presented in this book on the basis of the local density functional approximation. The emphasis is on realistic magnets for which the equations describing the many electron problem can only be solved by using computers. The great recent and continuing improvements of computers are to a large extent responsible for the progress in the field. Along with a detailed introduction to the density functional theory this book presents representative computational methods and provides the reader with a complete computer programme for the determination of the electronic structure of a magnet on a PC. A large part of the book is devoted to a detailed treatment of the connections between electronic properties and magnetism and how they differ in the various known magnetic systems. Current trends are exposed and explained for a large class of alloys and compounds. The modern field of artificially layered systems known as multilayers and their industrial applications are dealt with in detail. Finally an attempt is made to relate the rich thermodynamic properties of magnets to the ab initio results originating from the electronic structure.

Magnetism and Structure in Functional Materials Antoni Planes, Lluís Mañosa, Avadh Saxena, 2010-02-11 Magnetism and Structure in Functional Materials addresses three distinct but related topics: i) magnetoelastic materials such as magnetic martensites and magnetic shape memory alloys; ii) the magnetocaloric effect related to magnetostructural transitions; and iii) colossal magnetoresistance (CMR) and related manganites. The goal is to identify common underlying principles in these classes of materials that are relevant for optimizing various functionalities. The emergence of apparently different magnetic structural phenomena in disparate classes of materials clearly points to a need for common concepts in order to achieve a broader understanding of the interplay between magnetism and structure in this general class of new functional materials exhibiting ever more complex microstructure and function. The topic is interdisciplinary in nature and the contributors correspondingly include physicists, materials scientists, and engineers. Likewise the book will appeal to scientists from all these areas.

Magnetism in Heavy Fermion Systems Harry Brian Radousky, 2000 Magnetism in Heavy Fermion Systems is a review volume which covers an important subset of topics in the field of heavy fermion and non-Fermi liquid physics. It summarizes much of the experimental information in these areas and includes an article which discusses theoretical interpretations of the complex magnetic behavior of heavy fermion systems. The topics covered include heavy fermion superconductivity, muon spin relaxation in small moment heavy fermions, neutron scattering from heavy fermions, random localized magnetism in heavy fermions, and magnetism in Pr containing cuprates. One feature of the book which should be helpful to graduate students and new workers in the field is the

extensive references and a separate list of review articles

Universal Magnetism Edmund Shaftesbury, 1924

Fundamentals of Magnetism and Spintronics Atowar Rahman, 2022-09-07 Fundamentals of Magnetism and Spintronics develops the idea of magnetism understand its sources and other related matters step by step Fundamentals of Magnetism and Spintronics describes microscopic sources of magnetic field and explains why different bodies behave differently in the presence of an external magnetic field Different topics in Magnetism and Spintronics have been presented in simple ways using simple mathematics The objectives are to cover the basic concepts of Magnetism and Spintronics using simple models and to provide coverage of the subject matter as far as possible Chapters 1 to 3 have been devoted to define the microscopic source of magnetism and to define fundamental parameters of magnetism Chapter 4 to Chapter 11 have been devoted for the general properties of magnetic materials There has been tremendous research in the field of material science and magnetism and as a result remarkable success has been achieved in magnetic storage technology A new subject known as spintronics or magneto electronics has come up which is a novel kind of union of elements of material science magnetism and electrical engineering with a goal to create devices and architectures for digital electronics applications Chapter 12 has been devoted to introduce this subject to the students Simple pictures and heuristic descriptions have been given to introduce basic ideas of spintronics transport of spin polarized electrons mechanisms by which several magnetoelectronic devices operate and basic architectures of MRAM Contents Chapter 2 Angular momentum 21 Chapter 3 Some definitions 51 Chapter 4 Diamagnetic and Paramagnetic properties of Solids 81 Chapter 5 Magnetism of ordered systems 114 Chapter 6 Spin Waves Magnons 146 Chapter 7 Magnetic Energies and Magnetic Domains 157 Chapter 8 Magnetic Resonance Phenomena 204 Chapter 9 Magnetism in Thin Films 247 Chapter 10 Some Magnetic Phenomena 259 Chapter 11 Magnetic measurements 286 Chapter 12 Fundamentals of Spintronics 299 Problems 357 References 373

Mössbauer Spectroscopy Applied to Magnetism and Materials Science G.J Long, F. Grandjean, 2013-06-29 During the past 30 years materials science has developed into a full fledged field for basic and applied scientific enquiry Indeed materials scientists have devoted their efforts to creating new materials with improved electronic magnetic thermal mechanical and optical properties Often unnoticed these new materials are rapidly invading our homes and automobiles and may be found in our utensils electronic equipment textiles home appliances and electric motors Even though they may go unnoticed these new materials have either improved the efficiency and lifetime of these items or have reduced their weight or cost In particular magnetically ordered materials are useful in various applications such as motors magnetic imaging magnetic recording and magnetic levitation Hence much effort has been devoted to the development of better hard magnetic materials magnetic thin films and molecular magnets During the same period of time Mossbauer effect spectroscopy has grown from a laboratory curiosity to a mature spectroscopic technique a technique that probes solid state materials at specific atomic sites and yields microscopic information on the magnetic and electronic properties of these materials Iron 57 is the most commonly and easily used

Mossbauer effect isotope and of course is particularly relevant for the study of magnetic materials Various applications of Mossbauer spectroscopy to magnetic materials are discussed in the first six chapters of this volume Other isotopes such as zinc 67 and gadolinium 153 have recently been used to study the electronic properties of zinc compounds and the electronic and magnetic properties of rare earth transition metal compounds

Quantum Magnetism Ulrich Schollwöck, Johannes Richter, Damian J.J. Farnell, Raymond F. Bishop, 2008-05-14 The investigation of magnetic systems where quantum effects play a dominant role has become a very active branch of solid state physics research in its own right The first three chapters of the Quantum Magnetism survey conceptual problems and provide insights into the classes of systems considered namely one dimensional two dimensional and molecular magnets The following chapters introduce the methods used in the field of quantum magnetism including spin wave analysis exact diagonalization quantum field theory coupled cluster methods and the Bethe ansatz The book closes with a chapter on quantum phase transitions and a contribution that puts the wealth of phenomena into the context of experimental solid state physics Closing a gap in the literature this volume is intended both as an introductory text at postgraduate level and as a modern comprehensive reference for researchers in the field *The Magnetism of Amorphous Metals and Alloys* J.A. Fernandez-Baca, Wai-Yim Ching, 1995 <http://www.worldscientific.com/worldscibooks/10.1142/1712>

Computational Quantum Physics and Chemistry of Nanomaterials Mojmir Šob, 2021-04-01 This Special Issue of Nanomaterials collects a series of original research articles providing new insight into the application of computational quantum physics and chemistry in research on nanomaterials It illustrates the extension and diversity of the field and indicates some future directions It provides the reader with an overall view of the latest prospects in this fast evolving and cross disciplinary field *Magnetism and Magnetic Materials* R L White, K. A. Wickersheim, 2013-10-22

Magnetism and Magnetic Materials 1965 Digest A Survey of the Technical Literature of the Preceding Year focuses on the processes methodologies reactions technologies and advancements in magnetism and magnetic materials The selection first offers information on general theoretical problems including spin wave dispersion exchange integral magnetic ordering soluble models magnetic phase transitions and conduction electron spin polarization The text then ponders on neutron diffraction spin configurations and magnetic transitions and properties of transition metals and their alloys Topics include neutron scattering theory and equipment spin configurations and magnetic transitions magnetic behavior rare earth alloys and compounds and other alloys and compounds The publication takes a look at the properties of magnetically dilute alloys and rare earth metals and their alloys Discussions focus on rare earth intermetallic compounds transition metals in noble metals and other dilute alloys The text then examines the technical properties of soft magnetic materials magnetically hard materials thin films and nuclear magnetism The selection is a valuable source of data for readers interested in magnetism and magnetic materials *Proceedings of the Seventh Conference on Magnetism and Magnetic Materials* J.A. Osborn, NA American Institute of Physics, 2013-11-11 Papers presented at the Conference on Magnetism and Magnetic Materials Phoenix

Arizona November 13 16 1961 **Practical Instruction in Animal Magnetism** Joseph Philippe François Deleuze, 1879

21st Century Nanoscience – A Handbook Klaus D. Sattler, 2020-04-02 This 21st Century Nanoscience Handbook will be the most comprehensive up to date large reference work for the field of nanoscience Handbook of Nanophysics by the same editor published in the fall of 2010 embraced as the first comprehensive reference to consider both fundamental and applied aspects of nanophysics This follow up project has been conceived as a necessary expansion and full update that considers the significant advances made in the field since 2010 It goes well beyond the physics as warranted by recent developments in the field The fifth volume in a ten volume set covers exotic nanostructures and quantum systems Key Features Provides the most comprehensive up to date large reference work for the field Chapters written by international experts in the field Emphasises presentation and real results and applications This handbook distinguishes itself from other works by its breadth of coverage readability and timely topics The intended readership is very broad from students and instructors to engineers physicists chemists biologists biomedical researchers industry professionals governmental scientists and others whose work is impacted by nanotechnology It will be an indispensable resource in academic government and industry libraries worldwide The fields impacted by nanoscience extend from materials science and engineering to biotechnology biomedical engineering medicine electrical engineering pharmaceutical science computer technology aerospace engineering mechanical engineering food science and beyond Spin Dynamics in Confined Magnetic Structures II Burkard Hillebrands, Kamel

Ounadjela, 2003-09-04 This second volume of the book on spin dynamics in confined magnetic structures covers central aspects of spin dynamic phenomena so that researchers can find a comprehensive compilation of the current work in the field Introductory chapters help newcomers to understand the basic concepts and the more advanced chapters give the current state of the art for most spin dynamic issues in the milliseconds to femtoseconds range Both experimental techniques and theoretical work are discussed The comprehensive presentation of these developments makes this volume very timely and valuable for every researcher working in the field of magnetism It describes the new experimental techniques which have advanced this field very rapidly Among the techniques covered particular attention is given to those involving high temporal elemental and spatial resolution as well as to techniques involving magnetic field pulses with very short rise times and durations

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This book is crafted in an easy-to-understand language and is complemented by engaging illustrations. This book is highly recommended for anyone seeking to gain a comprehensive understanding of Magnetism In Disorder.

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