

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

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(Dated: July 24, 2017)

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_2YIrO_6 ($\text{A}=\text{Sr}$, and Ba) double perovskites and the fragile magnetism in $\text{R}_2\text{Os}_2\text{O}_7$ ($\text{R}=\text{rare earth}$) 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

T.J. Hicks



Magnetism In Disorder:

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 Y. J. Wang, C. H. Shang, 1996 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

The Magnetism of Amorphous Metals and Alloys J.A. Fernandez-Baca, Wai-Yim Ching, 1995 <http://www.worldscientific.com/worldscibooks/10.1142/1712>

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

Magnetism In Disorder T.J. Hicks, Universal Magnetism Edmund Shaftesbury, 1924

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

Theory of Itinerant Electron Magnetism Jürgen Kübler, 2021 The book in the broadest sense is an application of quantum mechanics and statistical mechanics to the field of magnetism It can be used for parts of a specialized course on material properties or solid state physics and magnetism

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

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 bal

Computational Quantum Physics and Chemistry of Nanomaterials Mojmír 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

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

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

Practical Instruction in Animal Magnetism Joseph Philippe François Deleuze, 1879 *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 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

Handbook of Magnetic Materials Ekkes H. Brück, 2017-11-13 Handbook of Magnetic Materials Volume 26 covers the expansion of magnetism over the last few decades and its applications in research notably the magnetism of several classes of novel materials that share the presence of magnetic moments with truly ferromagnetic materials The book is an ideal reference for scientists active in magnetism research providing readers with novel trends and achievements in magnetism Each article contains an extensive description given in graphical as well as tabular form with much emphasis placed on the

discussion of the experimental material within the framework of physics chemistry and material science Comprises topical review articles written by leading authorities Includes a variety of self contained introductions to a given area in the field of magnetism without requiring recourse to the published literature Introduces given topics in the field of magnetism Describes novel trends and achievements in magnetism

21st Century Nanoscience - A Handbook Klaus D. Sattler,2020-04-02

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Rock and Mineral Magnetism W. O'Reilly,2012-12-06 The past two decades have witnessed a revolution in the earth sciences The quantitative instrument based measurements and physical models of geophysics together with advances in technology have radically transformed the way in which the Earth and especially its crust is described The study of the magnetism of the rocks of the Earth s crust has played a major part in this transformation Rocks or more specifically their constituent magnetic minerals can be regarded as a measuring instrument provided by nature which can be employed in the service of the earth sciences Thus magnetic minerals are a recording magnetometer a goniometer or protractor recording the directions of flows fields and forces a clock a recording thermometer a position recorder a strain gauge an instrument for geological surveying a tracer in climatology and hydrology a tool in petrology No instrument is linear or free from noise and systematic errors and the performance of nature s instrument must be assessed and certified This has been the task of the research worker in rock and mineral magnetism

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Table of Contents Magnetism In Disorder

1. Understanding the eBook Magnetism In Disorder
 - The Rise of Digital Reading Magnetism In Disorder
 - Advantages of eBooks Over Traditional Books
2. Identifying Magnetism In Disorder
 - Exploring Different Genres
 - Considering Fiction vs. Non-Fiction
 - Determining Your Reading Goals
3. Choosing the Right eBook Platform
 - Popular eBook Platforms
 - Features to Look for in an Magnetism In Disorder
 - User-Friendly Interface
4. Exploring eBook Recommendations from Magnetism In Disorder
 - Personalized Recommendations
 - Magnetism In Disorder User Reviews and Ratings
 - Magnetism In Disorder and Bestseller Lists
5. Accessing Magnetism In Disorder Free and Paid eBooks

- Magnetism In Disorder Public Domain eBooks
- Magnetism In Disorder eBook Subscription Services
- Magnetism In Disorder Budget-Friendly Options
- 6. Navigating Magnetism In Disorder eBook Formats
 - ePub, PDF, MOBI, and More
 - Magnetism In Disorder Compatibility with Devices
 - Magnetism In Disorder Enhanced eBook Features
- 7. Enhancing Your Reading Experience
 - Adjustable Fonts and Text Sizes of Magnetism In Disorder
 - Highlighting and Note-Taking Magnetism In Disorder
 - Interactive Elements Magnetism In Disorder
- 8. Staying Engaged with Magnetism In Disorder
 - Joining Online Reading Communities
 - Participating in Virtual Book Clubs
 - Following Authors and Publishers Magnetism In Disorder
- 9. Balancing eBooks and Physical Books Magnetism In Disorder
 - Benefits of a Digital Library
 - Creating a Diverse Reading Collection Magnetism In Disorder
- 10. Overcoming Reading Challenges
 - Dealing with Digital Eye Strain
 - Minimizing Distractions
 - Managing Screen Time
- 11. Cultivating a Reading Routine Magnetism In Disorder
 - Setting Reading Goals Magnetism In Disorder
 - Carving Out Dedicated Reading Time
- 12. Sourcing Reliable Information of Magnetism In Disorder
 - Fact-Checking eBook Content of Magnetism In Disorder
 - Distinguishing Credible Sources
- 13. Promoting Lifelong Learning
 - Utilizing eBooks for Skill Development

- Exploring Educational eBooks

14. Embracing eBook Trends

- Integration of Multimedia Elements
- Interactive and Gamified eBooks

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