

# Lectures 21-22

## Solid state materials. Electronic structure and conductivity

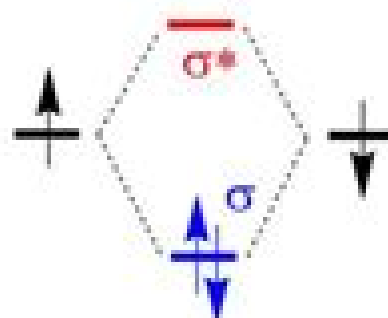
### 1) Band theory

- The electronic structure of **solids** can also be described by MO theory.
- A solid can be considered as a **supermolecule**.
- One mole of atoms ( $N_A$ ), each with  $X$  orbitals in the valence shell contributes  $X$  moles of atomic orbitals producing  $X$  moles of MO's.

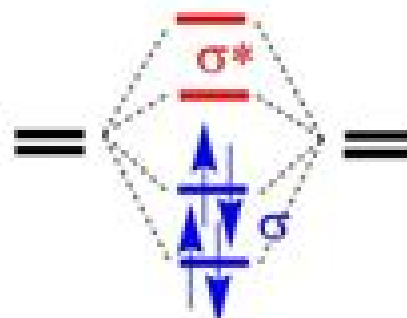
Consider qualitatively bonding between  $N$  *metal atoms* of  $ns^1$  configuration (Li, Na etc) arranged in a *chain*;  $N = 2, 4, N_A$ . Assume that  $X=1$  for simplicity.

- In the case of  $N \sim N_A$  atoms they form not **bonds** but **bands**.
- The band appearing in the *bonding* region is called **valence band**. The *antibonding* region is called **conduction band**.
- In the case of metals the **valence** and **conduction** bands are immediately **adjacent**.

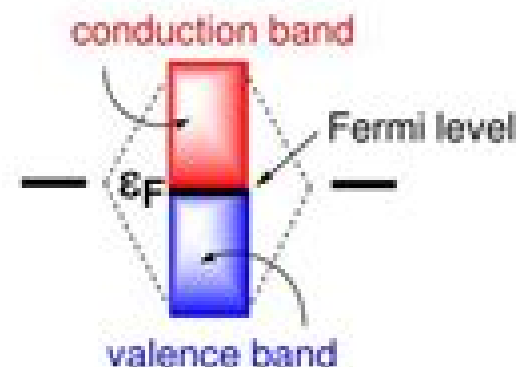
$N = 2$  Li atoms



4 Li atoms



$N_A$  Li atoms



# Electronic Structure Of Materials

**Guillaume Favre**



## **Electronic Structure Of Materials:**

**Electronic Structure of Materials** Adrian P. Sutton, 1993 In recent years researchers have increasingly recognized the dominant role of the local atomic environment in controlling the electronic structure and properties of materials This recognition has spawned the real space approach that provides a coherent framework for the study of perfect and defective crystals and non crystalline materials In addition to presenting these ideas this text details the reciprocal space approach exemplified in band theory and draws powerful links between the two approaches The book includes illustrations and examples of many up to date calculations based on density functional theory that are used today as predictive tools in materials science Throughout the book the mathematical complexity is kept to a minimum while comprehensive problem sets allow readers to master the fundamental concepts The text provides for students in materials science physics and chemistry a unique introduction to predictive modelling of the electronic structure and properties in today s materials *Electronic*

*Structure of Materials* Adrian P. Sutton, 1993-09-30 This book describes the modern real space approach to electronic structures and properties of crystalline and non crystalline materials in a form readily accessible to undergraduates in materials science physics and chemistry This book describes the modern real space approach to electronic structures and properties of crystalline and non crystalline materials in a form readily accessible to undergraduates in materials science physics and chemistry **Electronic Structure** Richard M. Martin, 2004-04-08 An important graduate textbook in condensed matter physics by highly regarded physicist

**Electronic Structure of Materials** Mireille Defranceschi, 2000

**Electronic Structure and the Properties of Solids** Walter A. Harrison, 1989-07-01 Should be widely read by practicing physicists chemists and materials scientists Philosophical Magazine In this comprehensive and innovative text Professor Harrison Stanford University offers a basic understanding of the electronic structure of covalent and ionic solids simple metals transition metals and their compounds The book illuminates the relationships of the electronic structures of these materials and shows how to calculate dielectric conducting and bonding properties for each Also described are various methods of approximating electronic structure providing insight and even quantitative results from the comparisons Dr Harrison has also included an especially helpful Solid State Table of the Elements that provides all the parameters needed to estimate almost any property of any solid with a hand held calculator using the techniques developed in the book Designed for graduate or advanced undergraduate students who have completed an undergraduate course in quantum mechanics or atomic and modern physics the text treats the relation between structure and properties comprehensively for all solids rather than for small classes of solids This makes it an indispensable reference for all who make use of approximative methods for electronic structure engineering semiconductor development and materials science The problems at the ends of the chapters are an important aspect of the book They clearly show that the calculations for systems and properties of genuine and current interest are actually quite elementary Prefaces Problems Tables Appendixes Solid State Table of the Elements

Bibliography Author and Subject Indexes Will doubtless exert a lasting influence on the solid state physics literature Physics Today Electronic Structure of Materials Rajendra Prasad, 2013-07-23 Most textbooks in the field are either too advanced for students or don't adequately cover current research topics Bridging this gap Electronic Structure of Materials helps advanced undergraduate and graduate students understand electronic structure methods and enables them to use these techniques in their work Developed from the author's lecture notes this classroom tested book takes a microscopic view of materials as composed of interacting electrons and nuclei It explains all the properties of materials in terms of basic quantities of electrons and nuclei such as electronic charge mass and atomic number Based on quantum mechanics this first principles approach does not have any adjustable parameters The first half of the text presents the fundamentals and methods of electronic structure Using numerous examples the second half illustrates applications of the methods to various materials including crystalline solids disordered substitutional alloys amorphous solids nanoclusters nanowires graphene topological insulators battery materials spintronic materials and materials under extreme conditions Every chapter starts at a basic level and gradually moves to more complex topics preparing students for more advanced work in the field End of chapter exercises also help students get a sense of numbers and visualize the physical picture associated with the problem Students are encouraged to practice with the electronic structure calculations via user friendly software packages

*Electronic Structure of Materials* Natalia Chezhina, Dmitry Korolev, 2019-04-01 This book is a short survey of magnetochemistry as a promising method for revealing the electronic structure of inorganic substances particularly solid oxide materials It is supported by five chapters that describe materials with various structures and applications showing how the method of magnetic dilution with the aid of other physical methods electron spin resonance magnetization Raman and Mossbauer spectroscopy and electrical conductivity accompanied by thorough structural and quantum mechanical studies may be used for describing the states of atoms and interatomic interactions in multicomponent oxide systems The book will serve as a guide for researchers in the field of various oxide materials since it shows the roots for selecting the best structures and qualitative and quantitative compositions of oxide materials on the basis of the knowledge about their electronic structure It is devoted to some of the most popular structures of multicomponent oxides among modern materials perovskites and pyrochlores giving a unified approach to their chemical structure Electronic Structure Methods for Complex Materials

Wai-Yim Ching, Paul Rulis, 2012-05-17 Density functional theory DFT has blossomed in the past few decades into a powerful tool that is used by experimentalists and theoreticians alike This book highlights the extensive contributions that the DFT based OLCAO method has made to progress in this field and it demonstrates its competitiveness for performing ab initio calculations on large and complex models of practical systems A brief historical account and introduction to the elements of the theory set the stage for discussions on semiconductors insulators crystalline metals and alloys complex crystals non crystalline solids and liquids microstructure containing systems and those containing impurities defects and surfaces

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**Materials** Natalia Chezhina, Dmitry Korolev, 2019-04-01 This book is a short survey of magnetochemistry as a promising method for revealing the electronic structure of inorganic substances particularly solid oxide materials It is supported by five chapters that describe materials with various structures and applications showing how the method of magnetic dilution with the aid of other physical methods electron spin resonance magnetization Raman and Mossbauer spectroscopy and electrical conductivity accompanied by thorough structural and quantum mechanical studies may be used for describing the states of atoms and interatomic interactions in multicomponent oxide systems The book will serve as a guide for researchers in the field of various oxide materials since it shows the roots for selecting the best structures and qualitative and quantitative compositions of oxide materials on the basis of the knowledge about their electronic structure It is devoted to some of the most popular structures of multicomponent oxides among modern materials perovskites and pyrochlores giving a unified approach to their chemical structure *Electronic Structure and Electronic Transitions in Layered Materials V.*

Grasso, 1986-06-30 This new volume in the series Physics and Chemistry of Materials with Layered Structures satisfies the need for a comprehensive review of the progress made in the decade 1972-1982 in the field of the electronic properties of layer compounds Some recent theoretical and experimental developments are highlighted by authoritative physicists active in current research The previous books of this series covering similar topics are volumes 3 and 4 The present review is mainly intended to fulfill the gap up to 1982 and part of 1983 I am indebted to all the authors for their friendly cooperation and continuous effort in preparing the contributions in their own fields of competence I am sure that both the expert scientists and the beginners in the field of the electronic properties of layered materials will find this book a valuable tool for their research work Warm thanks are due to Prof E Mooser General Editor of the series for his constant and authoritative advice This book has been conceived as a tribute to Prof Franco Bassani to whom the Italian tradition in the field of layer compounds as well as in other fields of solid state physics owes much The authors of this review have all benefited at some time of their professional life from close cooperation with him Istituto di Struttura della Materia VINCENZO GRASSO

Universit  di Messina IX V Grasso ed *Electronic Structure and Electronic Transitions in Layered Materials ix* *Electronic Structure Crystallography and Functional Motifs of Materials* Guo-Cong Guo, Xiao-Ming Jiang, 2024-01-08 *Electronic Structure Crystallography and Functional Motifs of Materials* Detailed resource on the method of electronic structure crystallography for revealing the experimental electronic structure and structure property relationships of functional materials *Electronic Structure Crystallography and Functional Motifs of Materials* describes electronic structure crystallography and functional motifs of materials two of the most challenging topics to realize the rational design of high performance functional materials emphasizing the physical properties and structure property relationships of functional materials using nonlinear optical materials as examples The text clearly illustrates how to extract experimental electronic

structure information and relevant physicochemical properties of materials based on the theories and methods in X ray crystallography and quantum chemistry Practical skills of charge density studies using experimental X ray sources are also covered which are particularly important for the future popularization and development of electron structure crystallography This book also introduces the related theories and refinement techniques involved in using scattering methods mainly X ray single crystal diffraction as well as polarized neutron scattering and Compton scattering to determine experimental electronic structures including the experimental electron density experimental electron wavefunction and experimental electron density matrix of crystalline materials Electronic Structure Crystallography and Functional Motifs of Materials includes information on Basic framework and assumptions of the first principle calculations density matrix and density function and Hartree Fock HF and Kohn Sham KS methods Analysis of topological atoms in molecules chemical interaction analysis coarse graining and energy partition of the density matrix and restricted space partition Principles of electronic structure measurement including thermal vibration analysis scattering experiments and refinement algorithm for experimental electronic structure Independent atom model multipole model X ray constrained wavefunction model and other electron density models Electronic Structure Crystallography and Functional Motifs of Materials is an ideal textbook or reference book for graduate students and researchers in chemistry physics and material sciences for studying the structures and properties of functional crystalline materials *Electronic Structure and Electronic Transitions in Layered Materials* V Grasso,1986-06-30 Electronic Structure Methods for Complex Materials Wai-Yim Ching,Paul Rulis,2012-05-17 This book details the application of the OLCAO method for calculating the properties of solids from fundamental principles to a wide array of material systems The method specializes in large and complex models and is able to compute a variety of useful properties including electronic optical and spectroscopic properties *Electronic Structure of Strongly Correlated Materials* Vladimir Anisimov,Yuri Izyumov,2010-07-23 Electronic structure and physical properties of strongly correlated materials containing elements with partially filled 3d 4d 4f and 5f electronic shells is analyzed by Dynamical Mean Field Theory DMFT DMFT is the most universal and effective tool used for the theoretical investigation of electronic states with strong correlation effects In the present book the basics of the method are given and its application to various material classes is shown The book is aimed at a broad readership theoretical physicists and experimentalists studying strongly correlated systems It also serves as a handbook for students and all those who want to be acquainted with fast developing filed of condensed matter physics **Special Issue: Electronic Structure of Materials** Mireille Defranceschi,2000

**Electronic Structure** Richard M. Martin,2004-04-08 The study of the electronic structure of materials is at a momentous stage with the emergence of computational methods and theoretical approaches Many properties of materials can now be determined directly from the fundamental equations for the electrons providing insights into critical problems in physics chemistry and materials science This book provides a unified exposition of the basic theory and methods of electronic

structure together with instructive examples of practical computational methods and real world applications Appropriate for both graduate students and practising scientists this book describes the approach most widely used today density functional theory with emphasis upon understanding the ideas practical methods and limitations Many references are provided to original papers pertinent reviews and widely available books Included in each chapter is a short list of the most relevant references and a set of exercises that reveal salient points and challenge the reader

Electronic Structure and Properties Frank Y. Fradin, 2013-10-22 Treatise on Materials Science and Technology Volume 21 Electronic Structure and Properties covers the developments in electron theory and electron spectroscopies The book discusses the electronic structure of perfect and defective solids the photoelectron spectroscopy as an electronic structure probe and the electron phonon interaction The text describes the elastic properties of transition metals the electrical resistivity of metals as well as the electronic structure of point defects in metals Metallurgists materials scientists materials engineers and students involved in the related fields will find the book useful

*Electronic Structure of Strongly Correlated Materials* Vladimir Anisimov, Yuri Izyumov, 2010 Electronic structure and physical properties of strongly correlated materials containing elements with partially filled 3d 4d 4f and 5f electronic shells is analyzed by Dynamical Mean Field Theory DMFT DMFT is the most universal and effective tool used for the theoretical investigation of electronic states with strong correlation effects In the present book the basics of the method are given and its application to various material classes is shown The book is aimed at a broad readership theoretical physicists and experimentalists studying strongly correlated systems It also serves as a handbook for students and all those who want to be acquainted with fast developing field of condensed matter physics

Electronic Structure of Rare-Earth Nickelates from First-Principles Harrison LaBollita, 2024-09-26 This thesis demonstrates the value of theoretical approaches in the discovery of new superconducting materials It reports a detailed study of the recently discovered nickel oxide nickelate superconductors using multiple first principles computational tools from density functional theory to dynamical mean field theory In the context of superconductivity discoveries have generally been linked to serendipitous experimental discovery this thesis reports some of the few examples of predictions of new superconductors that have later been realized in practice a prime example of the significance of the methodology it expounds Overall it represents a seminal systematic work in the electronic structure theory of the emergent field of nickelate superconductivity

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