1. Record Nr. UNINA9911019789603321

Autore	Guo Guo-Cong
Titolo	Electronic Structure Crystallography and Functional Motifs of Materials
Pubbl/distr/stampa	Newark : , : John Wiley & Sons, Incorporated, , 2024 ©2024
ISBN	9783527842339 3527842330 9783527842315 3527842314
Edizione	[1st ed.]
Descrizione fisica	1 online resource (243 pages)
Altri autori (Persone)	JiangXiao-Ming
Disciplina	548.85
Soggetti	Electronic structure Materials science
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di contenuto	Cover -- Title Page -- Copyright -- Contents -- About the Authors -- Foreword 1 -- Foreword 2 -- Preface -- Abbreviations -- Introduction -- Chapter 1 Overview of Electronic Structure Crystallography -- 1.1 Introduction -- 1.1.1 History of Electronic Structure Crystallography -- 1.1.2 The Beginnings of Xray Crystallography and Quantum Mechanics -- 1.1.3 The Nascent Period of Experimental Electronic Structure Research -- 1.1.4 Developments of Pseudoatom Models -- 1.1.5 Developments of Experimental Electrondensity Matrix Models -- 1.1.6 Developments of Experimental Electron Wavefunction Models -- 1.1.7 Developments in Electron DiffractionBased Studies of Electronic Structures -- 1.2 Basic Descriptors of Electronic Structure -- 1.2.1 Electron Density -- 1.2.2 Residual Density -- 1.2.3 Deformation Density -- 1.2.4 Electron Wavefunction and Density Matrix -- 1.3 Experimental Characterization of Electronic Structure -- 1.3.1 Experimental Electronic Structure Measurement with Xray Singlecrystal Diffractometer -- 1.3.1.1 Xray Source -- 1.3.1.2 Goniometer -- 1.3.1.3 Xray Detector -- 1.3.1.4 Cryogenic Systems -- 1.3.2 Key Aspects of Experimental Electronic Structure Measurement -- 1.3.2.1 Singlecrystal Samples -- 1.3.2.2 Measurement Process -- 1.3.2.3 Data

Correction -- 1.3.2.4 Examination of the Quality of Electronic Structure Refinement -- References -- Chapter 2 FirstPrinciples Calculations of the Electron Density Functions -- 2.1 Introduction -- 2.2 Basic Framework and Assumptions of the FirstPrinciples Calculations -- 2.3 Density Matrix and Density Function -- 2.3.1 Basic Definition -- 2.3.2 Electron Density -- 2.3.3 Momentum Density -- 2.4 Hartree-Fock (HF) and Kohn-Sham (KS) Methods -- 2.4.1 Basic Theoretical Framework -- 2.4.2 Periodic Solutions of Hartree-Fock (HF) and Kohn-Sham (KS) Equations.
2.4.3 Calculation of Crystal Density Matrix and Density Function -- 2.4.4 Pseudopotentials -- 2.4.5 Basis Set -- References -- Chapter 3 Topological Indices and Properties of Electronic Structures -- 3.1 Introduction -- 3.2 Analysis of Topological Atoms in Molecules -- 3.2.1 Topological Description of the Electron Density -- 3.2.2 Gradient Vector Field and Topological Atoms -- 3.2.3 Bond Path and Molecular Topological Graph -- 3.2.4 Laplacian -- 3.2.5 Topological Properties of Chemical Bonds -- 3.2.5.1 Electron Density at Bond Critical Points -- 3.2.5.2 Bond Radius and Bond Path Length -- 3.2.5.3 Laplacian of Electron Density at the Bond Critical Points -- 3.2.5.4 Ellipticity -- 3.2.5.5 Energy Density of Bond Critical Points -- 3.2.5.6 Delocalization Index and Bond Order -- 3.2.6 Topological Atomic Properties -- 3.2.6.1 Atomic Charges -- 3.2.6.2 Atomic Volume -- 3.2.6.3 Atomic Kinetic Energy -- 3.2.6.4 Laplacian -- 3.2.6.5 Total Atomic Energy -- 3.2.6.6 Atomic Dipole Moment -- 3.2.6.7 Atomic Quadrupole Moment -- 3.2.6.8 Atomic Information Entropy -- 3.3 Chemical Interaction Analysis -- 3.3.1 Source Function -- 3.3.2 Electron Localization Function -- 3.3.3 Reduced Density Gradient -- 3.4 Coarse Graining and Energy Partition of the Density Matrix -- 3.4.1 Partition of the Density Matrix in Real Space -- 3.4.2 Energy Partition -- 3.4.3 Electron Population Statistics -- 3.5 Restricted Space Partition -- 3.5.1 Restricted Partition -- 3.5.2 Restricted Electron Population Analysis -- 3.5.3 Quasicontinuous Distribution -- 3.5.4 Electron Localization Indicators (ELI) -- 3.5.4.1 Samespin Electron Pairs -- 3.5.4.2 Singlet and Triplet Electron Pairs -- 3.5.4.3 ELI in Momentum Space -- 3.6 Intermolecular Interaction Energy -- 3.6.1 Interaction Energy of Experimental Electron Density -- 3.6.2 Pseudoatomic Representation of Electrostatic Interactions.
3.6.2.1 Multipole Expansion Approximation -- 3.6.2.2 Exact Potential and Multipole Moment (EPMM) Model -- 3.6.2.3 Promolecular Approximation -- 3.6.3 Nonelectrostatic Interactions -- 3.6.4 Lattice Energy -- 3.6.5 Interaction Energies Obtained from Experimental Charge Analysis -- References -- Chapter 4 Principles of Electronic Structure Measurement -- 4.1 Introduction -- 4.2 Thermal Vibration Analysis -- 4.2.1 Lattice Dynamics -- 4.2.2 Atomic Displacement Parameters -- 4.2.3 Rigid Fragment Analysis -- 4.2.4 Neutron Diffractionassisted Analysis -- 4.2.4.1 Temperature -- 4.2.4.2 Absorption -- 4.2.4.3 Extinction -- 4.2.4.4 Thermal Diffuse Scattering -- 4.2.4.5 Multiple Scattering -- 4.3 Scattering Experiments -- 4.3.1 X ray Diffraction -- 4.3.2 Polarized Neutron Diffraction -- 4.3.3 Compton Scattering -- 4.4 Refinement Algorithm for Experimental Electronic Structure -- 4.4.1 Leastsquare Method -- 4.4.1.1 Mathematical -- 4.4.1.2 Leastsquare Refinement of Structure Factors -- 4.4.1.3 Parameterestimated variance and covariance -- 4.4.2 Maximum Entropy Method -- References -- Chapter 5 Pseudoatom Models -- 5.1 Introduction -- 5.2 Independent Atom Model -- 5.3 Kappa Model -- 5.4 Multipole Model -- 5.4.1 Multipole Spherical Harmonics -- 5.4.2 Real Spherical Harmonic Density Function -- 5.4.3 Radial Distribution Functions -- 5.4.4 Multipole Model Framework -- 5.4.5 Aspheric

Atomic Scattering Factors -- 5.4.6 Multipolar Model of Core Electron Expansion -- 5.5 Spin Density Model -- 5.5.1 Pure Spin Contribution -- 5.5.1.1 Atomic Orbital Model of Spin Density -- 5.5.1.2 Multipole Refinement of Spin Density -- 5.5.2 Spin and Orbital Contributions -- 5.5.3 Noncollinear Magnetism -- 5.5.4 Combinatorial Refinement of Electron Density and Spin Density -- 5.6 Other Electron Density Models -- 5.6.1 The Xray Atomic Orbital (XAO) Model.
5.6.1.1 Atomic Singleelectron Orbitals in a Crystal Field -- 5.6.1.2 Electron Density and Structure Factor -- 5.6.2 Xray Molecular Orbital Model (XMO) -- 5.6.2.1 Molecular Orbital and Electron Density -- 5.6.2.2 Structure Factors for Monocentric and Bicentric Terms -- 5.6.2.3 Processing of Temperature Factors -- 5.6.3 Molecular Orbitals with Variable Occupation Numbers Model (MOON) -- References -- Chapter 6 Density Matrix Model -- 6.1 Introduction -- 6.2 Density Matrix Model -- 6.2.1 Definition of the Density Matrix -- 6.2.2 Localized Model of the Density Matrix -- 6.3 Correlation of Density Matrix to Scattering Experiments -- 6.3.1 Dynamic Scattering Factor -- 6.3.2 Static Structure Factor -- 6.3.3 Elastic Scattering -- 6.3.4 Inelastic Scattering -- 6.4 Reconstruction and Refinement of the Density Matrix -- 6.4.1 Bayesian Method -- 6.4.2 Combined Refinement of Different Types of Data -- 6.4.3 Refinement of the One electron Reduced Density Matrix (1RDM) -- 6.4.4 Combinatorial Refinement of Structure Factor and Compton Profile Data -- 6.4.5 Spin resolved Oneorder Reduced Density Matrix (1SRDM) Refinement -- 6.4.5.1 Basic Framework -- 6.4.5.2 Molecular Modeling -- 6.4.5.3 Magnetic Structure Factor and Magnetic Compton Profile -- 6.4.5.4 Variation of the Basis Functions -- 6.4.5.5 Variation of Spin Population Matrices -- References -- Chapter 7 Electron Wavefunction Models -- 7.1 Introduction -- 7.2 Xray Constrained Wavefunction (XCW) Model -- 7.2.1 Mathematical Framework -- 7.2.2 Hirshfeld Atom Refinement -- 7.2.2.1 Selection of Wavefunction -- 7.2.2.2 Electron Density -- 7.2.2.3 Hirshfeld Atomic Partitioning Method -- 7.2.2.4 Calculation of the Structure Factor -- 7.2.3 Xray Constrained Wavefunction Refinement -- 7.2.3.1 Special Treatment for Thermal Vibrations -- 7.2.3.2 Density Matrix Representation of Structure Factor.
7.2.3.3 Experimental Constrained Wavefunction Refinement -- 7.2.4 Open Shell System Method -- 7.2.5 Treatment of Relativistic Effects -- 7.3 The XrayConstrained Extremely Localized Molecular Orbital Method -- 7.3.1 Theoretical Extremely Localized Molecular Orbitals -- 7.3.2 Refinement of the Experimentally Constrained Extremely Localized Molecular Orbitals -- References -- Chapter 8 Functional Electronic Structures and Functional Motif of Materials -- 8.1 Introduction -- 8.2 Material Functional Motif -- 8.2.1 Crystal Structure -- 8.2.2 Electronic Structure -- 8.2.3 Magnetic Structure -- 8.2.4 Modulated Defects -- 8.2.5 Statistical Defects -- 8.2.6 Local Defects -- 8.3 Functional Electronic Structures -- References -- Index -- EULA.

Sommario/riassunto

This book focuses on the electronic structure and functional motifs of materials, exploring both theoretical and experimental approaches in material science and chemistry. It covers the basic theory, experimental techniques, and refining models used to characterize the electronic structure of materials. The book emphasizes the role of X-ray diffraction and scattering methods in understanding material atomic arrangements. It aims to provide a comprehensive understanding of the electronic structure, essential for the development of novel materials. The authors, Prof. Guo-Cong Guo and Prof. Xiao-Ming Jiang, contribute their expertise in structural chemistry and material science. This book is intended for researchers and professionals in the fields of chemistry and material science.