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| Nota di bibliografia | Includes bibliographical references at the end of each chapters and index. |
| Nota di contenuto | Solid-State Photoemission and Related Methods; Preface; In Memoriam Lars Hedin (1930-2002); Contents; List of contributors; 1 Electronic structure theory for ground and excited state properties of materials; 1.1 Introduction; 1.2 Density functional theory and the FLAPW method; 1.2.1 Introduction; 1.2.2 Density-functional theory; 1.2.3 The FLAPW basis-set; 1.3 Electronic structure theory for excited states; 1.3.1 Band gaps and derivative discontinuities; 1.3.2 Band gaps and nonlocal potentials; 1.3.3 Quasiparticle calculations; 1.3.4 Density functional theory using non-local functionals<br>1.4 Application to semiconductor materials1.4.1 Bulk semiconductor materials; 1.4.2 Semiconductor/semiconductor interfaces; 1.4.3 Semiconductor/metal interfaces; 1.5 Applications of the first-principles FLAPW approach to studies of magnetism; 1.5.1 Magnetism; 1.5.2 Magneto-crystalline anisotropy in thin films; 1.5.3 Higher-order magneto-crystalline anisotropy; 1.5.4 Magnetostriction; 1.5.5 Magneto-optical effects; 1.5.6 Magnetic circular dichroism; References; |

2 Overview of core and valence photoemission; 2.1 Introduction; 2.2 Green function methods
2.2.1 Photoemission and the many-body problem2.2.2 Green functions and one-particle Schrodinger equation; 2.2.3 Elementary excitations in systems of interacting particles; 2.2.4 The self-energy; 2.2.5 Independent particle states and related methods; 2.2.6 Perturbation expansion; 2.2.7 Diagrams in many-body systems; 2.2.8 Spectral representation; 2.2.9 Photocurrent; 2.3 Three-stepmodel versusone-stepmodel; 2.4 Golden Rule; 2.4.1 Linear response in the external field; 2.4.2 Dipole approximation; 2.5 Initial state; 2.5.1 Core levels; 2.5.2 Valence bands; 2.6 Final state
2.6.1 Direct solution of Schrodinger equation2.6.2 Multiple scattering method; 2.7 Matrix elements: coreversusvalence levels; 2.8 Optical effects; 2.8.1 Resonant photoemission; 2.8.2 Photoemission by surface optical response fields; 2.9 Spin effects; 2.10 Computer codes for photoelectron diffraction and spectroscopy; References; 3 General theory of core electron photoemission; 3.1 Introduction; 3.2 Theory; 3.2.1 General considerations; 3.2.2 A model Hamiltonian with a priori determined parameters; 3.2.3 Extrinsic and intrinsic losses in core electron photoemission
3.2.4 Charge transfer and shake-down satellites3.2.5 Resonant photoemission; 3.2.6 Phonons and temperature effects; 3.3 Concluding remarks; References; 4 Valence band VUV spectra; 4.1 Introduction; 4.2 Electrons at crystal surfaces; 4.2.1 One-electronapproach; 4.2.2 Many-electronapproach; 4.3 Photoelectron spectroscopy; 4.3.1 Band mapping (peak positions); 4.3.2 Electron and hole lifetimes (peak widths); 4.3.3 Orbital orientation (peak intensities); 4.3.4 EDC spectra (profiles); 4.4 Summary; References
5 Angle-resolved photoelectron spectroscopy: From photoemission imaging to spatial resolution

Sommario/riassunto

Photoemission is one of the principal techniques for the characterization and investigation of condensed matter systems. The field has experienced many developments in recent years, which may also be put down to important achievements in closely related areas. This timely and up-to-date handbook is written by experts in the field who provide the background needed by both experimentalists and theorists. It represents an interesting framework for showing the connection between theory and experiment by bringing together different concepts in the investigation of the properties of materials. <br

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| Titolo | Modeling solvent environments : applications to simulations of biomolecules / / edited by Michael Feig |
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| ISBN | 9786612472329<br>9781282472327<br>1282472321<br>9783527629251<br>3527629254<br>9783527629268<br>3527629262 |
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| Altri autori (Persone) | FeigMichael |
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| Nota di contenuto | Modeling Solvent Environments: Applications to Simulations of Biomolecules; Contents; Preface; List of Contributors; 1: Biomolecular Solvation in Theory and Experiment; 1.1 Introduction; 1.2 Theoretical Views of Solvation; 1.2.1 Equilibrium Thermodynamics of Solvation; 1.2.2 Radial Distribution Functions; 1.2.3 Integral Equation Formalisms; 1.2.4 Kirkwood-Buff Theory; 1.2.5 Kinetic Effects of Solvation; 1.3 Computer Simulation Methods in the Study of Solvation; 1.3.1 Molecular Dynamics and Monte Carlo Simulations; 1.3.2 Water Models; 1.3.3 Solvent Structure and Dynamics from Simulations<br>1.3.4 Free Energy Simulations1.4 Experimental Methods in the Study of Solvation; 1.4.1 X-Ray/Neutron Diffraction and Scattering; 1.4.2 Nuclear Magnetic Relaxation; 1.4.3 Optical Spectroscopy; 1.4.4 Dielectric Dispersion; 1.5 Hydration of Proteins; 1.5.1 Protein Folding and Peptide Conformations in Aqueous Solvent; 1.5.2 Molecular Properties of Water Near Protein Surfaces; 1.5.3 Water Molecules at Protein-Ligand and Protein-Protein Interfaces; 1.6 Hydration of Nucleic |

acids; 1.7 Non-Aqueous Solvation; 1.7.1 Alcohols; 1.7.2 Urea; 1.7.3 Glycerol; 1.8 Summary; References
2: Model-Free "Solvent Modeling" in Chemistry and Biochemistry Based on the Statistical Mechanics of Liquids2.1 Introduction; 2.2 Outline of the RISM and 3D-RISM theories; 2.3 Partial Molar Volume of Proteins; 2.4 Detecting Water Molecules Trapped Inside Protein; 2.5 Selective Ion Binding by Protein; 2.6 Water Molecules Identified as a Substrate for Enzymatic Hydrolysis of Cellulose; 2.7 CO Escape Pathway in Myoglobin; 2.7.1 Effect of Protein Structure on the Distribution of Xe; 2.7.2 Partial Molar Volume Change Through the CO Escape Pathway of Myoglobin; 2.8 Perspective; References
3: Developing Force Fields From the Microscopic Structure of Solutions: The Kirkwood-Buff Approach3.1 Introduction; 3.2 Biomolecular Force Fields; 3.3 Examples of Problems with Current Force Fields; 3.4 Kirkwood-Buff Theory; 3.5 Applications of Kirkwood-Buff Theory; 3.6 The General KBFF Approach; 3.7 Technical Aspects of the KBFF Approach; 3.8 Results for Urea and Water Binary Solutions; 3.9 Preferential Interactions of Urea; 3.10 Conclusions and Future Directions; Acknowledgments; References; 4: Osmolyte Influence on Protein Stability: Perspectives of Theory and Experiment; 4.1 Introduction
4.2 Denaturing Osmolytes4.2.1 Does Urea Weaken Water Structure?; 4.2.2 Effect of Urea on Hydrophobic Interactions; 4.2.3 Direct Interaction of Urea with Proteins; 4.3 Protecting Osmolytes; 4.3.1 Do Protecting Osmolytes Increase Water Structure?; 4.3.2 Effect of Protecting Osmolytes on Hydrophobic Interactions; 4.4 Mixed Osmolytes; 4.5 Conclusions; Acknowledgments; References; 5: Modeling Aqueous Solvent Effects through Local Properties of Water; 5.1 The Role of Water and Cosolutes on Macromolecular Thermodynamics; 5.2 Forces Induced by Water in Aqueous Solutions 5.2.1 Interactions in Water-Accessible Regions of Proteins

Sommario/riassunto

A comprehensive view of the current methods for modeling solvent environments with contributions from the leading researchers in the field. Throughout, the emphasis is placed on the application of such models in simulation studies of biological processes, although the coverage is sufficiently broad to extend to other systems as well. As such, this monograph treats a full range of topics, from statistical mechanics-based approaches to popular mean field formalisms, coarse-grained solvent models, more established explicit, fully atomic solvent models, and recent advances in applying ab initio me