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Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references at the end of each chapters and index.
Nota di contenuto	Title Page; Copyright Page; Contents; Contributors; Preface; Chapter 1 Relativistic Configuration Interaction Calculations for Lanthanide and Actinide Anions; 1.1 Introduction; 1.2 Bound Rare Earth Anion States; 1.3 Lanthanide and Actinide Anion Survey; 1.3.1 Prior Results and Motivation for the Survey; 1.3.2 Techniques for Basis Set Construction and Analysis; 1.3.3 Discussion of Results; 1.4 Resonance and Photodetachment Cross Section of Anions; 1.4.1 The Configuration Interaction in the Continuum Formalism; 1.4.2 Calculation of the Final State Wavefunctions; Acknowledgments; References Chapter 2 Study of Actinides by Relativistic Coupled Cluster Methods2. 1 Introduction; 2.2 Methodology; 2.2.1 The Relativistic Hamiltonian; 2.2.2 Fock-Space Coupled Cluster Approach; 2.2.3 The Intermediate Hamiltonian CC method; 2.3 Applications to Actinides; 2.3.1 Actinium and Its Homologues: Interplay of Relativity and Correlation; 2.3.2 Thorium and Eka-thorium: Different Level Structure; 2.3.3 Rn-like actinide ions; 2.3.4 Electronic Spectrum of Superheavy Elements

Nobelium (Z=102) and Lawrencium (Z=103); 2.3.5 The Levels of U4+ and U5+: Dynamic Correlation and Breit Interaction
2.3.6 Relativistic Coupled Cluster Approach to Actinide Molecules2.4 Summary and Conclusion; References; Chapter 3 Relativistic All-Electron Approaches to the Study of f Element Chemistry; 3.1 Introduction; 3.2 Relativistic Hamiltonians; 3.2.1 General Aspects; 3.2.2 Four-Component Hamiltonians; 3.2.3 Two-Component Hamiltonians; 3.2.4 Numerical Example; 3.3 Choice of Basis Sets; 3.4 Electronic Structure Methods; 3.4.1 Coupled Cluster Approaches; 3.4.2 Multi-Reference Perturbation Theory; 3.4.3 (Time-Dependent) Density Functional Theory; 3.5 Conclusions and Outlook; Acknowledgments; References
Chapter 4 Low-Lying Excited States of Lanthanide Diatomics Studied by Four-Component Relativistic Configuration Interaction Methods4.1 Introduction; 4.2 Method of Calculation; 4.2.1 Quaternion Symmetry; 4.2.2 Basis Set and HFR/DC Method; 4.2.3 GOSCI and RASCI Methods; 4.3 Ground State; 4.3.1 CeO Ground State; 4.3.2 CeF Ground State; 4.3.3 Discussion of Bonding in CeO and CeF; 4.3.4 GdF Ground State; 4.3.5 Summary of the Chemical Bonds, of CeO, CeF, GdF; 4.4 Excited States; 4.4.1 CeO Excited States; 4.4.2 CeF Excited States; 4.4.3 GdF Excited States; 4.5 Conclusion; References
Chapter 5 The Complete-Active-Space Self-Consistent-Field Approach and Its Application to Molecular Complexes of the f-Elements5.1 Introduction; 5.1.1 Treatment of Relativistic Effects; 5.1.2 Basis Sets; 5.2 Identifying and Incorporating Electron Correlation; 5.2.1 The Hartree Product Wavefunction; 5.2.2 Slater Determinants and Fermi Correlation; 5.2.3 Coulomb Correlation; 5.3 Configuration Interaction and the Multiconfigurational Wavefunction; 5.3.1 The Configuration Interaction Approach; 5.3.2 CI and the Dissociation of H2; 5.3.3 Static Correlation and Crystal Field Splitting
5.3.4 Size Inconsistency and Coupled Cluster Theory

Sommario/riassunto

The f-elements and their compounds often possess an unusually complex electronic structure, governed by the high number of electronic states arising from open f-shells as well as large relativistic and electron correlation effects. A correct theoretical description of these elements poses the highest challenges to theory. Computational Methods in Lanthanide and Actinide Chemistry summarizes state-of-the-art electronic structure methods applicable for quantum chemical calculations of lanthanide and actinide systems and presents a broad overview of their most recent applications to

2. Record Nr. UNISA996390982103316

Autore	Alured Thomas
Titolo	The coppie of a letter vvritten to the Duke of Buckingham concerning the match with Spaine [[electronic resource]] : discovering what dangers would happen to this state by the Kings marrying with one of a contrary religion shewed by divers presidents
Pubbl/distr/stampa	Printed at London, : for George Tomlinson, 1642
Descrizione fisica	8 p
Soggetti	Great Britain Kings and rulers Early works to 1800
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Signed at end: Thomas Alured. Annotation on Thomason copy: "Septemb 2d". Reproduction of the original in the British Library.
Sommario/riassunto	eebo-0018