Record Nr. UNINA9910678279103321 Computational methods in lanthanide and actinide chemistry / / edited **Titolo** by Michael Dolg; contributors, Raymond Atta-Fynn [and forty others] Pubbl/distr/stampa Chichester, England:,: Wiley,, 2015 ©2015 **ISBN** 1-118-68828-7 1-118-68830-9 1-118-68829-5 Descrizione fisica 1 online resource (495 p.) Disciplina 546.41 Soggetti Rare earth metals Actinide elements Chemistry, Inorganic Lingua di pubblicazione Inglese **Formato** Materiale a stampa Livello bibliografico Monografia Description based upon print version of record. Note generali Includes bibliographical references at the end of each chapters and Nota di bibliografia index. Title Page; Copyright Page; Contents; Contributors; Preface; Chapter 1 Nota di contenuto 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+

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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

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