



# Computational Methods in Lanthanide and Actinide Chemistry

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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 atoms, molecules and solids. The book contains sixteen chapters, written by leading experts in method development as well as in theoretical investigations of f-element systems.

Topics covered include:

- Relativistic configuration interaction calculations for lanthanide and actinide anions
- Study of actinides by relativistic coupled cluster methods
- Relativistic all-electron approaches to the study of f- element chemistry
- Relativistic pseudopotentials and their applications
- Gaussian basis sets for lanthanide and actinide elements
- Applied computational actinide chemistry

This book will serve as a comprehensive reference work for quantum chemists and computational chemists, both those already working in, and those planning to enter the field of quantum chemistry for f-elements. Experimentalists will also find important information concerning the capabilities of modern quantum chemical methods to assist in the interpretation or even to predict the outcome of their experiments.

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