1. Record Nr. UNINA9910453539303321

Titolo	Recent advances in relativistic molecular theory [[electronic resource] /] / edited by Kimihiko Hirao, Yasuyuki Ishikawa
Pubbl/distr/stampa	River Edge, N.J. ; ; London, : World Scientific, c2004
ISBN	981-279-490-5
Descrizione fisica	1 online resource (343 p.)
Collana	Recent advances in computational chemistry ; ; v. 5
Altri autori (Persone)	HiraoK (Kimihiko) IshikawaYasuyuki
Disciplina	540
Soggetti	Molecular theory Electronic books.
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.
Nota di contenuto	AUTHOR LIST; PREFACE; CONTENTS; THE RELATIVISTIC ENERGY-CONSISTENT AB INITIO PSEUDOPOTENTIAL APPROACH AND ITS APPLICATIONTO LANTHANIDE AND ACTINIDE COMPOUNDS; 1. Introduction; 2. Energy-consistent ab initio Pseudopotentials; 2.1. Valence-only Model Hamiltonian; 2.2. Choice of the Pseudopotential Core; 2.3. Energy Adjustment; 2.4. Valence Basis Sets; 3. Calibration Studies; 3.1. Atoms; 3.2. Molecules; 4. Selected Applications; 5. Conclusions and Outlook; Acknowledgments; References; RECENT DEVELOPMENTS OF RELATIVISTIC MODEL COREPOTENTIAL METHOD; 1. Introduction 2. Model Core Potential (MCP) Method3. MCPs for Lanthanides; 3.1. Ionized states of atoms; 3.2. Applications to the ground state of CeO; 3.3. Application to low-lying states of GdO; 4. Relativistic Correlating Basis Functions; 4.1. Atomic correlating functions; 4.2. Atomic applications; 4.3. Molecular applications; 5. Concluding Remarks; Acknowledgments; References; SPIN-ORBIT MULTIREFERENCE CONFIGURATION INTERACTION METHOD AND APPLICATIONS TO SYSTEMS CONTAINING HEAVY ATOMS; 1. Introduction; 2. Spin-Orbit Operator and Use of the Wigner-EckartTheorem; 3. Spin-Orbit CI Methods 3.1. Calculation of Energies and Wave Functions3.2. Transition Moment Calculations; 4. Applications of SO-CI Methods; 5. Summary and

Outlook; Acknowledgments; References; Appendix; SPIN ORBIT COUPLING METHODS AND APPLICATIONS TO CHEMISTRY; I. Introduction; II. Theory and Methods; 1. general remarks; 2. electron correlation and SOC; III. Applications; 1. Hydrides of transition metals; 2. SOC in light diatomic molecules; 3. SOC in U and UF; 4. SOC in polyatomic molecules; Summary; Acknowledgements; References; TRANSGRESSING THEORY BOUNDARIES: THE GENERALIZED DOUGLAS-KROLL TRANSFORMATION
1. Introduction2. Two-component relativistic quantum chemistry; 2.1. Basic properties of Dirac 4-spinors; 2.2. Elimination techniques; 2.3. Transformation techniques; 3. The generalized Douglas-Kroll transformation; 3.1. General parametrization of unitary transformations; 3.2. Derivation of the standard Douglas-Kroll Hamiltonians; 3.3. DK transformation of the two-electron terms; 3.4. Implementation of the DK transformation; 4. Results; 4.1. One-electron systems; 4.2. Many-electron atoms; 5. Conclusion; References GENERALIZED-UHF THEORY FOR MAGNETIC PROPERTIES WITH QUASI-RELATIVISTIC HAMELTONIANS1. Introduction; 2. Magnetic shielding constant with spin-orbit interaction; 2.1. Hamiltonian and operators; 2.2. SO-UHF method; 2.3. SO-GUHFmethod; 3. Relation between quasi-relativistic theory and GUHF theory; 3.1. Orbital space for the general two-component Hamiltonian; 3.2. Quasi-relativistic GUHF method; 4. Computational aspects; 4.1. Basis sets; 4.2. Gauge-origin problem; 5. Results; 5.1. SO-UHF results; 5.2. SO-GUHF results; 5.3. Magnetic shielding constants of heavy elements: noble gases
5.4. Mercury-199 NMR

Sommario/riassunto

Relativistic effects, though minor in light atoms, increase rapidly in magnitude as the atomic number increases. For heavy atom species, it becomes necessary to discard the Schrodinger equation in favor of the Dirac equation. Construction of an effective many-body Hamiltonian that accurately accounts for both relativistic and electron correlation effects in many-electron systems is a challenge. It is only in the past 20-25 years that relativistic quantum chemistry has emerged as a field of research in its own right, and it seems certain that relativistic many-electron calculations of molecular