1. Record Nr. UNINA9910827419903321

Titolo	Reviews in computational chemistry . Volume 26 [[electronic resource] /] / edited by Kenneth B. Lipkowitz, Thomas R. Cundari, Donald B. Boyd
Pubbl/distr/stampa	Chichester, : Wiley, 2009
ISBN	1-282-00372-0 9786612003721 0-470-39954-6 0-470-39953-8
Edizione	[2nd ed.]
Descrizione fisica	1 online resource (570 p.)
Collana	Reviews in computational chemistry ; ; 26
Altri autori (Persone)	BoydDonald B LipkowitzKenny B CundariThomas R. <1964->
Disciplina	542.85 542/.8
Soggetti	Chemistry - Data processing Chemistry - Mathematics
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di contenuto	Reviews in Computational Chemistry Volume 26; Preface; Contents; Contributors; Contributors to Previous Volumes; 1. Computations of Noncovalent Interactions; Introduction; Challenges for Computing Interactions; Electron Correlation Problem; Basis Set Problem; Basis Set Superposition Errors and the Counterpoise Correction; Additive Basis/Correlation Approximations; Reducing Computational Cost; Truncated Basis Sets; Pauling Points; Resolution of the Identity and Local Correlation Approximations; Spin-Component-Scaled MP2; Explicitly Correlated R12 and F12 Methods Density Functional ApproachesSemiempirical Methods and Molecular Mechanics; Analysis Using Symmetry-Adapted Perturbation Theory; Concluding Remarks; Appendix: Extracting Energy Components from the SAPT2006 Program; Acknowledgments; References; 2. Reliable Electronic Structure Computations for Weak Noncovalent Interactions in Clusters; Introduction and Scope; Clusters and Weak Noncovalent Interactions; Computational Methods; Weak Noncovalent Interactions;

Historical Perspective; Some Notes about Terminology; Fundamental Concepts: A Tutorial; Model Systems and Theoretical Methods
Rigid Monomer ApproximationSupermolecular Dissociation and Interaction Energies; Counterpoise Corrections for Basis Set Superposition Error; Two-Body Approximation and Cooperative/Nonadditive Effects; Size Consistency and Extensivity of the Energy; Summary of Steps in Tutorial; High-Accuracy Computational Strategies; Primer on Electron Correlation; Primer on Atomic Orbital Basis Sets; Scaling Problem; Estimating E(int) at the CCSD(T) CBS Limit: Another Tutorial; Accurate Potential Energy Surfaces; Less Demanding Computational Strategies; Second-Order Møller-Plesset Perturbation Theory
Density Functional TheoryGuidelines; Other Computational Issues; Basis Set Superposition Error and Counterpoise Corrections; Beyond Interaction Energies: Geometries and Vibrational Frequencies; Concluding Remarks; Acknowledgments; References; 3. Excited States from Time-Dependent Density Functional Theory; Introduction; Overview; Ground-State Review; Formalism; Approximate Functionals; Basis Sets; Time-Dependent Theory; Runge-Gross Theorem; Kohn-Sham Equations; Linear Response; Approximations; Implementation and Basis Sets; Density Matrix Approach; Basis Sets; Convergence for Naphthalene
Double-Zeta Basis SetsPolarization Functions; Triple-Zeta Basis Sets; Diffuse Functions; Resolution of the Identity; Summary; Performance; Example: Naphthalene Results; Influence of the Ground-State Potential; Analyzing the Influence of the XC Kernel; Errors in Potential vs. Kernel; Understanding Linear Response TDDFT; Atoms as a Test Case; Quantum Defect; Testing TDDFT; Saving Standard Functionals; Electron Scattering; Beyond Standard Functionals; Double Excitations; Polymers; Solids; Charge Transfer; Other Topics; Ground-State XC Energy; Strong Fields; Electron Transport; Summary
Acknowledgments

Sommario/riassunto

Computational chemistry is increasingly used in conjunction with organic, inorganic, medicinal, biological, physical, and analytical chemistry, biotechnology, materials science, and chemical physics. This series is essential in keeping those individuals involved in these fields abreast of recent developments in computational chemistry.