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Basis Set Superposition Errors: Theory and PracticeIntroduction; Origin and Magnitude of BSSE; Magnitude of Error; Attempts at an Exact Theory; Counterpoise Correction Method; Energy Decomposition; Evaluation of Polarization and Charge Transfer Terms; Increased Functional Space; Localized Orbital Approach; Many-Body Perturbation Theory Versus Symmetry-Adapted Perturbation Theory; Secondary Corrections; Bond Functions; Basis Set Recommendations; Case Studies; Geometries; Dipole Moments; Interaction Energies; BSSE Corrected Interaction Energies; Many-Body Counterpoise Correction; Summary AppendixSample Input Deck for Counterpoise Corrections Using Gaussian 92 or 94; Sample Input Deck for Counterpoise Corrections Using GAMESS; References; Quantum Monte Carlo: Atoms, Molecules, Clusters, Liquids, and Solids; Introduction; History and Overview; Variational Quantum Monte Carlo; Diffusion Quantum Monte Carlo; Green's Function Quantum Monte Carlo; Node Structure; Importance Sampling; Trial Wavefunctions; Fixed-Node Calculations; Released-Node Calculations; Exact Cancellation Method; Difference Schemes; Excited States; Use of Pseudopotentials; A Sampling of Applications Potential Energy Surface for the Reaction H + H2 -- H2 + HBinding Energies for Silicon Hydrides; CuH Spectroscopic Constants; Clusters of Argon and HF: Energies, Structures, and Vibrational Frequency Shifts; Metallic Lithium; Homogeneous Electron Gas; Hydrocarbon Energetics; Vibrational States of Formaldehyde; Approaching Liquid Water; Reaction Path Zero-Point Energy; Transition State for Cyclooctatetraene Bond Shifting; Conclusions; Acknowledgments; References; Molecular Models of Water: Derivation and Description; Introduction; Properties of Neat Water Systems; Experimental Results
Results from Quantum Chemistry

Sommario/riassunto

THIS BOOK HAS SIX TUTORIALS AND REVIEWS WRITTEN BY INVITED EXPERTS. FIVE CHAPTERS TEACH TOPICS IN QUANTUM MECHANICS AND MOLECULAR SIMULATIONS. THE SIXTH CHAPTER EXPLAINS HOW PROGRAMS FOR CHEMICAL STRUCTURE DRAWING WORK. AN EDITORIAL DISCUSSES SOME OF THE MOST WELL-KNOWN PERSONAGES IN COMPUTATIONAL CHEMISTRY.FROM REVIEWS OF THE SERIES ""Anyone who is doing or intends to do computational research on molecular structure and design should seriously consider purchasing this book for his or her personal library.""-JOURNAL OF COMPUTATIONAL CHEMISTRY.""These reviews are becoming regard