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Perturbational Decomposition of the Cluster OperatorsPerturbation Theory Energies from the Coupled Cluster Hamiltonian; The (T) Correction; Computer Implementation of Coupled Cluster Theory; Factorization of the Coupled Cluster Equations; Matrix-Based Storage of Integrals and Amplitudes; Spatial Symmetry Simplifications; Spin Factorization of the Coupled Cluster Equations; Atomic-Orbital-Basis Algorithms; Current Research and Future Directions; Coupled Cluster Theory for Open-Shell Molecules; Spin-Restricted Triple-Excitation Corrections; Brueckner Orbitals in Coupled Cluster Theory

Future Research ProspectsAcknowledgments; References; Introduction to Zeolite Modeling; Introduction; Approaches to Zeolite Modeling; Computational Approaches; Scope of Zeolite Modeling; Models; Quantum Mechanical Models; Potential Models for Framework Modeling; Hybrid Models; Methods; Structure and Periodicity; Summation of Long-Range Interactions; Energy Minimization; Method of Molecular Dynamics; Monte Carlo Methods; Car-Parrinello Approach; Some Selected Applications; Framework Dynamics; Zeolite/Template Interactions: Tetrabutylammonium and Tetrapropylammonium in MEL and MFI Structures

Isomorphic Substitution

Sommario/riassunto

THIS VOLUME, WHICH IS DESIGNED FOR STAND-ALONE USE IN TEACHING AND RESEARCH, FOCUSES ON QUANTUM CHEMISTRY, AN AREA OF SCIENCE THAT MANY CONSIDER TO BE THE CENTRAL CORE OF COMPUTATIONAL CHEMISTRY. TUTORIALS AND REVIEWS COVER* HOW TO OBTAIN SIMPLE CHEMICAL INSIGHT AND CONCEPTS FROM DENSITY FUNCTIONAL THEORY CALCULATIONS,* HOW TO MODEL PHOTOCHEMICAL REACTIONS AND EXCITED STATES, AND* HOW TO COMPUTE ENTHALPIES OF FORMATION OF MOLECULES.* A FOURTH CHAPTER TRACES CANADIAN RESEARCH IN THE EVOLUTION OF COMPUTATIONAL CHEMISTRY.* ALSO INCLUDED WITH THIS VOLUME IS A SPECIAL TRIBUTE TO