1. Record Nr. UNINA9910139627103321

Autore	Reimers Jeffrey R
Titolo	Computational Methods for Large Systems : Electronic Structure Approaches for Biotechnology and Nanotechnology
Pubbl/distr/stampa	Hoboken, : Wiley, 2011
ISBN	1-283-20364-2 9786613203649 0-470-93077-2 0-470-93076-4
Descrizione fisica	1 online resource (683 p.)
Disciplina	620.50285 620/.50285
Soggetti	Nanostructured materials - Computer simulation Nanotechnology - Data processing Biotechnology - Data processing Electronics - Materials - Computer simulation
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di contenuto	COMPUTATIONAL METHODS FOR LARGE SYSTEMS; Contents; Contributors; Preface: Choosing the Right Method for Your Problem; A DFT: THE BASIC WORKHORSE; 1 Principles of Density Functional Theory: Equilibrium and Nonequilibrium Applications; 1.1 Equilibrium Theories; 1.2 Local Approximations; 1.3 Kohn-Sham Formulation; 1.4 Why DFT Is So Successful; 1.5 Exact Properties of DFTs; 1.6 Time-Dependent DFT; 1.7 TDDFT and Transport Calculations; 1.8 Modeling Reservoirs In and Out of Equilibrium; 2 SIESTA: A Linear-Scaling Method for Density Functional Calculations; 2.1 Introduction; 2.2 Methodology 2.3 Future Perspectives3 Large-Scale Plane-Wave-Based Density Functional Theory: Formalism, Parallelization, and Applications; 3.1 Introduction; 3.2 Plane-Wave Basis Set; 3.3 Pseudopotential Plane-Wave Method; 3.4 Charged Systems; 3.5 Exact Exchange; 3.6 Wavefunction Optimization for Plane-Wave Methods; 3.7 Car-Parrinello Molecular Dynamics; 3.8 Parallelization; 3.9 AIMD Simulations of Highly Charged Ions in Solution; 3.10 Conclusions; B HIGHER-ACCURACY METHODS

4 Quantum Monte Carlo, Or, Solving the Many-Particle Schrodinger Equation Accurately While Retaining Favorable Scaling with System Size4.1 Introduction; 4.2 Variational Monte Carlo; 4.3 Wavefunctions and Their Optimization; 4.4 Diffusion Monte Carlo; 4.5 Bits and Pieces; 4.6 Applications; 4.7 Conclusions; 5 Coupled-Cluster Calculations for Large Molecular and Extended Systems; 5.1 Introduction; 5.2 Theory; 5.3 General Structure of Parallel Coupled-Cluster Codes; 5.4 Large-Scale Coupled-Cluster Calculations; 5.5 Conclusions
6 Strongly Correlated Electrons: Renormalized Band Structure Theory and Quantum Chemical Methods6.1 Introduction; 6.2 Measure of the Strength of Electron Correlations; 6.3 Renormalized Band Structure Theory; 6.4 Quantum Chemical Methods; 6.5 Conclusions; C MORE-ECONOMICAL METHODS; 7 The Energy-Based Fragmentation Approach for Ab Initio Calculations of Large Systems; 7.1 Introduction; 7.2 The Energy-Based Fragmentation Approach and Its Generalized Version; 7.3 Results and Discussion; 7.4 Conclusions; 7.5 Appendix: Illustrative Example of the GEBF Procedure
8 MNDO-like Semiempirical Molecular Orbital Theory and Its Application to Large Systems8.1 Basic Theory; 8.2 Parameterization; 8.3 Natural History or Evolution of MNDO-like Methods; 8.4 Large Systems; 9 Self-Consistent-Charge Density Functional Tight-Binding Method: An Efficient Approximation of Density Functional Theory; 9.1 Introduction; 9.2 Theory; 9.3 Performance of Standard SCC-DFTB; 9.4 Extensions of Standard SCC-DFTB; 9.5 Conclusions; 10 Introduction to Effective Low-Energy Hamiltonians in Condensed Matter Physics and Chemistry; 10.1 Brief Introduction to Second Quantization Notation 10.2 Huckel or Tight-Binding Model

Sommario/riassunto

While its results normally complement the information obtained by chemical experiments, computer computations can in some cases predict unobserved chemical phenomena Electronic-Structure Computational Methods for Large Systems gives readers a simple description of modern electronic-structure techniques. It shows what techniques are pertinent for particular problems in biotechnology and nanotechnology and provides a balanced treatment of topics that teach strengths and weaknesses, appropriate and inappropriate methods. It's a book that will enhance the your calculating confidence and improve yo