1. Record Nr. UNINA9910458625303321

Titolo	Introduction to modern methods of quantum many-body theory and their applications [[electronic resource] /] / editors, Adelchi Fabrocini, Stefano Fantoni, Eckhard Krotscheck
Pubbl/distr/stampa	River Edge, NJ, : World Scientific, c2002
ISBN	981-277-707-5
Descrizione fisica	1 online resource (428 p.)
Collana	Series on advances in quantum many-body theory ; ; v. 7
Altri autori (Persone)	FabrociniA FantoniS (Stefano) KrotscheckEckhard
Disciplina	530.14/4
Soggetti	Many-body problem Electronic books.
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Lecture notes of the second European Summer School on Microscopic Quantum Many-Body Theories and their Applications, held in Miramare, Trieste, Italy, on September 3-14, 2001.
Nota di bibliografia	Includes bibliographical references and indexes.
Nota di contenuto	CONTENTS ; PREFACE ; Chapter 1 DENSITY FUNCTIONAL THEORY ; 1. Introduction ; 1.1. Units and notation ; 1.2. Hartree-Fock theory ; 1.3. Homogeneous electron gas ; 1.3.1. Free electrons ; 1.3.2. Exchange energy ; 2. What is density functional theory? ; 2.1. Hohenberg-Kohn theorem 2.2. A simple example: the Thomas-Fermi theory 2.2.1. Variational equation of Thomas-Fermi theory ; 2.2.2. Thomas-Fermi atom ; 2.2.3. An example ; 3. Kohn-Sham theory ; 3.1. Local density approximation ; 3.2. Spin and the local spin density approximation 3.3. The generalized gradient approximation 4. Numerical methods for the Kohn-Sham equation ; 4.0.1. Exact exchange ; 4.0.2. 0(N) methods ; 5. Some applications and limitations of DFT ; 5.1. Two examples of condensed matter ;

5.2. Vibrations ; 5.3. NMR chemical shifts
6. Limitations of DFT 7. Time-dependent density functional theory: the equations
; 7.1. Optical properties ; 7.1.1. f-sum rule
; 7.2. Methods to solve the TDDFT equations
; 7.2.1. Linear response formula ; 7.3. Dynamic polarizability ; 7.4. Dielectric function
8. TDDFT: numerical aspects 8.1. Configuration matrix method ; 8.2. Linear response method
; 8.3. Sternheimer method ; 8.4. Real time method
; 9. Applications of TDDFT ; 9.1. Simple metal clusters ; 9.2. Carbon structures
; 9.3. Diamond ; 9.4. Other applications
9.5. Limitations

Sommario/riassunto

This invaluable book contains pedagogical articles on the dominant nonstochastic methods of microscopic many-body theories - the methods of density functional theory, coupled cluster theory, and correlated basis functions - in their widest sense. Other articles introduce students to applications of these methods in front-line research, such as Bose-Einstein condensates, the nuclear many-body problem, and the dynamics of quantum liquids. These keynote articles are supplemented by experimental reviews on intimately connected topics that are of current relevance. The book addresses the striking

2. Record Nr. UNINA9910794942803321

Autore	He Meng
Titolo	Synthesis of chiral rare earth and alkaline earth compounds : magnetism and catalytic studies / / von M.S.-Chem. Meng He
Pubbl/distr/stampa	Gottingen, [Germany] : , : Cuvillier Verlag, , 2016 ©2016
ISBN	3-7369-8330-1
Edizione	[1. Auflage.]
Descrizione fisica	1 online resource (126 pages) : illustrations (some color), tables, graphs
Disciplina	546.3
Soggetti	Rare earth metal compounds Rare earth metal catalysts Catalysis
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di bibliografia	Includes bibliographical references.