1. Record Nr. UNINA9910792254203321

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Titolo	Time-dependent density-functional theory [[electronic resource]] : concepts and applications / / Carsten Ullrich
Pubbl/distr/stampa	Oxford, : Oxford University Press, c2012
ISBN	0-19-162744-5 0-19-884193-0 1-283-42682-X 0-19-162691-0 9786613426826
Descrizione fisica	1 online resource (541 p.)
Collana	Oxford graduate texts
Classificazione	UL 2000
Disciplina	541.28
Soggetti	Density functionals Mathematical physics
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Cover; Contents; List of abbreviations; 1 Introduction; 1.1 A survey of time-dependent phenomena; 1.2 Preview of and guide to this book; 2 Review of ground-state density-functional theory; 2.1 The formal framework of DFT; 2.2 Exact properties; 2.3 Approximate functionals; PART I: THE BASIC FORMALISM OF TDDFT; 3 Fundamental existence theorems; 3.1 Time-dependent many-body systems; 3.2 The Runge-Gross theorem; 3.3 The van Leeuwen theorem; 4 The time-dependent Kohn-Sham scheme; 4.1 The time-dependent Kohn-Sham equation; 4.2 Spin-dependent systems; 4.3 The adiabatic approximation 4.4 The meaning of self-consistency in DFT and TDDFT4.5 Numerical time propagation; 5 Time-dependent observables; 5.1 Explicit density functionals; 5.2 Implicit density functionals; 5.3 The time-dependent energy; 6 Properties of the time-dependent xc potential; 6.1 What is the universal xc functional?; 6.2 Some exact conditions; 6.3 Galilean invariance and the harmonic potential theorem; 6.4 Memory and causality; 6.5 Initial-state dependence; 6.6 Time-dependent variational principles; 6.7 Discontinuity upon change of particle number; PART II: LINEAR RESPONSE AND EXCITATION ENERGIES

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Sommario/riassunto

Time-dependent density-functional theory (TDDFT) describes the quantum dynamics of interacting electronic many-body systems formally exactly and in a practical and efficient manner. TDDFT has become the leading method for calculating excitation energies and optical properties of large molecules, with accuracies that rival traditional wave-function based methods, but at a fraction of the computational cost.This book is the first graduate-level text on the concepts and applications of TDDFT, including many examples and exercises, and extensive coverage of the literature. The book begins with a s