1. Record Nr. UNINA9910451907203321

Titolo	Atoms, molecules and clusters in electric fields : theoretical approaches to the calculation of electric polarizability / / editor, George Maroulis
Pubbl/distr/stampa	London : , : Imperial College Press, , [2006] ©2006
ISBN	1-281-86738-1 9786611867386 1-86094-886-3
Descrizione fisica	1 online resource (693 p.)
Collana	Series in computational, numerical and mathematical methods in sciences and engineering, , 1793-3439 ; ; v. 1
Disciplina	539.7
Soggetti	Polarizability (Electricity) Atoms Molecules Atomic spectroscopy Cluster theory (Nuclear physics) Collision spectroscopy Electronic books.
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.
Nota di contenuto	Preface; Contents; 1 Atomic Static Dipole Polarizabilites; 1 Introduction; 2 Theory; 3 Hydrogenic Systems; 4 Multi-Electron Atoms. The Static Dipole Polarizabilities from Z=1 to 119; 5 Trends and Correlation with other Properties; 6 Atomic Dipole Polarizabilities from Density Functional Theory; 7 Conclusion; Acknowledgment; References; 2 First-Order ZPVA Correction to First Hyperpolarizabilities of Mono-Substituted Benzene Molecules; 1 Introduction; 2 Methodology; 3 Applications; Acknowledgment; References; 3 Polarizability and Hyperpolarizability in Small Silicon Clusters; 1 Introduction 2 Computational methodology 3 Results and discussion; 4 Conclusions; Acknowledgments; References; 4 Theoretical Calculations of the Static Dipole Polarizability of Atoms and Small Atomic Clusters; 1 Introduction; 2 Theory; 3 Results and Discussion; 4 Concluding

Remarks and Outlook; References; 5 Elongation Method for Polymers and Its Application to Nonlinear Optics; 1 Introduction; 2 The elongation method; 3 Applications of the elongation method; 4 Toward Linear Scaling; 5 Application of the elongation method to nonlinear optics; 6 Summary and future prospects; Acknowledgments; References
6 Responses of Molecular Vibrations to Intermolecular Electrostatic Interactions and their Effects on Vibrational Spectroscopic Features1 Introduction; 2 Basic Formulas; 3 Structural Changes Induced by Electric Field and Their Consequences in Vibrational Properties; 4 Modulation of the Electric Fields in Liquids: Field-Modulating Modes (FMMs); 5 Effect of Electrostatic Interactions on the Low-Frequency Vibrational Spectra of Liquids; 6 How to Recognize the Vibrational Modes with Large Effects of Electrostatic Interactions: Intensity-Carrying Modes (ICMs)
7 Electrostatic Vibrational Coupling between Molecules: Transition Dipole Coupling (TDC)8 Conclusions; Acknowledgments; References; 7 The (Hyper)polarizabilities of Liquid Water Modeled Using Coupled Cluster/Molecular Mechanics Response Theory Methods; 1 Introduction; 2 Coupled Cluster Theory for States in Vacuum; 3 Solvent Models; 4 Response Theory and Molecular Properties for Solvated Molecules; 5 Electric Properties of Molecules in Condensed Phases; 6 Conclusions; Acknowledgments; References
8 The Discrete Solvent Reaction Field Model: A Quantum Mechanics/Molecular Mechanics Model for Calculating Nonlinear Optical Properties of Molecules in Condensed Phase1 Introduction; 2 The discrete solvent reaction field model; 3 Calculating macroscopic and microscopic properties with a QM/MM model; 4 Selected applications; 5 Summary and Outlook; References; 9 Extraordinary First Hyperpolarizabilities from Loosely Bound Electron in Dipole-Bound Anions: (HF)N- (N = 2 3 4); 1 Introduction; 2 Calculational methods and numerical results; 3 Conclusion; Acknowledgments; References
10 Third-Order Nonlinear Optical Properties of Open-Shell and/or Charged Molecular Systems

Sommario/riassunto

With the central importance of electric polarizability and hyperpolarizability for a wide spectrum of activities, this book charts the trends in the accurate theoretical determination of these properties in specialized fields. The contributions include reviews and original papers that extend from methodology to applications in specific areas of primary importance such as cluster science and organic synthesis of molecules with specific properties.