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Nota di contenuto	CONTENTS ; Preface ; 1 One-Electron Equations for Embedded Electron Density: Challenge for Theory and Practical Payoffs in Multi-Level Modelling of Complex Polyatomic Systems ; 1 Introduction ; 2 The formalism ; 3 Approximating the unknown components of the =8 functional 4 Extension - Localized excited states in condensed matter 5 Numerical implementation ; 6 Applications ; 7 Concluding remarks ; Appendix A Functional derivatives: Generalized Gradient Approximation ; Appendix B The exchange-correlation functional in Local Density Approximation Appendix C Open-shell systems References ; 2 Density-Functional Based Investigation of Molecular Magnets ; 1 Exchange and Spin-Orbit Coupling in Molecules ; 2 Molecular Magnets ; 3 DFT: Theoretical and Computational Framework ; 4 Predicting Magnetic Properties of Molecules and Clusters 5 Electronic Structure of the Fe8 Molecular Magnet 6 Mn12-Acetate and Its Derivatives ; 7 The Mn4 Monomer and Dimer ; 8 The Co4 Molecular

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3 Vibrational Spectra by Electron Impact: Theoretical Models for Intensities 1 Introduction ; 2 Static-exchange approximation ; 3 Discrete Momentum Representation (DMR) of the Lippmann-Schwinger equation
; 4 Electron energy loss spectrum of propane
; 5 Assessment of the DMR method
6 General remarks on ab initio calculations of vibrationally inelastic electron scattering

Sommario/riassunto

There have been important developments in the last decade: computers are faster and more powerful, code features are enhanced and more efficient, and larger molecules can be studied - not only in vacuum but also in a solvent or in crystal. Researchers are using new techniques to study larger systems and obtain more accurate results. This is impetus for the development of more efficient methods based on the first-principle multi-level simulations appropriate for complex species. Among the cutting-edge methods and studies reviewed in this decennial volume of the series are the Density Function