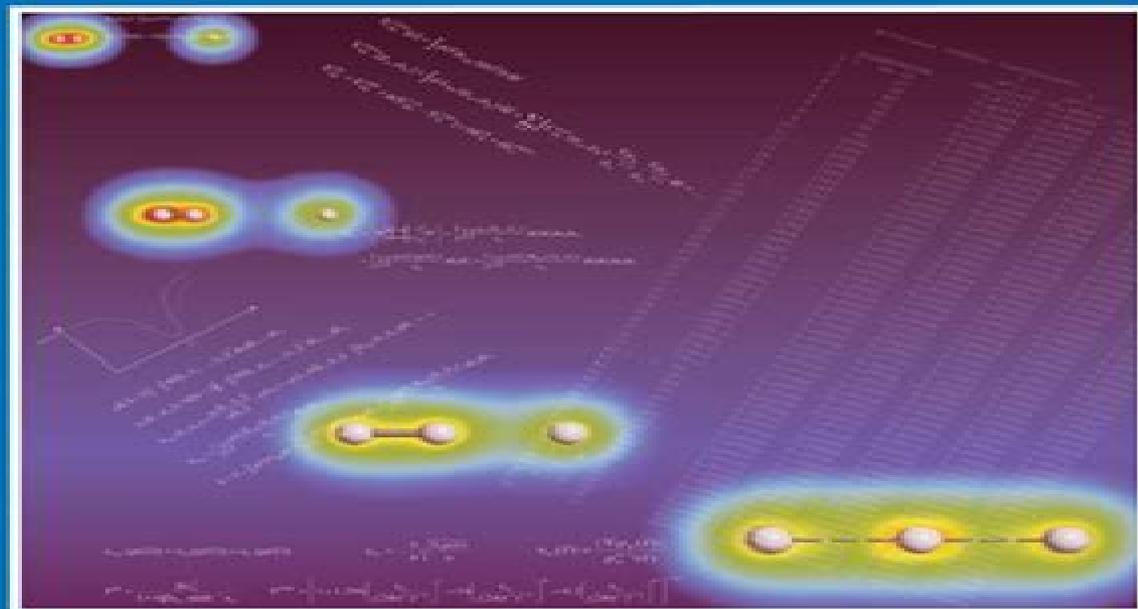


Wolfram Koch, Max C. Holthausen

A Chemist's Guide to Density Functional Theory

Second Edition



Chemists Guide To Density Functional Theory

John M. Herbert



Chemists Guide To Density Functional Theory:

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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 self contained review of ground state DFT followed by a detailed and pedagogical treatment of the formal framework of TDDFT It is explained how excitation energies can be calculated from linear response TDDFT Among the more advanced topics are time dependent current density functional theory orbital functionals and many body theory Many applications are discussed including molecular excitations ultrafast and strong field phenomena excitons in solids van der Waals interactions nanoscale transport and molecular dynamics

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Chérif F. Matta,2010-01-14 Divided into five major parts the two volumes of this ready reference cover the tailoring of theoretical methods for biochemical computations as well as the many kinds of biomolecules reaction and transition state elucidation conformational flexibility determination and drug design Throughout the chapters gradually build up from introductory level to comprehensive reviews of the latest research and include all important compound classes such as DNA RNA enzymes vitamins and heterocyclic compounds The result is in depth and vital knowledge for both readers already working in the field as well as those entering it Includes contributions by Prof Ada Yonath Nobel Prize in Chemistry 2009 and Prof Jerome Karle Nobel Prize in Chemistry 1985

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Lakhtakia,2004-09-24 Despite some 20 years of research history nanotechnology is still widely regarded as being at an embryonic stage of development This text provides guidance on the state of the art to the growing numbers of nanotechnology researchers helping to shape the contours of both experimental research and theoretical research

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Introduction to the Physics and Chemistry of Materials Robert J. Naumann, 2009 Preparing students for graduate work in materials science and engineering this applications oriented text emphasizes cutting edge technology to provide a clear picture of how the principles of materials apply to exciting breakthroughs and promising new fields **Bulletin of the Chemical Society of Japan** Nihon Kagakkai, 2004

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