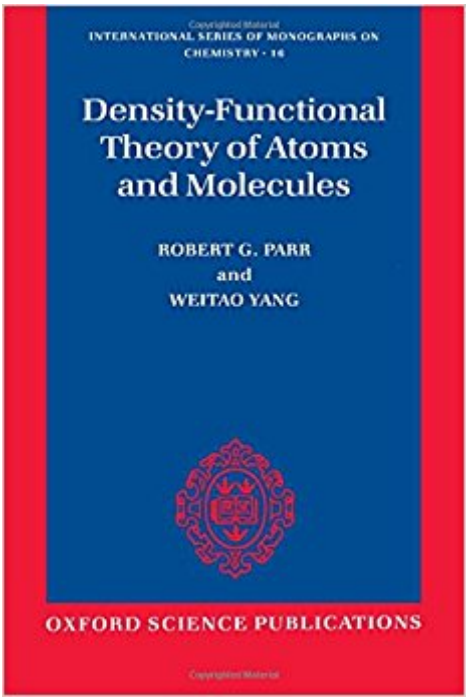
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Density-Functional Theory Of Atoms And Molecules (International Series Of Monographs On Chemistry)



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Synopsis

This book is a rigorous, unified account of the fundamental principles of the density-functional theory of the electronic structure of matter and its applications to atoms and molecules. Containing a detailed discussion of the chemical potential and its derivatives, it provides an understanding of the concepts of electronegativity, hardness and softness, and chemical reactivity. Both the Hohenberg-Kohn-Sham and the Levy-Lieb derivations of the basic theorems are presented, and extensive references to the literature are included. Two introductory chapters and several appendices provide all the background material necessary beyond a knowledge of elementary quantum theory. The book is intended for physicists, chemists, and advanced students in chemistry.

Book Information

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"The theory of atoms, molecules and solids is largely dependent on good approximate solutions to appropriate quantum mechanical many-electron systems. Thus the appearance in recent years, of a new practical way to generate such solutions has met with considerable interest. The method is the density-functional method (DFT) in the local density approximation (LDA). . . . R.G. Parr and W. Yang are experienced professionals in this area . . . Their book is a thorough and solid introduction to the DFT. . . . I found the book well written, accurate and helpful. I recommend it." --Annual Nuclear Energy"Gives an excellent summary of the foundations and, much more briefly, of some of the applications of this electron density theory . . . . well written and important book." --The Times

Higher Education Supplement"The author’s goal of giving ’a coherent account of the (density-functional) theory as it stands today’ has been attained in this excellent book." --Theoretica Chimica Acta"This book is an excellent rigorous introduction to the ideas of density functional theory, couched in the language of density matrices that is familiar to theoretical chemists. It is well-written and authoritative, fills a void in the literature, and should be part of the library of practicing theoretical chemists and physicists." --Journal of the American Chemical Society"In the book, Parr summarizes, in a rigorous and fairly mathematical way, the basic theorems related to the density-functional method. Much emphasis is placed on a thorough review of the work done by his own students.. . . Basic principles are emphasized and explained in elegant mathematical detail. Various approximations of the exchange and correlation potential are carefully examined. The book provides the essential perspective and background needed by an investigator who wants to continue to progress in the field." --American Scientist

Robert G. Parr and Yang Weitao are both at University of North Carolina at Chapel Hill.

"Density functional theory" sounds like a tough topic in a science curriculum. It is indeed, but in the long run it is a valuable tool to explore the properties of matter a it undergoes chemical and physical tranformations, say water vapour interacting with infrared energy, a protein folding itself to attain a characteristic structure that catalizes a chemical reaction, the coupling between DNA nanowires with other conductors to make a molecular switch, and the reduction of nitrogen oxides over iron atoms embedded in a zeolite among many more.Of course there is a long way yet to be walked between the theory and its many applications, nonetheless there you have the fundamental principles that govern the behavior of matter and the DFT is a model that offers a good way to undertand them.The style is straight as a scientific monograph is used to be. You’ll need lots of paper, a bunch of sharp pencils and plenty of time to work your path trough, tough. That is because it is aimed to graduate students and professionals, rather than an introductory text.

Density functional theory has been used in solid state physics for many decades. It has recently become popular in quantum chemistry. The authors have made seminal contributions to the field and their insight is distilled into this book. The focus of this book is on understanding the physics and chemistry underlying density functional theory - it does not concern itself with computatioonal details of the methodology or specific applications to different systems. Parr and Yang’s book has now become a classic in the field, a must-buy for any student or researcher of density functional

theory in chemistry.

I've never met anyone who was "into" DFT and did not like this book... except me. I think it is the most over-rated book on ab initio theory out there. I liked Szabo and Ostlund and Helgaker et al's books because they were detailed enough that you could not know Hartree-Fock or MP2, but after reading them, you could write a HF or MP2 program. I didn't know DFT before I read this book and I still couldn't write a DFT program after reading it. To me, the text seemed more philisophical than applicable, but considering the limited scope of this book, you would expect it to be more detailed than what it really is.

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