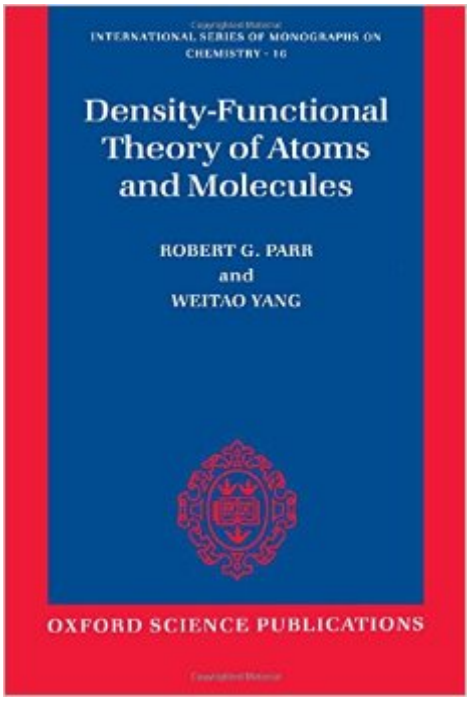
Density-Functional Theory Of Atoms And Molecules (International Series Of Monographs On Chemistry)



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

Series: International Series of Monographs on Chemistry (Book 16)
Paperback: 352 pages
Publisher: Oxford University Press (May 26, 1994)
Language: English
ISBN-10: 0195092767
ISBN-13: 978-0195092769
Product Dimensions: 9.2 x 0.8 x 6.2 inches
Shipping Weight: 1 pounds (View shipping rates and policies)
Average Customer Review: 4.0 out of 5 starsÂ Â See all reviewsÂ (3 customer reviews)
Best Sellers Rank: #1,637,182 in Books (See Top 100 in Books) #92 inÂ Books > Science & Math > Chemistry > Physical & Theoretical > Quantum Chemistry #456 inÂ Books > Science & Math > Chemistry > Physical & Theoretical > Physical Chemistry #1023 inÂ Books > Science & Math > Physics > Nuclear Physics

Customer Reviews

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.

"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.

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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