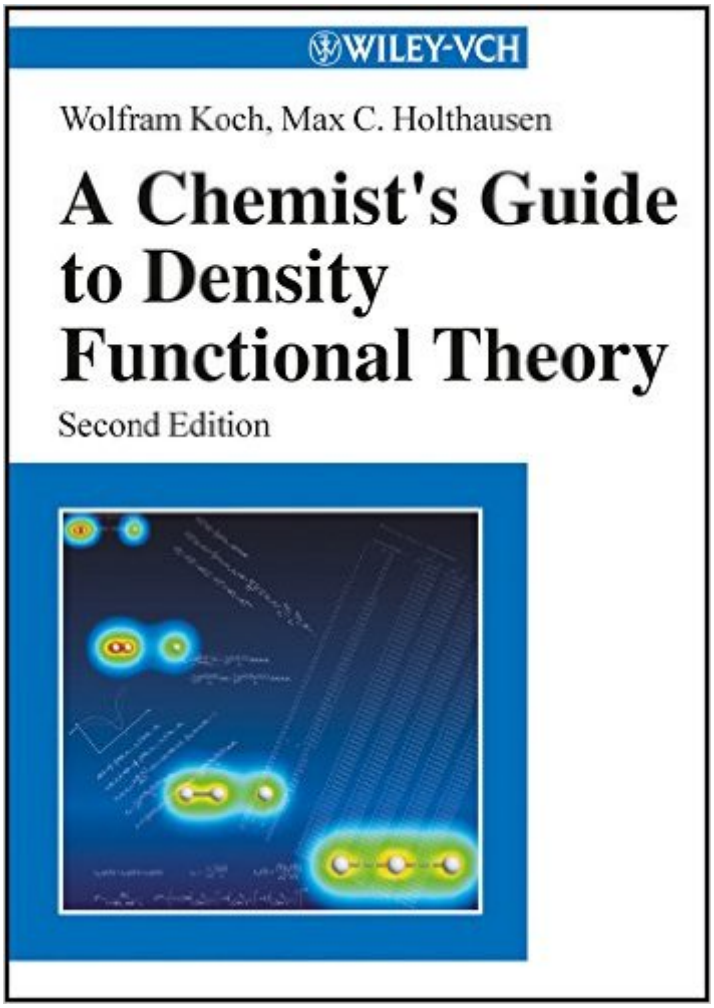
A Chemist's Guide To Density Functional Theory, 2nd Edition



Synopsis

"Chemists familiar with conventional quantum mechanics will applaud and benefit greatly from this particularly instructive, thorough and clearly written exposition of density functional theory: its basis, concepts, terms, implementation, and performance in diverse applications. Users of DFT for structure, energy, and molecular property computations, as well as reaction mechanism studies, are guided to the optimum choices of the most effective methods. Well done!" Paul von Ragu? Schleyer "A conspicuous hole in the computational chemist's library is nicely filled by this book, which provides a wide-ranging and pragmatic view of the subject.[...It] should justifiably become the favorite text on the subject for practioneers who aim to use DFT to solve chemical problems." J. F. Stanton, J. Am. Chem. Soc. "The authors' aim is to guide the chemist through basic theoretical and related technical aspects of DFT at an easy-to-understand theoretical level. They succeed admirably." P. C. H. Mitchell, Appl. Organomet. Chem. "The authors have done an excellent service to the chemical community. [...] A Chemist's Guide to Density Functional Theory is exactly what the title suggests. It should be an invaluable source of insight and knowledge for many chemists using DFT approaches to solve chemical problems." M. Kaupp, Angew. Chem.

Book Information

Paperback: 313 pages
Publisher: Wiley-VCH; 2 edition (July 11, 2001)
Language: English
ISBN-10: 3527303723
ISBN-13: 978-3527303724
Product Dimensions: 6.8 x 0.7 x 9.7 inches
Shipping Weight: 1.4 pounds (View shipping rates and policies)
Average Customer Review: 4.8 out of 5 starsÂ Â See all reviewsÂ (6 customer reviews)
Best Sellers Rank: #1,011,376 in Books (See Top 100 in Books) #61 inÂ Books > Science & Math > Chemistry > Physical & Theoretical > Quantum Chemistry #805 inÂ Books > Science & Math > Experiments, Instruments & Measurement > Methodology & Statistics #881 inÂ Books > Medical Books > Medicine > Internal Medicine > Pathology > Clinical Chemistry

Customer Reviews

Computational and Theoretical chemists concerned with the applications of canonical quantum chemistry (molecular orbital) methods to chemically interesting problems know too well how (computationally) demanding is going beyond the Hartree-Fock (HF) approximation by employing

the so called post-HF methods. Hence, very often they must resort on using Density Functional Theory (DFT). Here, however, they need to confront themselves with the terminology invented by their physics collegues: Kohn-Sham orbitals, Fermi hole, local and non-local spin-density functionals, generalized gradient approximation, pseudopotentials, and so forth. Any terminology is associated to a certain model of thought, which requires lot of efforts to be fully comprehended.The book of Koch and Holthausen represents a praiseworthy attempt of presenting the basic concepts of DFT to research chemists. This 300-pages book is organized in two parts and it contains 13 chapters. Part A is concerned with the definition of the (DFT) model, while Part B discusses the performance of the model in dealing with molecular structures, vibrational frequencies, thermochemical, electrical and magnetic properties, H-bonds, and chemical reactivity. A rich bibliography is appended at the end of the book. Clearly written and logically organized, this book can be considered "THE Chemists's Guide to DFT" and it deserves five stars.

From a physicist's point of view this book is very clear at explaining Density Functional Theory (DFT). The authors use many chemical examples, but still can be applied to physics. Many physics books on DFT assume the reader knows most of the material so skips many important details that can leave the reader confused. Surprisingly, these chemists spend entire chapters on just about every piece of DFT. They even give many examples, using the Hydrogen molecule as an example quite a few times.This book is fairly recent, published in 2001. It talks about many DFT codes used today and important functionals such as B3LYP. The book is a little relaxed on the math, so if you are wanting to see some of the detailed math I suggest "Density-Functional Theory of Atoms and Molecules" by Parr & Yang as a good companion book.

Now just beginning to show its years, this is a clear and authoritative guide to the theory and practice of density functional methods - now the clear choice for a wide range of applications especially for organiometallic systems.

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