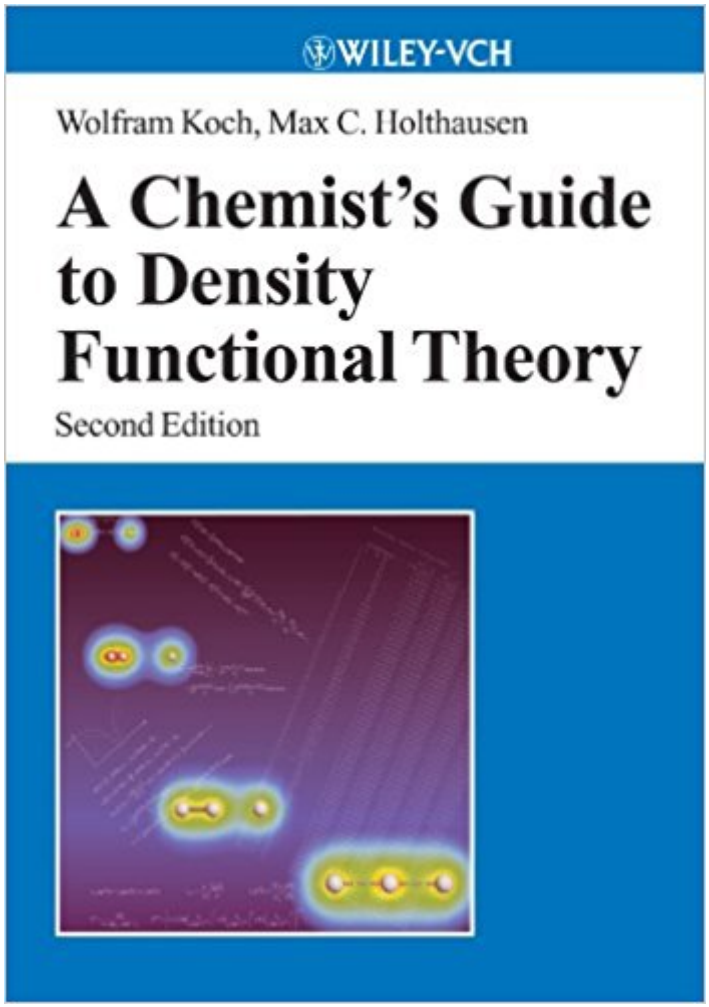
A Chemist's Guide To Density Functional Theory, 2nd Edition



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 RaguÃƒÂ Ã Â¿Ã Â Â 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

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Customer Reviews

..."Wolfram Koch und Max Holthausen schafften es meisterlich, sowohl ein Lehrwerk f]r Anfdnger als auch ein einfaches Nachschlagewerk f]r Experten auf dem Gebiet der Dichtefunktionaltheorie-Methoden zu konzipieren. Dies wurde mvglich durch die Aufteilung des

Buches in zwei gro_e Teile: Theorie und Praxis. Wdhrend die Theorie sich in verstdndlicher Weise auf das Nvtigste beschrdnkt, werden im Praxisteil nahezu alle]blichen quantenchemischen Fragestellungen eingehend besprochen ? und dies exemplarisch anhand aufbereiteter Originalvervffentlichungen." wissenschaft-online

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.

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.

This book presents the Density functional Theory (DFT), for Chemists. It is divided in two parts: (A)The Definition of the Model - where the theory is presented; (B) The Performance of the Model - where the applications are explored. If you are interested in Computational Chemistry and want to learn DFT, then this book is for you.

This book is an excellent introduction to density functional theory. And it is not difficult to read straight through.

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.

Unlike Parr and Yang’s Density-Functional Theory of Atoms and Molecules, this book doesn’t have many rigorous while lengthy derivations. However, it gives readers a clear clue for DFT ,and most importantly, a way to appreciate this theory as a chemist. I think this book is a perfect complement for Parr and Yang’s book.

Functional Medicine, Vol. 2: Protocols for Common Inflammatory Disorders (Inflammation Mastery & Functional Inflammology) The Chemist The Chemist's Companion: A Handbook of Practical Data, Techniques, and References A Chemist in the White House: From the Manhattan Project to the End of the Cold War