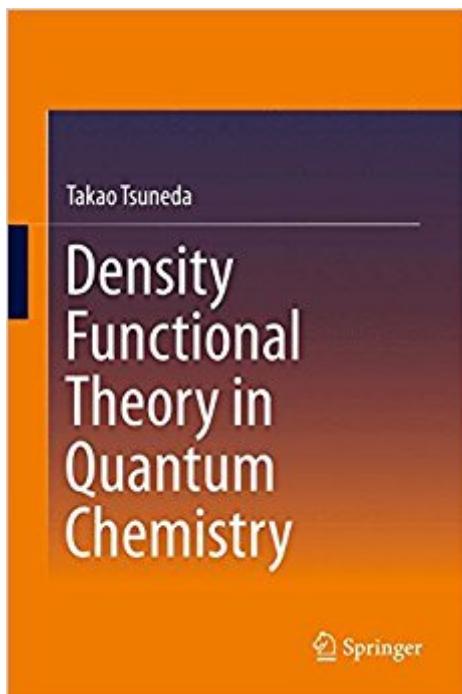


The book was found

Density Functional Theory In Quantum Chemistry



Synopsis

In this book, density functional theory (DFT) is introduced within the overall context of quantum chemistry. DFT has become the most frequently used theory in quantum chemistry calculations. However, thus far, there has been no book on the fundamentals of DFT that uses the terminology and methodology of quantum chemistry, which is familiar to many chemists, including experimentalists. This book first reviews the basic concepts and historical background of quantum chemistry and then explains those of DFT, showing how the latter fits into the bigger picture. Recent interesting topics of DFT in chemistry are also targeted. In particular, the physical meanings of state-of-the-art exchange-correlation functionals and their corrections are described in detail. Owing to its unconventionality, this book is certain to be of great interest not only to chemists but also to solid state physicists.

Book Information

Hardcover: 200 pages

Publisher: Springer; 2014 edition (February 20, 2014)

Language: English

ISBN-10: 4431548246

ISBN-13: 978-4431548249

Product Dimensions: 6.1 x 0.5 x 9.2 inches

Shipping Weight: 1.1 pounds (View shipping rates and policies)

Average Customer Review: Be the first to review this item

Best Sellers Rank: #1,192,375 in Books (See Top 100 in Books) #59 in Books > Science & Math > Chemistry > Physical & Theoretical > Quantum Chemistry #394 in Books > Science & Math > Physics > Solid-State Physics #823 in Books > Science & Math > Physics > Electromagnetism

Customer Reviews

In this book, density functional theory (DFT) is introduced within the overall context of quantum chemistry. DFT has become the most frequently used theory in quantum chemistry calculations. However, thus far, there has been no book on the fundamentals of DFT that uses the terminology and methodology of quantum chemistry, which is familiar to many chemists, including experimentalists. This book first reviews the basic concepts and historical background of quantum chemistry and then explains those of DFT, showing how the latter fits into the bigger picture. Recent interesting topics of DFT in chemistry are also targeted. In particular, the physical meanings of

state-of-the-art exchange-correlation functionals and their corrections are described in detail. Owing to its unconventionality, this book is certain to be of great interest not only to chemists but also to solid state physicists.

[Download to continue reading...](#)

Density Functional Theory in Quantum Chemistry Density-Functional Theory of Atoms and Molecules (International Series of Monographs on Chemistry) Osteoporosis: How To Reverse Osteoporosis, Build Bone Density And Regain Your Life (Osteoporosis, Bone Density, Strong Bones, Healthy Bones, Osteoporosis Cure) Advanced Molecular Quantum Mechanics: An Introduction to Relativistic Quantum Mechanics and the Quantum Theory of Radiation (Studies in Chemical Physics) A Chemist's Guide to Density Functional Theory Time-Dependent Density-Functional Theory: Concepts and Applications (Oxford Graduate Texts) A Chemist's Guide to Density Functional Theory, 2nd Edition Patai's 1992 Guide to the Chemistry of Functional Groups (Patai's Chemistry of Functional Groups) The Chemistry of Double-Bonded Functional Groups, Supplement A3, 2 Part Set (Patai's Chemistry of Functional Groups) Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory (Dover Books on Chemistry) Recent Advances in the Theory of Chemical and Physical Systems: Proceedings of the 9th European Workshop on Quantum Systems in Chemistry and Physics ... in Theoretical Chemistry and Physics) Covariant Loop Quantum Gravity: An Elementary Introduction to Quantum Gravity and Spinfoam Theory (Cambridge Monographs on Mathematical Physics) The Quantum Mechanics Solver: How to Apply Quantum Theory to Modern Physics Study Guide: Ace Organic Chemistry I - The EASY Guide to Ace Organic Chemistry I: (Organic Chemistry Study Guide, Organic Chemistry Review, Concepts, Reaction Mechanisms and Summaries) Ace General Chemistry I and II (The EASY Guide to Ace General Chemistry I and II): General Chemistry Study Guide, General Chemistry Review The Chemistry of Organic Silicon Compounds, Vol. 2, Part 1-3 (Patai's Chemistry of Functional Groups) Wheater's Functional Histology: A Text and Colour Atlas, 6e (FUNCTIONAL HISTOLOGY (WHEATER'S)) Wheater's Functional Histology: A Text and Colour Atlas (Book with CD-ROM) (Functional Histology (Wheater's)) Functional Programming in JavaScript: How to improve your JavaScript programs using functional techniques Nolte's The Human Brain: An Introduction to its Functional Anatomy With STUDENT CONSULT Online Access, 6e (Human Brain: An Introduction to Its Functional Anatomy (Nolt)

[Contact Us](#)

[DMCA](#)

Privacy

FAQ & Help