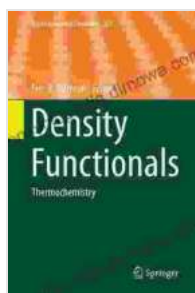


Unleash the Power of Density Functionals: Unraveling Thermochemistry with Topics in Current Chemistry

In the realm of quantum chemistry, the advent of density functional theory (DFT) has revolutionized our understanding of molecular systems. DFT provides a potent tool for exploring the electronic structure and properties of atoms, molecules, and materials. Among its many applications, DFT is particularly adept at unraveling thermochemical data, paving the way for accurate predictions of reaction energies, molecular enthalpies, and a plethora of other thermodynamic parameters.

Within the esteemed Topics in Current Chemistry series, the latest installment, "Density Functionals Thermochemistry," delves deep into this fascinating subject. This comprehensive volume, spanning 365 pages, brings together a team of renowned experts, each contributing their specialized knowledge to shed light on the latest advancements in DFT-based thermochemistry.



Density Functionals: Thermochemistry (Topics in Current Chemistry Book 365)

★★★★★ 5 out of 5

Language : English
File size : 5257 KB
Text-to-Speech : Enabled
Enhanced typesetting : Enabled
Print length : 300 pages

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A Journey Through DFT Thermochemistry

The book opens with a historical perspective, tracing the development of DFT from its humble beginnings to its current status as a ubiquitous tool in modern chemistry. The chapter authors provide a lucid exposition of the underlying principles of DFT, making it accessible even to those new to the field.

Subsequent chapters delve into the practical application of DFT for thermochemical studies. Readers will find insightful discussions on the calculation of reaction energies, molecular enthalpies, and free energies using various DFT functionals. The authors meticulously assess the strengths and limitations of different functionals, empowering readers to make informed choices for their own research endeavors.

Exploring Specialized Applications

Beyond the fundamental principles, "Density Functionals Thermochemistry" ventures into specialized applications where DFT has demonstrated its prowess. One chapter focuses on the application of DFT to study the thermodynamics of complex materials, such as polymers and biomolecules. Another chapter explores the use of DFT in conjunction with machine learning algorithms to enhance the accuracy and efficiency of thermochemical predictions.

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- **In-depth Understanding of DFT Thermochemistry:** Gain a thorough grasp of the underlying principles, methodologies, and applications of DFT for thermochemical studies.
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- **Valuable Resource for Researchers and Educators:** Serve as an invaluable reference for researchers and educators working in the fields of quantum chemistry, computational chemistry, and physical chemistry.
- **Cutting-Edge Insights from Experts:** Benefit from the collective wisdom of renowned experts in DFT thermochemistry, ensuring you are up-to-date with the latest advancements in the field.

"Density Functionals Thermochemistry" is an indispensable guide for researchers, educators, and students seeking to harness the immense power of DFT for thermochemical studies. Its comprehensive coverage, practical insights, and exploration of advanced applications make it an

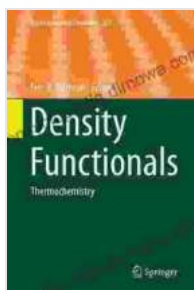
invaluable resource for anyone interested in unraveling the complexities of molecular systems at the quantum level.

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Secure your copy of "Density Functionals Thermochemistry: Topics in Current Chemistry 365" today and unlock the transformative power of DFT for your thermochemical investigations. Let this comprehensive guide illuminate your path towards groundbreaking discoveries in the world of quantum chemistry and beyond.

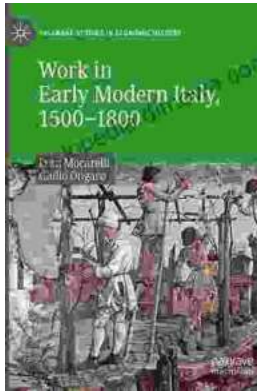
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