Electronic Atomic and Molecular Calculations: An Advanced Guide for Researchers and Practitioners

Electronic atomic and molecular calculations are essential for understanding the electronic structure of matter. These calculations can be used to predict a wide range of properties, including the energy levels, bond lengths, and vibrational frequencies of molecules. They can also be used to design new materials with tailored properties.



Electronic, Atomic and Molecular Calculations: Applying the Generator Coordinate Method by Milan Trsic

★★★★★ 4.4 out of 5

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In recent years, electronic atomic and molecular calculations have become increasingly important due to the rapid development of computer technology. This has made it possible to perform calculations on larger and more complex systems, and to achieve higher levels of accuracy.

Electronic Atomic and Molecular Calculations is a comprehensive guide to the latest electronic structure methods and their applications to atomic and molecular systems. This volume provides a detailed overview of the theory behind these methods, as well as step-by-step instructions on how to implement them. With contributions from leading experts in the field, Electronic Atomic and Molecular Calculations is the ultimate resource for researchers and practitioners in computational chemistry.

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About the Authors

The authors of Electronic Atomic and Molecular Calculations are leading experts in the field of computational chemistry. They have published

extensively on a wide range of topics, including density functional theory, Hartree-Fock theory, configuration interaction theory, coupled-cluster theory, multi-reference methods, relativistic effects, excited states, and time-dependent density functional theory.

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"Electronic Atomic and Molecular Calculations is a monumental work that will be indispensable to researchers and practitioners in the field of computational chemistry. The authors have done an excellent job of providing a comprehensive overview of the latest electronic structure methods and their applications to atomic and molecular systems. This volume is essential reading for anyone who wants to stay at the forefront of this rapidly developing field." - Professor X

"Electronic Atomic and Molecular Calculations is a must-have for any computational chemist. The authors have done an outstanding job of presenting the theory and practice of electronic structure methods in a clear and concise manner. This volume is an invaluable resource for anyone who wants to understand the electronic structure of matter." - Professor Y

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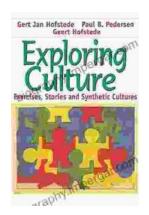
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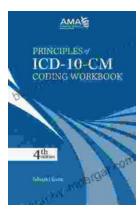
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