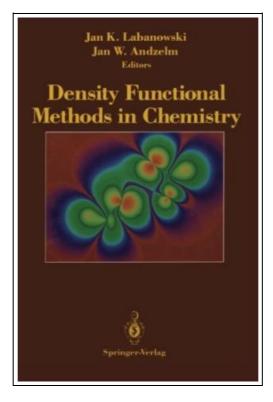
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Springer-Verlag New York Inc., United States, 2011. Paperback. Condition: New. Language: English. Brand New Book ***** Print on Demand ******. Predicting molecular structure and energy and explaining the nature of bonding are central goals in quantum chemistry. With this book, the editors assert that the density functional (DF) method satisfies these goals and has come into its own as an advanced method of computational chemistry. The wealth of applications presented in the book, ranging from solid state sys- tems and polymers to organic and organo-metallic molecules, metallic clus- ters, and biological complexes, prove that DF is becoming a widely used computational tool in chemistry. Progress in the methodology and its imple- mentation documented by the contributions in this book demonstrate that DF calculations are both accurate and efficient. In fact, the results of DF calculations may pleasantly surprise many chem- ists. Even the simplest approximation of DF, the local spin density method (LSD), yields molecular structures typical of ab initio correlated methods. The next level of theory, the nonlocal spin density method, predicts the energies of molecular processes within a few kcallmol or less. Like the Hartree-Fock (HF) and configuration interaction (CI) methods, the DF method is based only on fundamental physical constants. Therefore, it does not require semiempirical parameters and can be applied to any molecular system and to metallic phases. However, DF s greatest advantage is that it can be applied to much larger systems than those approachable by tradition- al ab initio methods, especially when compared with correlated ab initio methods. Softcover reprint of the original 1st ed. 1991.





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