



Density-Functional Theory of Atoms and Molecules (International Series of Monographs on Chemistry, No. 16)

Robert G. Parr, Yang Weitao

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This book is a rigorous, unified account of the fundamental principles of the density-functional theory of the electronic structure of matter and its applications to atoms and molecules. Containing a detailed discussion of the chemical potential and its derivatives, it provides an understanding of the concepts of electronegativity, hardness and softness, and chemical reactivity. Both the Hohenberg-Kohn-Sham and the Levy-Lieb derivations of the basic theorems are presented, and extensive references to the literature are included. Two introductory chapters and several appendices provide all the background material necessary beyond a knowledge of elementary quantum theory.



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