

DENSITY FUNCTIONAL THEORY OF ATOMS AND MOLECULES BY ROBERT G PARR YANG WEITAO%0A

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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

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Density Functional Theory of Atoms and Molecules

Topics discussed include the concept of electronegativity, the concept of an atom in a molecule, calculation of electronegativities from the X method, the concept of pressure, Gibbs-Duhem equation, Maxwell relations, stability conditions, and local density functional theory.

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Book Review Density-functional theory of atoms and molecules. R.G. Parr and W. Yang, Oxford University Press, New York, Oxford, 1989. IX + 333 pp. Price 45.00

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