# Density Functional Theory of Molecules, Clusters and Solids


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Rapid advances are taking place in the application of density functional theory (DFT) to describe complex electronic structures, to accurately treat large systems and to predict physical and chemical properties. Both theoretical content and computational methodology are developing at a pace which offers researchers new opportunities in areas such as quantum chemistry, cluster science, and solid state physics. This volume contains ten contributions by leading scientists in the field and provides an authoritative overview of the most important developments. The book focuses on the following themes: determining adequate approximations for the many-body problem of electronic correlations; how to transform these approximations into computational algorithms; applications to discover and predict properties of electronic systems; and developing the theory. For researchers in surface chemistry, catalysis, ceramics and inorganic chemistry.

作者介绍:

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## 标签

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## 书评

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