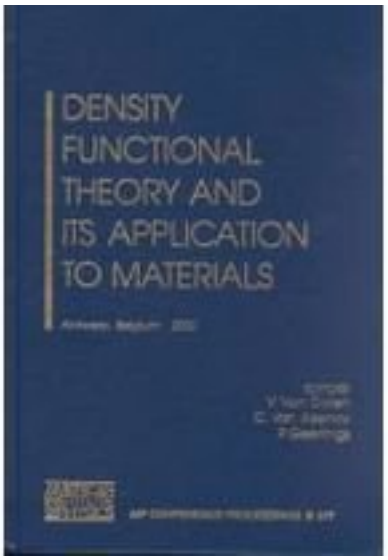
Density Functional Theory and Its Application to Materials



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An overview of the state of the art in density functional theory is presented. Not only the recent theoretical developments but also the achievements in calculating mechanical and electronic properties of molecules, polymers, and solids are described. Recent developments related to the construction of exchange-correlation functionals used in density functional theory for ground and excited states are presented. Applications to materials modeling in general as well as to nanotubes, quantum dots, and artificial molecules are incorporated. Topics such as optical excitations, critical temperatures of superconductors, and state-of-the-art Monte Carlo calculations are also discussed.

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