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Nota di contenuto	Advanced Calculations for Defects in Materials: Electronic Structure Methods; Contents; List of Contributors; 1 Advances in Electronic Structure Methods for Defects and Impurities in Solids; 1.1 Introduction; 1.2 Formalism and Computational Approach; 1.2.1 Defect Formation Energies and Concentrations; 1.2.2 Transition Levels or Ionization Energies; 1.2.3 Practical Aspects; 1.3 The DFT-LDA/GGA Band-Gap Problem and Possible Approaches to Overcome It; 1.3.1 LDA + U for Materials with Semicore States; 1.3.2 Hybrid Functionals; 1.3.3 Many-Body Perturbation Theory in the GW Approximation 1.3.4 Modified Pseudopotentials 1.4 Summary; References; 2 Accuracy of Quantum Monte Carlo Methods for Point Defects in Solids; 2.1 Introduction; 2.2 Quantum Monte Carlo Method; 2.2.1 Controlled

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Sommario/riassunto

This book investigates the possible ways of improvement by applying more sophisticated electronic structure methods as well as corrections and alternatives to the supercell model. In particular, the merits of hybrid and screened functionals, as well as of the +U methods are assessed in comparison to various perturbative and Quantum Monte Carlo many body theories. The inclusion of excitonic effects is also discussed by way of solving the Bethe-Salpeter equation or by using time-dependent DFT, based on GW or hybrid functional calculations. Particular attention is paid to overcome the side effect