1. Record Nr. UNINA9910876633903321

Titolo	Advanced calculations for defects in materials : electronic structure methods / / edited by Audrius Alkauskas ... [et al.]
Pubbl/distr/stampa	Weinheim, Germany, : Wiley-VCH, 2011
ISBN	3-527-63853-9 1-283-17365-4 9786613173652 3-527-63852-0 3-527-63854-7
Descrizione fisica	1 online resource (404 p.)
Altri autori (Persone)	AlkauskasAudrius
Disciplina	620.112 620.1127
Soggetti	Materials - Testing Solids
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and index.
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 Pseudopotentials1.4 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 Approximations; 2.2.1.1 Time Step; 2.2.1.2 Configuration Population; 2.2.1.3 Basis Set; 2.2.1.4 Simulation Cell; 2.2.2 Uncontrolled Approximations; 2.2.2.1 Fixed-Node Approximation; 2.2.2.2 Pseudopotential; 2.2.2.3 Pseudopotential Locality; 2.3 Review of Previous DMC Defect Calculations; 2.3.1 Diamond Vacancy; 2.3.2 MgO

Schottky Defect; 2.3.3 Si Interstitial Defects; 2.4 Results; 2.4.1 Time Step
2.4.2 Pseudopotential2.4.3 Fixed-Node Approximation; 2.5 Conclusion; References; 3 Electronic Properties of Interfaces and Defects from Many-body Perturbation Theory: Recent Developments and Applications; 3.1 Introduction; 3.2 Many-Body Perturbation Theory; 3.2.1 Hedin.s Equations; 3.2.2 GW Approximation; 3.2.3 Beyond the GW Approximation; 3.3 Practical Implementation of GW and Recent Developments Beyond; 3.3.1 Perturbative Approach; 3.3.2 QP Self-Consistent GW; 3.3.3 Plasmon Pole Models Versus Direct Calculation of the Frequency Integral; 3.3.4 The Extrapolar Method
3.3.4.1 Polarizability with a Limited Number of Empty States3.3.4.2 Self-Energy with a Limited Number of Empty States; 3.3.5 MBPT in the PAW Framework; 3.4 QP Corrections to the BOs at Interfaces; 3.5 QP Corrections for Defects; 3.6 Conclusions and Prospects; References; 4 Accelerating GW Calculations with Optimal Polarizability Basis; 4.1 Introduction; 4.2 The GW Approximation; 4.3 The Method: Optimal Polarizability Basis; 4.4 Implementation and Validation; 4.4.1 Benzene; 4.4.2 Bulk Si; 4.4.3 Vitreous Silica; 4.5 Example: Point Defects in a-Si3N4; 4.5.1 Model Generation
4.5.2 Model Structure4.5.3 Electronic Structure; 4.6 Conclusions; References; 5 Calculation of Semiconductor Band Structures and Defects by the Screened Exchange Density Functional; 5.1 Introduction; 5.2 Screened Exchange Functional; 5.3 Bulk Band Structures and Defects; 5.3.1 Band Structure of ZnO; 5.3.2 Defects of ZnO; 5.3.3 Band Structure of MgO; 5.3.4 Band Structures of SnO2 and CdO; 5.3.5 Band Structure and Defects of HfO2; 5.3.6 BiFeO3; 5.4 Summary; References; 6 Accurate Treatment of Solids with the HSE Screened Hybrid; 6.1 Introduction and Basics of Density Functional Theory
6.2 Band Gaps

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