

1. Record Nr.	UNISA996395520103316
Autore	Sorocold Thomas <1561-1617.>
Titolo	Supplications of saints [[electronic resource] ] : A booke of prayers and prayes. In foure parts ... wherein are three most excellent prayers, made by the late famous Queen Elizabeth. // By Tho. Sorocold
Pubbl/distr/stampa	London, : Printed by T. S[nodham] for Nicholas Bourne, and are to be sold at his shop, at the south entry of the Royall Exchange, 1619
Edizione	[The eight [sic] edition, enlarged..]
Descrizione fisica	[30], 90, 87-417, [5] p
Altri autori (Persone)	Elizabeth, Queen of England, <1533-1603.>
Soggetti	Prayers Devotional exercises
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Printer from STC. Signatures: A-TÂ <sup>1</sup> Â <sup>2</sup> . Headpieces, initials. Errors in paging; nos. 87-90 repeated in pagination. Imperfect: leaf N11 wanting. Reproduction of original in: Library of Congress.
Nota di contenuto	(from t.p.): 1. Daniels deuotion 2. Pauls assembly 3. Dauids suite 4. Moses song [brace] praiers for [brace] 1. Thrice euey day 2. Companies 3. Euey one alone 4. Praises and graces.
Sommario/riassunto	eebo-0078

2. Record Nr.	UNINA9911019145203321
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	9786613173652 9783527638536 3527638539 9781283173650 1283173654 9783527638529 3527638520 9783527638543 3527638547
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 Pseudopotential 2.4.3 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 Extrapolation Method  
 3.3.4.1 Polarizability with a Limited Number of Empty States 3.3.4.2 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  $\alpha$ - $\text{Si}_3\text{N}_4$ ; 4.5.1 Model Generation  
 4.5.2 Model Structure 4.5.3 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  $\text{SnO}_2$  and CdO; 5.3.5 Band Structure and Defects of  $\text{HfO}_2$ ; 5.3.6  $\text{BiFeO}_3$ ; 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

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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

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