

1. Record Nr.	UNINA9910821880203321
Titolo	Computational approaches to energy materials // edited by Richard Catlow, Aron Walsh, Alexey A. Sokol
Pubbl/distr/stampa	Chichester, West Sussex, United Kingdom, : John Wiley & Sons Inc., 2013
ISBN	9781118551462 111855146X 9781118551448 1118551443 9781299465251 1299465250 9781118551455 1118551451
Edizione	[1st ed.]
Descrizione fisica	1 online resource (320 p.)
Classificazione	SCI013050
Altri autori (Persone)	CatlowC. R. A <1947-> (Charles Richard Arthur) WalshAron SokolAlexey A
Disciplina	621.31
Soggetti	Energy storage - Mathematical models Electron distribution - Mathematical models Energy conversion - Mathematical models
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	Computational Approaches to Energy Materials; Contents; About the Editors; List of Contributors; Preface; Acknowledgments; 1 Computational Techniques; 1.1 Introduction; 1.2 Atomistic Simulations; 1.2.1 Basic Concepts; 1.2.2 Parameterization; 1.2.3 Parameter Sets; 1.2.4 Implementation; 1.3 Electronic Structure Techniques; 1.3.1 Wavefunction Methods; 1.3.1.1 Hartree-Fock Theory; 1.3.1.2 Post-Hartree-Fock Approaches; 1.3.1.3 Semi-empirical Wavefunction Methods; 1.3.2 Density Functional Theory; 1.3.2.1 Exchange-Correlation Functionals; 1.3.2.2 Semi-empirical Density Functional Approaches

1.3.3 Excited States  
1.4 Multiscale Approaches; 1.4.1 Hybrid QM/MM Embedding Techniques; 1.4.2 Beyond Atomistic Models; 1.5 Boundary Conditions; 1.6 Point-Defect Simulations; 1.6.1 Mott-Littleton Approach; 1.6.2 Periodic Supercell Approach; 1.7 Summary; References;  
2 Energy Generation: Solar Energy; 2.1 Thin-Film Photovoltaics; 2.2 First-Principles Methods for Electronic Excitations; 2.2.1 Hedin's Equations and the GW Approximation; 2.2.2 Hybrid Functionals; 2.2.3 Bethe-Salpeter Equation; 2.2.4 Model Kernels for TDDFT; 2.3 Examples of Applications; 2.3.1 Cu-Based Thin-Film Absorbers  
2.3.2 Delafossite Transparent Conductive Oxides  
2.4 Conclusions; References;  
3 Energy Generation: Nuclear Energy; 3.1 Introduction; 3.2 Radiation Effects in Nuclear Materials; 3.2.1 Fission; 3.2.1.1 Structural Materials; 3.2.1.2 Fuel; 3.2.1.3 Cladding; 3.2.2 Fusion; 3.2.2.1 Structural Materials; 3.2.2.2 Plasma-Facing Materials; 3.2.3 Waste Disposal; 3.3 Modeling Radiation Effects; 3.3.1 BCA Modeling; 3.3.2 Molecular Dynamics; 3.3.2.1 Cascade Simulations; 3.3.2.2 Sputtering Simulations; 3.3.3 Monte Carlo Simulations; 3.3.3.1 Kinetic Monte Carlo; 3.3.3.2 Object Kinetic Monte Carlo  
3.3.3.3 Transition Rates  
3.3.3.4 Examples; 3.3.4 Cluster Dynamics; 3.3.4.1 Examples; 3.3.4.2 Comparison with OKMC; 3.3.5 Density Functional Theory; 3.3.5.1 Interatomic Potentials; 3.3.5.2 Transition Rates; 3.4 Summary and Outlook; References;  
4 Energy Storage: Rechargeable Lithium Batteries; 4.1 Introduction; 4.2 Overview of Computational Approaches; 4.3 Li-Ion Batteries; 4.4 Cell Voltages and Structural Phase Stability; 4.5 Li-Ion Diffusion and Defect Properties; 4.6 Surfaces and Morphology; 4.7 Current Trends and Future Directions; 4.8 Concluding Remarks; References  
5 Energy Storage: Hydrogen  
5.1 Introduction; 5.2 Computational Approach in Hydrogen Storage Research; 5.3 Chemisorption Approach; 5.4 Physisorption Approach; 5.5 Spillover Approach; 5.6 Kubas-Type Approach; 5.7 Conclusion; References;  
6 Energy Conversion: Solid Oxide Fuel Cells; 6.1 Introduction; 6.2 Computational Details; 6.3 Cathode Materials and Reactions; 6.3.1 Surfaces: LaMnO<sub>3</sub> and (La,Sr)MnO<sub>3</sub> Perovskites; 6.3.1.1 Surface Termination, Surface Point Defects; 6.3.1.2 Oxygen Adsorption and Diffusion; 6.3.1.3 Rate-Determining Step of the Surface Reaction  
6.3.2 Bulk Properties of Multicomponent Perovskites

## Sommario/riassunto

"Outlining their strengths, limitations, contemporary, and future applications, Computational Approaches to Energy Materials is the first authoritative resource to present a broad survey of computational techniques for the development of energy materials. Printed in full color to aid interpretation of materials simulations, this accessible and much-needed text includes all current methodologies based on electronic structure, interatomic potential, and hybrid methods. The methodological components are integrated into a comprehensive survey of applications, addressing the major themes in energy research"--

"This authoritative but accessible text is the first book on the market presenting a broad survey of computational techniques for the development of energy materials, outlining their strengths, limitations, contemporary and future applications"--

2. Record Nr.	UNINA9911019709203321
Autore	Küenzlen Jürgen
Titolo	Anchor Technology in Concrete and Masonry for Practitioners and Engineers : With Recommendations for the Execution and Evaluation of Job Site Tests
Pubbl/distr/stampa	Newark : , : Wilhelm Ernst & Sohn Verlag fur Architektur und Technische, , 2025 ©2025
ISBN	9783433608623 3433608628 9783433608630 3433608636 9783433608654 3433608652
Edizione	[1st ed.]
Descrizione fisica	1 online resource (309 pages)
Collana	Bauingenieur-Praxis Series
Altri autori (Persone)	SchellerEckehard BeckerRainer ImmelThorsten
Soggetti	Anchorage (Structural engineering) Concrete construction
Lingua di pubblicazione	Tedesco
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di contenuto	Cover -- Title Page -- Copyright -- Advertisement -- Contents -- About the Authors -- Advertisement -- Chapter 1 Introduction -- 1.1 General -- 1.2 By Way of an Introduction: A Real Conversation About Anchors in a Private Situation -- 1.3 Anchor Technology for Professionals -- Chapter 2 European Regulations -- 2.1 General -- 2.2 European Technical Assessment (ETA) -- 2.3 CE Marking -- 2.4 The Most Important Regulations Referred to in this Book -- 2.4.1 European and International Standards (DIN EN, ISO) -- 2.4.2 Laws, Directives, Technical Rules -- 2.4.3 European Technical Approval Guidelines (ETAG), European Assessment Documents (EAD) and Technical Reports (TR) -- 2.4.4 European 'Approvals' (ETAs) -- 2.4.5 Test Reports -- Chapter 3 Base Material – In What Material Do I

Want To Fasten My Anchors? -- 3.1 General -- 3.2 Identifying the Base Material on the Construction Site -- 3.2.1 Identifying the Base Material by Means of Construction Documents -- 3.2.1.1 Concrete -- 3.2.1.2 Masonry -- 3.2.2 Identifying the Base Material Without Construction Documents -- 3.2.2.1 Drilling a Test Hole -- 3.2.2.2 Options for Determining the Concrete Compressive Strength

---

Sommario/riassunto

Anchor Technology in Concrete and Masonry for Practitioners and Engineers provides a comprehensive guide for professionals involved in the installation and evaluation of anchors in construction materials. Authored by experts Jürgen Künzlen, Eckehard Scheller, Rainer Becker, and Thorsten Immel, the book covers European regulations, material properties, environmental influences, and anchor systems. It offers detailed discussions on the proper selection and installation of anchors in concrete and masonry, addressing various external conditions such as temperature, fire, and corrosion. The book aims to fill a knowledge gap in the industry by offering practical advice and scientific insights for ensuring safe and effective fastening. It is intended for civil engineers, construction professionals, and researchers who seek to understand the intricacies of anchor technology.

---