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1.3.3 Excited States1.4 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 Oxides2.4 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 Rates3.3.3.4 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: Hydrogen5.1 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: LaMnO3 and (La,Sr) MnO3 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"--
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