1. Record Nr. UNINA9910872195703321

Titolo	Computational Design of Battery Materials / / edited by Dorian A. H. Hanaor
Pubbl/distr/stampa	Cham : , : Springer International Publishing : , : Imprint : Springer, , 2024
ISBN	9783031473036 9783031473029
Edizione	[1st ed. 2024.]
Descrizione fisica	1 online resource (589 pages)
Collana	Topics in Applied Physics, , 1437-0859 ; ; 150
Disciplina	621.312424
Soggetti	Materials Catalysis Force and energy Materials science - Data processing Electric batteries Machine learning Condensed matter Chemistry, Physical and theoretical Materials for Energy and Catalysis Computational Materials Science Batteries Machine Learning Two-dimensional Materials Theoretical Chemistry
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di bibliografia	Includes bibliographical references.
Nota di contenuto	Battery materials: Bringing it all together for tomorrow’s energy storage needs -- Atomistic Simulations of Battery Materials and Processes -- Ab Initio Interfacial Electrochemistry Applied to Understanding, Tuning and Designing Battery Chemistry -- Electrolyte-Electrode Interfaces: A Review of Computer Simulations -- Many-particle Na-ion dynamics in NaMPO4 olivine phosphates (M=Mn, Fe) -- Crystal Structure Prediction for Battery Materials -- Nanoscale Modelling of Substitutional Disorder

in Battery Materials -- Machine learning methods for the design of battery manufacturing processes -- Machine learning methods for the design of battery manufacturing processes -- Applications of Ab Initio Molecular Dynamics for Modeling Batteries -- Forming a Chemically-Guided Basis for Cathode Materials with Reduced Biological Impact using Combined Density Functional Theory and Thermodynamics Modeling -- Oxygen Redox in Battery Cathodes: A Brief Overview -- Theoretical Investigation of Layered Anode Materials -- Design of Improved Cathode Materials by Intermixing Transition Metals in Sodium-Iron Sulphate and Sodium Manganate for Sodium-Ion Batteries -- Sodium Intercalation into Graphite and Graphene Complexes towards Advanced Sodium-Ion Battery Anode Materials -- Combining molecular simulations with modern experiments to design ionic liquid-based battery electrolytes -- Design of battery materials via defects and doping -- Role of Adsorption Energy in the Design of Battery Materials: A DFT Perspective.

Sommario/riassunto

This book presents an essential survey of the state of the art in the application of diverse computational methods to the interpretation, prediction, and design of high-performance battery materials. Rechargeable batteries have become one of the most important technologies supporting the global transition from fossil fuels to renewable energy sources. Aided by the growth of high-performance computing and machine learning technologies, computational methods are being applied to design the battery materials of the future and pave the way to a more sustainable energy economy. In this contributed collection, leading battery material researchers from across the globe share their methods, insights, and expert knowledge in the application of computational methods for battery material design and interpretation. With chapters featuring an array of computational techniques applied to model the relevant properties of cathodes, anodes, and electrolytes, this book provides the ideal starting point for any researcher looking to integrate computational tools in the development of next-generation battery materials and processes.