

| | |
|-------------------------|---|
| 1. Record Nr. | UNINA9910566697403321 |
| Titolo | Transition metal oxides for electrochemical energystorage // edited by Jagjit Nanda, Veronica Augustyn |
| Pubbl/distr/stampa | Weinheim, Germany : , : Wiley-VCH GmbH, , [2022] ©2022 |
| ISBN | 3-527-81725-5 3-527-81722-0 |
| Descrizione fisica | 1 online resource (435 pages) |
| Disciplina | 621.3126 |
| Soggetti | Transition metal oxides Electronic books. |
| Lingua di pubblicazione | Inglese |
| Formato | Materiale a stampa |
| Livello bibliografico | Monografia |
| Nota di bibliografia | Includes bibliographical references and index. |
| Nota di contenuto | Cover -- Title Page -- Copyright -- Contents -- Foreword -- Chapter 1 An Overview of Transition Metal Oxides for Electrochemical Energy Storage -- 1.1 Fundamentals of Electrochemical Cells -- 1.2 Lilon Batteries: Basic Principles and TMO Electrodes -- 1.3 Brief History of Lithiumlon Batteries -- 1.4 The Role of Advanced Characterization and Computing Resources -- 1.5 Beyond Lithiumlon Batteries -- Acknowledgments -- References -- Chapter 2 Metal-IonCoupled Electron Transfer Kinetics in IntercalationBased Transition Metal Oxides* -- 2.1 Introduction -- 2.2 Thermodynamic Control -- 2.3 Diffusional Control -- 2.4 Kinetic Control -- 2.5 Effect of Surface Layers on Ion Transfer Kinetics -- 2.6 Slow Desolvation as a Limiting Intercalation Step -- 2.7 Concluding Remarks -- References -- Chapter 3 NextGeneration CobaltFree Cathodes - A Prospective Solution to the Battery Industry's Cobalt Problem* -- 3.1 Introduction -- 3.2 Potential of CobaltFree Cathode Materials -- 3.3 Layered Cathodes -- 3.3.1 Conventional Layered Cathodes -- 3.3.2 Binary Layered NiRich Cathode Materials -- 3.3.3 Ternary Layered NiRich Cathode Materials -- 3.4 Spinel and Olivine Cathodes -- 3.5 Disordered Rocksalt (DRX) Cathodes -- 3.6 Challenges in Commercial Adoption of New Cobalt Free Chemistries -- 3.6.1 Synthesis of Cathode Precursors -- 3.6.2 Synthesis of Final Cathode Powders -- 3.6.3 Electrode Fabrication -- |

3.6.4 Battery Assembly -- 3.7 Summary and Perspective --
Acknowledgments -- Conflict of Interest -- References -- Chapter 4
Transition Metal Oxide Anodes for Electrochemical Energy Storage in
Lithium and Sodium Ion Batteries* -- 4.1 Introduction -- 4.2 Potential
Advantages and Challenges of the Conversion Mechanism -- 4.3
Transition Metal Oxides as Anode Materials -- 4.3.1 Iron Oxide (Fe_3O_4 ,
 Fe_2O_3) -- 4.3.2 Cobalt Oxide (CoO , Co_3O_4).
4.3.3 Manganese Oxide (MnO , Mn_3O_4 , MnO_2) -- 4.3.4 Copper Oxide
(Cu_2O , CuO) -- 4.3.5 Nickel Oxide (NiO) -- 4.3.6 Ruthenium Oxide
(RuO_2) -- 4.3.7 Other Transition Metal Oxides -- 4.4 Summary and
Outlook -- References -- Chapter 5 Layered Nalon Transition Metal
Oxide Electrodes for Sodium Ion Batteries -- 5.1 Introduction -- 5.2
Layered Transition Metal Oxides -- 5.2.1 Structural Classification --
5.2.2 Single Transition Metal Based Layered Transition Metal Oxides --
5.2.3 Mixed Metal Based Layered Transition Metal Oxides -- 5.2.4
Anionic Redox Activity for High Capacity -- 5.3 Summary and Outlook
-- References -- Chapter 6 Anionic Redox Reaction in Li Excess High
Capacity Transition Metal Oxides -- 6.1 Stoichiometric Layered Oxides
for Rechargeable Lithium Batteries -- 6.2 Li Excess Rocksalt Oxides as
High Capacity Positive Electrode Materials -- 6.3 Reversible and
Irreversible Anionic Redox for Li_3NbO_4 and Li_2TiO_3 Based Oxides --
6.4 Activation of Anionic Redox by Chemical Bonds with High Ionic
Characters -- 6.5 Li_4MoO_5 as a Host Structure for Lithium Excess
Oxides -- 6.6 Extremely Reversible Anionic Redox for Li_2RuO_3 System
-- 6.7 Anionic Redox for Sodium Storage Applications -- 6.8 Future
Perspectives of Anionic Redox for Energy Storage Applications --
References -- Chapter 7 Transition Metal Oxides in Aqueous
Electrolytes -- 7.1 Introduction: Opportunities and Challenges of
Aqueous Batteries -- 7.2 Electrochemistry of Aqueous Batteries --
7.2.1 Potential Window -- 7.2.2 Diverse Charge Transfer and Storage
Processes in Aqueous Batteries -- 7.2.2.1 Overview of Various Storage
Mechanisms -- 7.2.2.2 Semiquantitative Analysis of Storage
Mechanism from Sweeping Voltammetry Analysis -- 7.2.2.3 Storage
Mechanisms in Electrolyte with Different pH Values -- 7.3 Transition
Metal Oxides for Aqueous EES -- 7.3.1 Manganese Compounds.
7.3.1.1 Crystal Structures of Manganese Oxides for Aqueous Storage --
7.3.1.2 Compositing Manganese Oxides with Other Additives -- 7.3.1.3
Surface Engineering Crystal Facets, Edge Sites, and Bulk/Nano Size
Domain -- 7.3.1.4 Doping and Defect Chemistry -- 7.3.1.5 Pre
intercalated Species -- 7.3.2 Ni Compounds -- 7.3.3 Vanadium
Compounds -- 7.3.3.1 Li or Na Vanadates -- 7.3.4 Iron Compounds --
7.3.4.1 $\text{Fe}/\text{Fe}_3\text{O}_4$ -- 7.3.4.2 $\text{Fe}_2\text{O}_3/\text{FeOOH}$ -- 7.4 Conclusion --
Acknowledgments -- References -- Chapter 8 Nanostructured
Transition Metal Oxides for Electrochemical Energy Storage -- 8.1
Fundamental Electrochemistry of Nanostructured TMOs -- 8.1.1
Thermodynamics of Charge Storage in Nanostructured TMOs -- 8.1.2
Kinetics of Charge Storage in Nanostructured TMOs -- 8.2 Emerging
Nanostructured TMOs -- 8.2.1 Nanostructured TMO Cathodes for LIBs
-- 8.2.2 Nanostructured Binary TMOs for Conversion Type Charge
Storage -- 8.2.3 Nanostructured Binary TMOs for Intercalation Type
Charge Storage -- 8.3 Implementation of Nanostructured TMOs in
Electrode Architectures -- 8.3.1 One Dimensional and Two Dimensional
Architectures -- 8.3.1.1 Nanowires and Nanotubes -- 8.3.2 Three
Dimensional Architectures -- 8.3.2.1 Assemblies -- 8.3.2.2 Foams --
8.3.2.3 Aerogels -- 8.4 Conclusions -- References -- Chapter 9
Interfaces in Oxide Based Li Metal Batteries* -- 9.1 Introduction -- 9.2
Solid Oxide Electrolytes -- 9.3 Cathode: Toward True Solid -- 9.3.1
Origin of Interfacial Impedance and Current Pressing Issues at

Cathode/Solid Electrolyte Interfaces -- 9.3.1.1 Interfacial Reaction During Cell Fabrication -- 9.3.1.2 Electrochemical Oxidation and Chemical Reaction During Cycle -- 9.3.1.3 Chemomechanical Degradation During Cycling -- 9.3.2 Strategies and Approaches Toward Enhanced Stability and Performance -- 9.3.2.1 Cathode Coating. 9.3.2.2 Geometric Arrangement Concerns and Strategies Toward Maximizing Reaction Sites -- 9.3.2.3 Conductive Additives in Solid State Cathode -- 9.4 Anode: Adopting Lithium Metal in the Solid -- 9.4.1 Li/Solid-Electrolyte Interface: Chemical, Electrochemical, and Mechanical Considerations, Including Mitigation Strategies -- 9.4.2 Li Dendrite Formation and Propagation in Solid Electrolytes: Challenges and Strategies -- 9.5 Outlook and Perspective -- Acknowledgments -- Contributions -- Ethics Declarations -- References -- Chapter 10 Degradation and Life Performance of Transition Metal Oxide Cathodes used in Lithium Ion Batteries -- 10.1 Introduction -- 10.2 Degradation Trends -- 10.3 Transition Metal Oxide Cathodes -- 10.3.1 Spinel Cathodes -- 10.3.2 NCM System of Cathodes -- 10.3.3 NCMA Cathodes -- 10.4 Degradation Mechanism -- 10.5 Concluding Remarks -- References -- Chapter 11 Mechanical Behavior of Transition Metal Oxide Based Battery Materials -- 11.1 Introduction -- 11.2 Mechanical Responses to Compositional Changes -- 11.2.1 Volume Changes and Deformation in Electrode Particles -- 11.2.2 Particle Fracture -- 11.3 Impact of Strain Energy on Chemical Phenomena -- 11.3.1 Thermodynamics -- 11.3.2 TwoPhase Equilibrium -- 11.4 Solid Electrolytes -- 11.4.1 Electrode/Electrolyte Interfaces -- 11.4.2 Electrolyte Fracture -- 11.5 Summary -- References -- Chapter 12 SolidState NMR and EPR Characterization of TransitionMetal Oxides for Electrochemical Energy Storage -- 12.1 Introduction -- 12.2 Brief Introduction of NMR Basics -- 12.2.1 Nuclear Spins -- 12.2.2 NMR Spin Interactions -- 12.2.3 Paramagnetic Interactions and Experimental Approaches to Achieve High Spectral Resolution -- 12.3 Multinuclear NMR Studies of Transitionmetaloxide Cathodes -- 12.3.1 Li Extraction and Insertion Dynamics -- 12.3.2 O Evolution -- 12.4 EPR Studies -- 12.5 Summary. References -- Chapter 13 In Situ and In Operando Neutron Diffraction of Transition Metal Oxides for Electrochemical Storage -- 13.1 Introduction -- 13.1.1 Neutron Diffraction and Transition Metal Oxides -- 13.1.1.1 Neutron Reflectometry -- 13.1.1.2 SmallAngle Neutron Scattering -- 13.1.1.3 Quasielastic and Inelastic Neutron Scattering -- 13.1.2 Neutron Diffraction Instrumentation -- 13.1.3 In Situ and In Operando Neutron Diffraction -- 13.2 Device Operation -- 13.2.1 Experimental Design and Approach to the RealTime Analysis of Battery Materials -- 13.2.2 Advancements in Understanding Electrode Structure During Battery Operation -- 13.3 Gas and Temperature Studies -- 13.3.1 Experimental Design and Approach to the In Situ Study of Solid Oxide FuelCell (SOFC) Electrodes -- 13.3.2 Advancements in Understanding Solid Oxide FuelCell Electrode Function -- 13.4 Materials Formation and Synthesis -- 13.5 ShortRange Structure -- 13.6 Outlook -- Acknowledgments -- References -- Chapter 14 Synchrotron Xray Spectroscopy and Imaging for Metal Oxide Intercalation Cathode Chemistry -- 14.1 Introduction -- 14.2 Xray Absorption Spectroscopy -- 14.2.1 Soft Xray Absorption Spectroscopy -- 14.2.2 Hard Xray Absorption Spectroscopy -- 14.3 RealSpace Xray Spectroscopic Imaging -- 14.3.1 2D FullField Xray Imaging -- 14.3.2 Xray Tomographic Imaging -- 14.4 Conclusion -- References -- Chapter 15 AtomicScale Simulations of the Solid Electrolyte Li₇La₃Zr₂O₁₂ -- 15.1 Introduction -- 15.1.1 Motivation -- 15.1.2 Solid Electrolytes -- 15.1.3 Li₇La₃Zr₂O₁₂ (LLZO) -- 15.1.4 Challenges

-- 15.2 Elastic Properties of $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ -- 15.3 Potential Failure Modes Arising from LLZO Microstructure -- 15.4 Conclusions -- Acknowledgements -- References.

Chapter 16 Machine Learning and Data Intensive Methods for Accelerating the Development of Rechargeable Battery Chemistries: A Review.
