Contents

Preface *xix*

1 **Fundamentals of Nanomaterials in Energy Systems** *1*
Ricardo Antonio Escalona-Villalpando, Fabiola Ilian Espinosa-Lagunes, Luis Gerardo Arriaga Hurtado, and Janet Ledesma-García
1.1 Introduction *1*
1.1.1 Nanomaterials in Battery Systems *2*
1.1.2 Nanomaterials in Fuel Cells *5*
1.1.3 Nanocatalysts for Fuel Oxidation *6*
1.1.4 Nanomaterials for Photovoltaic Cells *7*
1.1.5 Nanomaterials for the Application of Capacitors *9*
1.1.6 Carbon Nanomaterials *9*
1.1.6.1 Activated Carbon *10*
1.1.7 Metal Oxides/hydroxides *10*
1.1.8 Conductive Polymers *11*
1.2 Conclusions *12*
References *12*

2 **Basics of Surface Defects: Types, Formation, and Impact** *17*
H. Rojas-Chávez, M.A. Valdés-Madrigal, and J. M. Juárez-García
2.1 Introduction *17*
2.2 Surface Defect Typology *18*
2.2.1 Grain Boundaries *18*
2.2.2 Twins *19*
2.2.3 Stacking Faults (Piling-Up Faults) *20*
2.2.4 Phase Boundaries *20*
2.2.5 External Surfaces (Free Surfaces) *20*
2.3 Surface Defect Formation *21*
2.4 Impact of 2D Defects *23*
2.4.1 Energy Production *23*
2.4.2 Energy Storage *25*
2.5 Concluding Remarks *25*
References *26*

3 Fundamentals of Interfacial Defects in Materials Science: Types, Formation, and Classification *29*
J. Moroni Mora Muñoz, I. Olvera Rodríguez, L. J. Salazar-Gastélum, and R. Castellanos-Espinoza
3.1 Interfacial Defects *29*
3.2 Grain Boundaries: Low-Angle and High-Angle Grain Boundaries *29*
3.2.1 Low-Angle Grain Boundaries (LAGBs) *30*
3.2.2 High-Angle Grain Boundaries (HAGBs) *30*
3.2.3 Coherent Phase Boundaries *31*
3.2.4 Semi-coherent Phase Boundaries *31*
3.2.5 Incoherent Phase Boundaries *32*
3.3 Twin Boundaries: Symmetrical Interfaces Within a Crystal *32*
3.3.1 Growth Twins and Annealing Twins *32*
3.3.2 Deformation Twins *33*
3.4 Free Surface Defects: Influence on Solid Interface Interactions with Other Phases *33*
3.4.1 Nature and Formation of Free Surface Defects *33*
3.4.2 Influence of Free Surface Defects at Solid–Liquid Interfaces *34*
3.4.3 Engineering-Free Surface Defects for Optimized Material Performance *35*
3.5 Impact of Interfacial Defects on the Material Properties *35*
3.5.1 Impact of Interfacial Defects on Mechanical Properties: Enhancing Strength, Toughness, and Durability *35*
3.6 Grain Boundaries and Strengthening Mechanisms *36*
3.6.1 Dislocations: Phonon Interactions and Thermal Conductivity Reduction *36*
3.6.2 Voids: Interruptions in Thermal Pathways *37*
3.6.3 Free Surface Defects: Enhancing or Impeding Thermal Conductivity *37*
3.7 Optical and Photocatalytic Properties: Enhancing Light Absorption and Catalysis *37*
3.7.1 Recombination Centers and Lower Charge Mobility: Grain Boundaries *37*
3.7.2 Voids: Scattering Centers Affecting Light Absorption *38*
3.7.3 Phase Mismatches: Challenges in Band Alignment and Charge Transfer *38*
3.8 Free Surface Defects: Impact on Surface States and Carrier Dynamics *39*
3.8.1 Barrier and Chemical Properties: Enhancing Permeability and Selectivity *39*
3.8.2 Grain Boundaries: Facilitating Enhanced Permeability *39*
3.8.3 Dislocations: Influence on Molecular Pathways *40*
3.8.4 Phase Mismatches: Challenges in Selective Transport *40*
3.9 Role of Free Surface Defects on the Enhanced Permeability *41*
3.9.1 Catalysis and Surface Reactivity: Free Surface Defects *41*
3.9.1.1 Grain Boundaries: Enhanced Catalytic Activity *41*

3.9.2 Voids: Balancing Surface Area and Stability *41*
3.9.3 Phase Mismatches: Effects on Charge Movement and Efficiency *42*
3.9.4 Free Surface Defects: Increasing Surface Reactivity *42*
3.10 Conclusions *43*
References *43*

4 Thermodynamics and Kinetics of Formation of Surface and Interfacial Defects *47*
Juan Hernández-Tecorralco and Carlos M. Ramos-Castillo
4.1 Defects in Thermodynamic Equilibrium *47*
4.1.1 Configurational Entropy *47*
4.1.2 Thermodynamics of Defect Reactions *50*
4.1.3 Charged Point Defects and Their Ionization *50*
4.1.4 Schottky Defects *52*
4.1.5 Oxygen Partial Pressure Dependence of Schottky Defects *52*
4.1.6 Frenkel Defects *52*
4.2 The Kinetics of Defect Formation *53*
4.2.1 Arrhenius Equation and Thermally Activated Processes *54*
4.2.2 Mechanism of Defect Formation *55*
4.2.3 Diffusion and Fick's Laws *56*
4.3 Summary *58*
References *58*

5 Defects as Catalytic Sites in Energy Chemistry *61*
Beatriz Ruiz Camacho, Adriana Medina Ramírez, and José de Jesús Ramírez Minguela
5.1 Defects as Active Sites *61*
5.2 Defects as Active Sites for Electrochemical Reactions *62*
5.2.1 Oxygen Reduction Reaction (ORR) *63*
5.2.2 Hydrogen and Oxygen Evolution Reactions (HER/OER) *64*
5.2.3 CO_2 Reduction Reaction (CO_2RR) *66*
5.2.4 Nitrogen Photoreduction to Ammonia (NH_3) *67*
5.3 Synthesis Methods for Defects *68*
5.3.1 Preparation Methods of Vacancy Defects *68*
5.3.2 Preparation Methods of Doping Defects *69*
5.4 Identification of Defects *70*
5.4.1 X-Ray Diffraction (XRD) *70*
5.4.2 Electron Microscopy (TEM, HRTEM/STEM) *70*
5.4.3 X-Ray Photoelectrons Spectroscopy (XPS) *71*
5.4.4 Raman Spectroscopy *71*
5.4.5 Electron Paramagnetic Resonance (EPR) Spectroscopy *71*
5.4.6 X-Ray Absorption Spectroscopy (XAS) *71*
5.5 Conclusion and Perspectives *71*
References *72*

6 Advanced Characterization Techniques for Defect and Interface Engineering *75*
José Béjar and Alfredo Aguilar-Elguezabal
6.1 Introduction *75*
6.2 Electron Microscopy Techniques *75*
6.3 X-Ray Diffraction (XRD) *77*
6.4 X-Ray Photoelectron Spectroscopy (XPS) *79*
6.5 Raman Spectroscopy *80*
6.6 Electron Paramagnetic Resonance (EPR) *82*
6.7 Fourier Transform Infrared (FTIR) Spectroscopy *85*
6.8 Conclusions *86*
References *86*

7 Computational Modeling of Defects in Nanomaterials *89*
Carlos M. Ramos-Castillo and Juan Hernández-Tecorralco
7.1 Defects Stability by Density Functional Theory *89*
7.1.1 Fundamentals on Density Functional Theory *89*
7.1.2 Defect Formation Energy *94*
7.1.3 Electronic Structure of Defects *95*
7.2 Electronic Descriptors in Catalysis *97*
7.2.1 The d-Band Center in Defective Materials *98*
7.2.2 The Newns–Anderson Model for Chemisorption *98*
7.2.3 Computational Hydrogen Electrode *101*
7.2.4 Example: Layered Double Hydroxide with Oxygen Vacancies *104*
7.2.5 Solvent Effects *105*
7.2.6 Outlook *105*
References *106*

8 Defect Healing and Control Strategies in Energy Systems *109*
César Coello-Mauléón, Carlos Guzmán-Martínez, and Noé Arjona
8.1 Introduction to Self-Healing Systems *109*
8.2 Thermodynamics and Kinetics Implication on Self-Healing Systems *110*
8.3 Mechanism Inside of Self-Healing *112*
8.4 Coupled Self-Healing in Electrodes, Electrolytes, and Interfaces *115*
8.5 Real-Time Monitoring *120*
8.6 Future Perspectives *122*
References *123*

9 Future Frontiers in Defect Science for Advanced Energy Technologies *127*
Lorena Álvarez Contreras, Noé Arjona, and Minerva Guerra Balcázar
9.1 Introduction *127*
9.2 Evolving Paradigms: Trends and Prospects in Defect-Driven Nanomaterials *128*

9.2.1 Advanced Characterization of Defects in Energy Materials *129*
9.2.2 Expanding the Role of Defect Engineering Beyond Catalysis *129*
9.2.3 Real-Time Tracking of Defect Evolution *131*
9.3 Intersection with Other Disciplines: Collaborations and Synergies *133*
9.3.1 Computational Materials Science and Data-Driven Approaches *133*
9.3.2 Bioinspired Design and Nanofabrication *134*
9.3.3 Industrial Partnerships and Translational Research *135*
9.4 Roadmap for Future Research in Surface and Interfacial Defects in Nanomaterials *136*
9.4.1 Future Research Thrusts in Defect Engineering *138*
9.5 Conclusions *139*
References *139*

10 Defects and Interface Engineering of MXenes: Heterojunction Hybrid Catalysts for Hydrogen Production *143*
Divyadharshini Satheesh, Gouranga Maharana, Rekha Pachaiappan, Kovendhan Manavalan, and D. Paul Joseph
10.1 Defects *143*
10.1.1 Point Defects *143*
10.1.2 Line Defects *144*
10.1.3 Planar Defects *144*
10.1.4 Volume Defects *144*
10.2 Interface Engineering: A Brief Introduction *145*
10.2.1 Interfacial Engineering in Nanomaterials *145*
10.3 Influence of Defects and Interfaces on the Characteristics of Materials *145*
10.3.1 Doping Strategy for Interface Technique *146*
10.3.2 Morphological Interface *146*
10.4 Introduction to Hydrogen Production *147*
10.4.1 What Is Hydrogen? *147*
10.4.2 How Is Hydrogen Produced? *147*
10.4.2.1 Steam-Reforming Method *147*
10.4.2.2 Hydrogen from Biomass *149*
10.4.2.3 Electrochemical Hydrogen Generation *149*
10.5 2D MXenes for Hydrogen Evolution Reactions *149*
10.5.1 Synthesis of MXenes *150*
10.5.1.1 Fluoride Etching Technique *150*
10.5.1.2 Alkali Etching Method *151*
10.5.1.3 Water-Free Etching Technique *151*
10.5.2 Single MXene for HER Studies *153*
10.5.3 Heterostructures of MXene for HER *154*
10.5.4 Characteristics of MXenes in Electrocatalysis *157*
10.6 Conclusion *158*
10.7 Future Perspectives *158*
References *159*

11 Defect and Interface Engineering in Electrocatalytic CO_2 Reduction *163*
Narmadha Maharajan, Sampathkumar Prakasam, and Suresh Chinnathambi
11.1 Introduction *163*
11.2 Types of Defects *164*
11.3 Methods to Create Defects *165*
11.3.1 Thermal Treatment *165*
11.3.2 Plasma Etching *166*
11.3.3 Elemental Doping *166*
11.3.4 Defects Creation by Using Chemicals *166*
11.3.5 Phase Transformation *166*
11.3.6 Ion Exchange Membrane *166*
11.4 Characterization of Defects *166*
11.5 Defect Engineering in Metal Electrocatalysts *167*
11.5.1 Impact of Creating Vacancies in CO_2RR *167*
11.5.1.1 Role of Anion and Cation Vacancy for Generation of Defects *168*
11.5.2 Influence of Lattice Defects in CO_2RR *168*
11.5.2.1 Lattice Strain *169*
11.5.2.2 Lattice Disorder *170*
11.5.3 Grain Boundaries in CO_2RR *170*
11.6 Effect of Surface Defect Sites on CO_2RR *170*
11.6.1 Impact of Defects in Single/Bimetallic Materials *171*
11.6.2 Defect-Induced Metal Alloys for CO_2RR *171*
11.6.3 Impact of Defects on Metal Oxides and its CO_2RR *171*
11.6.4 Surface and Defect Aspects in Metal Sulfide Electrocatalysts *172*
11.6.5 Role of Defects in Metal Nitrides for CO_2RR *172*
11.7 Impact of Defects in Carbon-Based Materials for CO_2RR *173*
11.8 Intrinsic Defect *173*
11.9 Single-Metal Atom Sites *174*
11.10 Challenges and Perspectives in CO_2RR *175*
11.11 Conclusion *176*
Acknowledgement *176*
References *176*

12 Defect and Interface Engineering in Fuel Production *179*
I. Velázquez-Hernández and M. Estévez
12.1 Catalytic Defects in Alternative Fuel Synthesis *179*
12.2 Interfacial Considerations in Fuel Production *180*
12.2.1 Heterogeneous Catalyst Interfaces *180*
12.2.2 Metal–Support Interactions (MSIs) *182*
12.3 Defect-Engineered Nanomaterials for Precision Fuel Synthesis *183*
12.3.1 Defect-Mediated Pathways for Alternative Fuel Production *183*
12.3.1.1 CO_2 Reduction *183*
12.3.1.2 Methanol Synthesis *183*
12.3.1.3 Ammonia Synthesis *183*

12.3.1.4 Biodiesel Production *184*
12.4 Innovative Catalysts for Sustainable Fuel Synthesis *185*
12.4.1 Single-Atom Catalysts (SACs) *185*
12.4.2 MXene-Based Catalysts *186*
12.5 Integration of Defects in Electrochemical Fuel Production *186*
12.6 Conclusions *187*
References *187*

13 Defect and Interface Engineering in Electrochemical Valorization of Biomass to Value-Added Chemicals *191*
Sampathkumar Prakasam, Narmadha Maharajan, and Suresh Chinnathambi
13.1 Introduction *191*
13.2 Defect Engineering and Its Types *193*
13.2.1 Point Defects *193*
13.2.2 Extended Defects *194*
13.3 Biomass Valorization and Its Types *194*
13.3.1 Biorefinery Concept *194*
13.3.2 Thermochemical Conversion *194*
13.3.2.1 Pyrolysis, Combustion, and Gasification *194*
13.3.3 Biochemical Conversion *195*
13.3.3.1 Fermentation, Anaerobic Digestion, and Enzymatic Hydrolysis *195*
13.3.4 Hydrothermal Processing *195*
13.3.5 Supercritical Fluid Processing *195*
13.3.6 Electrochemical Valorization *195*
13.4 Defects and Interface Engineering in Electrochemical Valorization of Biomass *196*
13.4.1 Defect-Induced Chemical and Fuel Synthesis from Cellulose and Hemicellulose *196*
13.4.1.1 Synthesis of Polyols *196*
13.4.1.2 Electro-valorization of Glycerol *198*
13.4.1.3 Electro-valorization of Furans *199*
13.4.1.4 5-Hydroxymethyl Furfural (5-HMF) *200*
13.4.1.5 Electro-valorization of Furfural *200*
13.4.1.6 Chemical Intermediates and Fuels from Lignin *203*
13.5 Challenges in Electrochemical Biomass Valorization *204*
13.6 Future Perspectives and Conclusions *204*
References *205*

14 Defect and Interface Engineering in Fuel Cells *209*
Minerva Guerra Balcázar, Carlos Guzmán Martínez, and Alejandra Álvarez López
14.1 Impact of Defects on Electrocatalytic Activity *209*
14.2 Defects on Noble Metal-Based Catalysts *210*
14.3 Defects in Alternative Non-platinum Catalysts *213*

14.4 Carbon-Based Materials and Their Modification with Defects *214*
14.5 Conclusions and Future Perspectives *214*
References *215*

15 Defect and Interface Engineering in Electrolyzers *217*
J.C. Cruz, B. Pamplona Solis, K. García Uitz, and M.P. Gurrola
15.1 Introduction to Electrolyzers *217*
15.1.1 Proton Exchange Membrane Electrolyzer (PEMEL) *218*
15.1.2 Alkaline Electrolyzer *219*
15.2 Materials Used as Catalysts in Electrolyzers *219*
15.2.1 Electrocatalysts for PEMEL *221*
15.2.2 Electrocatalysts for AEL *221*
15.2.3 Pourbaix Diagram for Water Electrolysis *222*
15.3 Components of an Electrolysis System *224*
15.3.1 Components of an AEL-Type Electrolyzer *224*
15.3.2 Components of a PEMEL-Type Electrolyzer *225*
15.4 Common Problems in Materials Engineering *225*
15.4.1 AEL System *225*
15.4.2 PEMEL System *226*
15.5 Future Trends of PEMEL, AEL, and AEMEL *226*
15.6 Conclusions *227*
References *228*

16 Defect and Interface Engineering for the Oxygen Reduction Reaction *233*
Heriberto Cruz-Martínez, Lidia Santiago-Silva, Brenda García-Hilerio, and Víctor A. Franco-Luján
16.1 Introduction *233*
16.2 Types and Effects of Defects in Graphene for ORR *234*
16.3 Roles of Vacancies in Graphene for ORR *234*
16.4 Roles of Doping in Graphene for ORR *237*
16.5 Conclusions *240*
Acknowledgments *241*
References *241*

17 Defect and Interface Engineering in Li-Ion Batteries *247*
Jesús Adrián Díaz–Real
17.1 Introduction *247*
17.2 Defect Engineering in Li-Ion Batteries *248*
17.2.1 Types of Defects and Their Mechanisms *248*
17.2.1.1 Point Defects *248*
17.2.1.2 Extended Defects *248*
17.2.1.3 Planar Defects *249*
17.2.2 Effects on Electrochemical Performance *249*
17.2.2.1 Charge Transport *249*
17.2.2.2 Structural Stability *249*

17.2.2.3 Energy Density and Capacity *249*
17.2.3 Methods for Defect Creation and Control *250*
17.2.3.1 Chemical Doping *250*
17.2.3.2 Thermal and Mechanical Treatments *250*
17.2.3.3 Non-equilibrium Synthesis *250*
17.2.4 Challenges and Future Directions *250*
17.3 Interface Engineering in Li-Ion Batteries *251*
17.3.1 Role of Interfaces in Battery Performance *251*
17.3.2 Strategies for Interface Optimization *251*
17.3.2.1 Surface Coatings and Modifications *251*
17.3.2.2 Interface Doping *252*
17.3.2.3 Solid–Electrolyte Interface (SEI) Engineering *252*
17.3.2.4 Advanced Surface Engineering Techniques *252*
17.3.3 Case Studies in Interface Engineering *252*
17.3.4 Challenges and Future Directions *252*
17.4 Experimental Techniques and Analytical Methods *253*
17.4.1 Characterization of Defect Analysis *253*
17.4.1.1 Microscopy-Based Techniques *253*
17.4.1.2 Spectroscopy-Based Techniques *253*
17.4.1.3 Crystallographic Techniques *254*
17.4.2 Interfacial Characterization Techniques *254*
17.4.2.1 Ex Situ Techniques *254*
17.4.2.2 In Situ and Operando Techniques *254*
17.4.3 Emerging Techniques *255*
17.5 Challenges and Future Directions *255*
17.5.1 Challenges in Defect and Interface Engineering *255*
17.5.1.1 Defect Density vs Material Stability *255*
17.5.1.2 Interfacial Degradation *256*
17.5.1.3 Manufacturability and Scalability of Processes *256*
17.5.2 Future Directions *256*
17.6 Conclusions *257*
References *258*

18 Defects and Interface Engineering in Na-Ion Batteries *261*
Zhen-Yi Gu, Xiao-Tong Wang, Xin-Xin Zhao, and Xing-Long Wu
18.1 Defects in Electrode Materials *261*
18.1.1 Defect Type *261*
18.1.2 Defect-Modulated Pure Phase *263*
18.2 Interface Engineering *264*
18.2.1 Air Stability *264*
18.2.2 Electrode–Electrolyte Interphase *266*
18.2.3 Solid-State Electrolyte *269*
18.2.4 Binder *270*
18.3 Summary *272*
References *273*

19 **Defect and Interface Engineering in K-Ion Batteries** *277*
Yahreli Audeves-Audeves, Raúl Castellanos-Espinoza, and Minerva Guerra Balcázar
19.1 Introduction to Potassium-Ion Batteries *277*
19.2 Defect Engineering in Materials of Potassium-Ion Batteries *279*
19.3 Defects in Anode Materials Used in PIBs *280*
19.3.1 Intrinsic Defect Carbon-Based Materials *281*
19.3.1.1 Vacancies in Carbon-Based Anodes *281*
19.3.2 Edge-Defect in Carbon-Based Anodes *281*
19.3.3 Extrinsic Defects Carbon-Based Materials *282*
19.3.3.1 Vacancies/Doping in Carbon-Based Anodes *282*
19.3.3.2 Vacancies/Doping with Order-in-Disorder Engineering in Carbon-Based Anodes *282*
19.3.4 Intercalation and Storage of Metal Ions in Graphite Anodes *283*
19.4 Defects in Cathode Materials Used in PIBs *283*
19.4.1 Prussian Blue Analogs (PBAs) *284*
19.4.2 MXenes *285*
19.4.3 Transition Metal Oxides *285*
19.4.4 Polyanionic Compounds *286*
19.4.5 Transition Metal Sulfides *286*
19.5 Recent Advances in PIBs Through Defect/Interface Engineering *287*
19.6 Applications and Future Perspectives *287*
References *288*

20 **Defect and Interface Engineering in Lithium-Air Batteries** *293*
Lorena Álvarez Contreras and J. Antonio Cruz-Navarro
20.1 Electrochemical Dynamics of Li-Air Systems *293*
20.2 Defect-Driven Modulation of Lithium Reactivity *294*
20.3 Interface Engineering for Precision Oxygen Reaction *295*
20.4 Defect-Induced Stability Enhancements *296*
20.5 Interfaces and Long-Term Cyclability in Li-Air Systems *302*
20.6 Future Perspectives in Defect and Interface Engineering for Li-Air Batteries *303*
20.7 Conclusion *304*
References *305*

21 **Defect and Interface Engineering in Zinc-Air Batteries** *309*
Alejandro Arredondo-Espínola and Noé Arjona
21.1 Introduction to Zinc-Air Batteries *309*
21.2 Types of Bifunctional Electrocatalyst for ZABs *311*
21.2.1 Noble Metals *311*
21.2.2 Transition Metals *312*
21.2.3 Carbonaceous Materials *312*
21.3 Defect and Interface Engineering Applied to Electrocatalysts *313*

21.3.1 Heteroatomic Doping *313*
21.3.2 Edge Sites *313*
21.3.3 Strain Defects *314*
21.3.4 Vacancies *315*
21.4 Interface and Defect Engineering Applied to Different Rechargeable Zinc-air Batteries *315*
21.4.1 Aqueous/Flow Zinc-Air Batteries *315*
21.4.2 Flexible Zinc-Air Batteries *320*
21.5 Conclusions and Perspectives *322*
References *322*

22 Addressing Surface and Interfacial Defects in Lithium–Sulfur Batteries *327*
Alexander Suárez-Barajas and Noé Arjona
22.1 Introduction *327*
22.2 Lithium–Sulfur Batteries: Benefits and Mechanisms *328*
22.2.1 Fundamental Advantages *328*
22.3 Challenges in Lithium–Sulfur Batteries *328*
22.3.1 Volumetric Expansion of Sulfur *329*
22.3.2 Low Conductivity of Sulfur *329*
22.3.3 Polysulfide Dissolution and the Shuttle Effect *329*
22.3.4 Lithium Metal Anode Challenges *330*
22.4 Impact of Surface and Interfacial Defects in LSBs *330*
22.5 The Effect on Sulfur Cathodes in Li–S Batteries *331*
22.5.1 Heterostructures: Enhancing Redox Kinetics *331*
22.5.2 Vacancies: Unlocking Active Sites *331*
22.5.3 Doping: Tailoring Electronic Properties *332*
22.5.4 Single-Atom Catalysts: Redefining Efficiency *333*
22.6 Effects of Surface Defects on Separators and Their Role in Addressing Li–S Battery Challenges *334*
22.6.1 Engineering Vacancies in Separator Materials *334*
22.6.2 Doping to Enhance Separator Functionality *335*
22.6.3 Heterostructures for Synergistic Performance *335*
22.6.4 Single-Atom Catalysts (SACs) for Precision Catalysis *336*
22.7 Surface and Interfacial Defects in Lithium Metal Anodes for Li–S Batteries *337*
22.7.1 Protective Coatings and Interlayers *337*
22.7.2 Stable SEI Formation *338*
22.7.3 Non-Dendritic Lithiation and Uniform Lithium Deposition *339*
22.8 Conclusions and Future Perspectives *340*
References *340*

23 Engineering Defects in Advanced Battery Systems *343*
María Fernanda Bósquez-Cáceres, Juan P. Tafur, and Vivian Morera Córdova
23.1 Introduction to Advanced Battery Technologies *343*

23.1.1 Overview of Current Battery Technologies *343*
23.1.2 Current Limitations in Battery Technologies *345*
23.1.3 Opportunities Offered by Defect Engineering *345*
23.2 Fundamentals of Defect Engineering in Batteries *346*
23.2.1 Types of Defects in Battery Materials and Their Impact on Electrochemical Properties *346*
23.2.2 Defect Formation Mechanisms and Methodologies of Insertion in Battery Materials *349*
23.2.3 Characterization Techniques for Defect Analysis *350*
23.2.4 Defect Modeling *351*
23.3 Case Studies: Enhancing the Performance of Advanced Battery Systems *351*
23.3.1 Defect Engineering in Anode Materials *351*
23.3.2 Defect Engineering in Cathode Materials *353*
23.3.3 Defect Engineering in Solid Electrolytes *354*
23.3.4 Interface Engineering for Improved Battery Performance *355*
23.4 Challenges and Future Perspectives in Defect Engineering *356*
23.4.1 Current Limitations in the Implementation of Defect Engineering for Batteries *356*
23.4.2 Future Perspectives *357*
References *357*

24 Defect and Interface Engineering in Electrochemical Pseudocapacitors Based on Carbon *361*
Zhipeng Sun and Xiaoyan Shi
24.1 Introduction *361*
24.2 Defect Engineering in Carbon Materials: Insights and Applications *361*
24.2.1 Classification of Defects in Carbon Materials *361*
24.2.1.1 Intrinsic Defects *362*
24.2.1.2 Extrinsic Defects *363*
24.2.1.3 Metal-Free Heteroatom-Doped Defects *363*
24.2.1.4 Charge-Dominated Mechanisms: Nitrogen Doping *364*
24.2.1.5 Halogen Doping: A Versatile Strategy *364*
24.2.1.6 Silicon, Boron, and Phosphorus Doping *365*
24.2.1.7 Sulfur Doping and Electron Spin Contribution *365*
24.3 Strategies for Defect Engineering *365*
24.3.1 Carbon Strategies for Introducing Intrinsic Defects in Carbon Materials *366*
24.3.2 Carbon Strategies for Introducing Extrinsic Defects in Carbon Materials *367*
24.3.3 Challenges and Future Directions *368*
24.4 Defect Characterization in Carbon Materials *368*
24.4.1 Direct Visualization of Carbon Defects *368*
24.4.2 Indirect Observation of Carbon Defects *369*
24.4.3 Comprehensive Characterization of Carbon Defects *370*

24.5 Applications in Electrochemical Pseudocapacitor Systems *370*
24.5.1 Supercapacitors *370*
24.5.2 Hybrid Capacitors *373*
24.5.2.1 Lithium-Ion Hybrid Capacitors (LIHCs) *373*
24.5.2.2 Sodium-Ion Hybrid Capacitors (SIHCs) *373*
24.5.2.3 Potassium-Ion Hybrid Capacitors (PIHCs) *374*
24.5.2.4 Zinc-Ion Hybrid Capacitors (ZIHCs) *375*
24.6 Surface/Interface Engineering *376*
24.6.1 Functionalization *377*
24.6.2 Interface Engineering *377*
24.6.3 Characterization *377*
24.6.4 Applications in Electrochemical Pseudocapacitor Systems *377*
24.7 Future Perspectives *379*
24.8 Conclusion *380*
References *380*

25 Metal Oxide-Based Electrochemical Supercapacitors: Performance Enhancement by Defects and Interface Engineering *383*
Poovitha Ganesan, Yuvashree Jayavelu, D. Paul Joseph, V. Ganesh, Rathika Rajendran, and Kovendhan Manavalan
25.1 Introduction *383*
25.1.1 Background of Various Energy Storage Device *385*
25.1.1.1 Fuel Cell *385*
25.1.1.2 Capacitor *385*
25.1.1.3 Battery *386*
25.2 Classification of Supercapacitor *386*
25.2.1 Electric Double-Layer Capacitor (EDLC) *386*
25.2.2 Pseudocapacitor *387*
25.2.3 Hybrid Supercapacitors *389*
25.2.3.1 Symmetric and Asymmetric Supercapacitors *389*
25.2.3.2 Battery-Type Supercapacitors *390*
25.3 Supercapacitor Components *391*
25.3.1 Electrode *391*
25.3.2 Electrolyte *391*
25.3.3 Separator *392*
25.3.4 Current Collectors *392*
25.4 Synthesis Strategies for Electrode Materials *393*
25.4.1 Hydrothermal Method *393*
25.4.2 Solvothermal Method *393*
25.4.3 Sol–Gel Method *394*
25.4.4 Chemical Precipitation Method *394*
25.4.5 Electrochemical Deposition Method *394*
25.5 Defect and Interface Engineering in Pseudocapacitors *394*
25.5.1 Oxygen Vacancy Defects *395*

25.5.2 Heteroatom Doping *395*
25.6 Characterization Techniques for Defects and Interface Analysis *397*
25.6.1 Physiochemical Characterization Technique *397*
25.6.2 Electrochemical Characterization Techniques *398*
25.6.2.1 Cyclic Voltammetry *398*
25.6.2.2 Galvanostatic Charge–Discharge Analysis *398*
25.6.2.3 Electrochemical Impedance Spectroscopy *398*
25.7 Conclusion *400*
References *400*

26 Defect and Interface Engineering in Electrochemical Pseudocapacitors Based on Pseudocapacitive Materials *405*
Próspero Acevedo-Peña
26.1 Introduction *405*
26.2 MXenes *406*
26.3 Transition Metal Nitrides *411*
26.4 Conducting Polymers *414*
References *416*

Index *419*