

1. Record Nr.	UNINA9910830155403321
Autore	Li Yuliang
Titolo	Graphdiyne : fundamentals and applications in renewable energy and electronics // Yuliang Li
Pubbl/distr/stampa	Hoboken, New Jersey : , : John Wiley & Sons, Inc., , [2022] ©2022
ISBN	3-527-82847-8 3-527-82848-6
Descrizione fisica	1 online resource (395 pages)
Disciplina	620.115
Soggetti	Nanostructured materials Nanostructured materials - Analysis
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di contenuto	Cover -- Title Page -- Copyright -- Contents -- Preface -- Chapter 1 Introduction -- 1.1 The Development of Carbon Materials -- 1.2 Models and Nomenclature -- 1.3 Brief Introduction of Graphdiyne -- References -- Chapter 2 Basic Structure and Band Gap Engineering: Theoretical Study of GDYs -- 2.1 Structures -- 2.1.1 Theoretical Prediction and Classification -- 2.1.2 Geometric Structures of GDYs -- 2.2 Electronic Structures -- 2.2.1 Dirac Cones in , , and 6,6,12 Graphynes -- 2.2.2 Semiconductor Properties of Graphynes -- 2.2.3 Electronic Structures Comparison of GDYs -- 2.2.4 Structure and Size Based Electronic Properties -- 2.2.5 StrainDependent Electronic Properties -- 2.3 Mechanical Properties -- 2.3.1 Mechanical Properties of GDYs -- 2.3.2 Mechanical Properties of Graphyne -- 2.3.3 Mechanical Properties of Graphdiyne -- 2.3.4 Mechanical Properties of Graphynes Family -- 2.3.5 The Influence Factors on the Mechanical Properties of GDYs -- 2.4 Layers Structure of Bulk GDYs -- 2.4.1 Stacking Modes for Bilayer Graphyne -- 2.4.2 Stacking Modes for Bilayer Graphyne -- 2.4.3 Stacking Modes for Bilayer Graphdiyne -- 2.4.4 Identification on the Stacking Structures of GDY -- 2.5 Band Gap Engineering of GDYs -- 2.5.1 Influences of Nonmetal Doping -- 2.5.2 Influences of Chemical Modification and Functionalization -- 2.5.3 Tunable Band Gap Under Strain -- 2.5.4 Graphyne Nanoribbons Under

Strain or Electric Field -- References -- Chapter 3 GDY Synthesis and Characterization -- 3.1 Synthesis -- 3.1.1 Basic Chemistry -- 3.1.2 Cu Surface Mediated Synthesis -- 3.1.3 Template Synthesis -- 3.1.4 Interfacial Synthesis -- 3.1.5 Vapor-Liquid-Solid (VLS) Growth -- 3.1.6 Chemical Vapor Deposition (CVD) Growth -- 3.1.7 Explosion Approach -- 3.2 Characterization -- 3.2.1 Raman Spectroscopy -- 3.2.2 X-ray Photoelectron Spectroscopy (XPS). 3.2.3 X-ray Absorption Spectroscopy (XAS) -- 3.2.4 Microscope Technology -- 3.2.5 X-ray Diffraction (XRD) Technique -- 3.2.6 Others -- 3.3 Summary -- References -- Chapter 4 Functionalization of GDYs -- 4.1 Heteroatom Doping -- 4.1.1 Nitrogen and Phosphorus Doping -- 4.1.2 Halogen Doping -- 4.1.3 Sulfur, Boron, Hydrogen, and Other Nonmetal Heteroatoms -- 4.1.4 Dual Heteroatom Doping -- 4.2 Metal Decoration -- 4.2.1 Metal Atomic Decoration -- 4.2.2 Metallic Compounds -- 4.3 Absorption of Guest Molecules -- References -- Chapter 5 Graphdiyne-Based Materials in Catalytic Applications -- 5.1 Graphdiyne-Based Zero-Valent Metal Atomic Catalysts -- 5.1.1 Synthetic Strategy for GDY-Based ACs -- 5.1.2 Adsorption Geometry and Electronic Structures of GDY-Based ACs -- 5.1.3 Morphology and Valence States of GDY-Based ACs -- 5.1.4 Application of GDY-Based ACs -- 5.1.4.1 Applied for Water Splitting -- 5.1.4.2 Applied for Ammonia Synthesis at Ambient Conditions -- 5.1.4.3 Applied for Oxygen Reduction Reaction -- 5.1.4.4 Applied for Organic Reactions -- 5.2 GDY-Based Heterojunction Catalysts -- 5.2.1 Hydrogen Evolution Reaction on GDY-Based Heteros -- 5.2.2 Oxygen Evolution Reaction on GDY-Based Heterojunction -- 5.2.3 Photo/Photoelectrocatalytic Oxygen Evolution Reaction -- 5.2.4 Applied for Overall Water Splitting -- 5.2.5 Applied for Other Catalysis -- 5.3 Graphdiyne-Based Metal Free Catalysts -- 5.3.1 Applied for Water Splitting -- 5.3.2 Applied for Oxygen Reduction Reactions -- 5.3.3 Applied for Photocatalysis -- References -- Chapter 6 Graphdiyne-Based Materials in Rechargeable Batteries Applications -- 6.1 Introduction -- 6.2 Lithium-Ion Battery Anodes -- 6.3 Graphdiyne Derivatives for LIB Anodes -- 6.4 Sodium Ion Battery Anodes -- 6.5 Electrochemical Interface -- 6.5.1 Function of Interface -- 6.5.2 Protection for LIBs Anodes. 6.5.3 Protection for LIB Cathodes -- 6.6 Lithium-Sulfur Battery -- 6.7 Lithium Metal Anodes -- 6.8 Supercapacitor Electrodes -- 6.9 Fuel Cells -- References -- Chapter 7 Graphdiyne-Based Materials in Solar Cells Applications -- 7.1 Perovskite Solar Cells -- 7.1.1 Graphdiyne Based Materials in Interfacial Layers -- 7.1.2 Graphdiyne-Based Materials in Active Layers -- 7.2 Organic Solar Cells -- 7.3 Others -- 7.3.1 Quantum Dots Solar Cells -- 7.3.2 Dye-Sensitized Solar Cells -- 7.4 Future Perspectives -- References -- Chapter 8 Graphdiyne: Electronics, Thermoelectrics, and Magnetism Applications -- 8.1 Electronic Devices -- 8.2 Optic Devices -- 8.3 Thermoelectric Materials -- 8.4 Magnetism -- References -- Chapter 9 Graphdiyne-Based Materials in Sensors and Separation Applications -- 9.1 Sensors -- 9.1.1 Biomolecules Sensor -- 9.1.1.1 DNA Detection -- 9.1.1.2 RNA and Amino Acids Detection -- 9.1.2 Small Molecule Detection Sensor -- 9.1.2.1 Gas Sensor -- 9.1.2.2 Humidity Detection -- 9.1.2.3 Hydrogen Peroxide Detection -- 9.1.2.4 Glucose Detection -- 9.1.3 Other Sensors -- 9.2 Separation -- 9.2.1 Gas Separation -- 9.2.1.1 Hydrogen Separation -- 9.2.1.2 Oxygen Separation -- 9.2.1.3 Carbon Dioxide Separation -- 9.2.1.4 Helium Separation -- 9.2.2 Oil/Water Separation -- 9.3 Conclusion and Perspective -- References -- Chapter 10 Perspectives -- 10.1 Chemical Synthesis Methodology and Aggregate Structures of Graphdiyne -- 10.2 Controllable Preparation of Highly Ordered Graphdiyne -- 10.3 Fundamental Physical Properties

