Carbon-based Nanomaterials for Green Applications

Edited by

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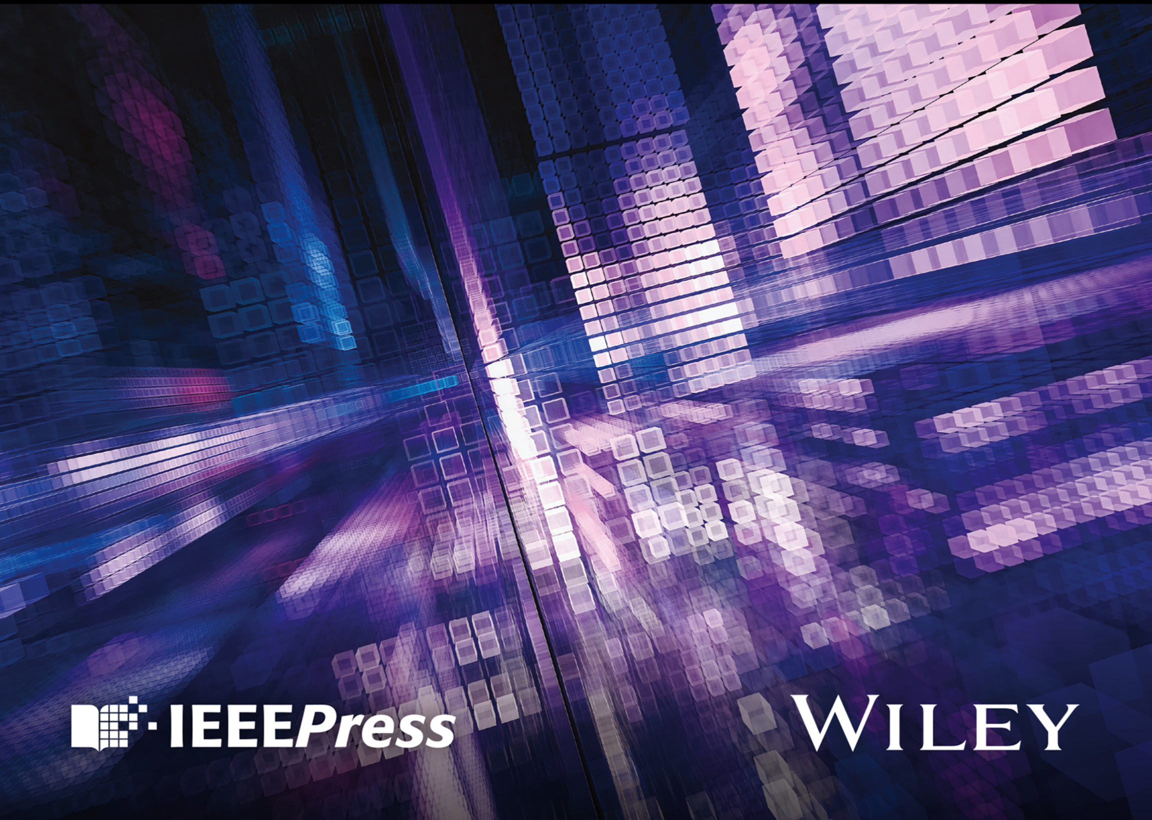

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Contents

About the Editors *xxv*
List of Contributors *xxix*
Preface *xxxvii*
Acknowledgments *xxxix*

1 Green Energy: An Introduction, Present, and Future Prospective *1*
Manoj Singh Adhikari, Raju Patel, Manoj Sindhwani, and Shippu Sachdeva
1.1 Introduction *1*
1.2 Present Status of Green Energy *3*
1.3 Global Renewable Energy Capacity *4*
1.4 Leading Green Energy Technologies *5*
1.5 Challenges in Green Energy Adoption *7*
1.6 Prospects of Green Energy *8*
1.7 Sustainable Practices in Green Energy *10*
1.8 Case Studies of Successful Green Energy Projects *12*
1.9 Policy and Regulatory Framework for Green Energy *13*
1.10 Opportunities and Challenges in the Evolution to a Green Energy Future *14*
1.10.1 Opportunities *14*
1.10.2 Challenges *16*
1.11 Conclusion *16*
References *17*

2 Properties of Carbon-Based Nanomaterials and Techniques for Characterization *21*
Ravi Tejasvi
2.1 Introduction *21*
2.1.1 Carbon Nanotubes *21*
2.1.2 Graphene *22*
2.1.3 Graphene Oxide *22*
2.1.4 Fullerenes *22*

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2.2 Significance in Green Energy *22*
2.2.1 Energy Storage *23*
2.2.2 Solar Energy *23*
2.2.3 Catalysis and Fuel Cells *23*
2.2.4 Thermal Management *23*
2.2.5 Environmental Remediation *23*
2.3 Techniques for Characterization of Properties of Carbon Nanomaterials *24*
2.3.1 Electrical Conductivity *25*
2.3.2 Thermal Conductivity *28*
2.3.3 Mechanical Strength *29*
2.3.4 Surface Area Characterization *30*
2.3.5 Scanning Electron Microscopy *32*
2.3.6 Energy Dispersive X-ray Spectroscopy *33*
2.3.7 Transmission Electron Microscopy *34*
2.3.8 Electron Energy Loss Spectroscopy *37*
2.3.9 Atomic Force Microscopy *38*
2.3.10 Raman Spectroscopy *39*
2.3.11 Photoluminescence *40*
2.3.12 Time-Resolved Photoluminescence *41*
2.3.13 Thermal Gravimetric Analysis and Differential Scanning Calorimetry *42*
2.3.14 Fourier Transform Infrared Spectroscopy *43*
2.3.15 UV-Vis-NIR Spectroscopy *44*
2.3.16 X-ray Photoelectron Spectroscopy *45*
2.3.17 Small Angle X-ray Scattering *47*
2.3.18 X-ray Diffraction Analysis *48*
2.3.19 Scanning Electrochemical Microscopy *49*
2.3.20 Electrochemical Impedance Spectroscopy *50*
2.4 Conclusion *51*
References *52*

3 Green Energy: Present and Future Prospectives *57*
Irtiqa Amin, Quraazah Akeemu Amin, and Harpreet Kaur
3.1 Introduction *57*
3.1.1 Systematic Review Survey Reports *59*
3.2 Sustainable Energy Resources *62*
3.2.1 Wind Energy *63*
3.2.1.1 Applications of Wind Turbine Systems *65*
3.2.1.2 Advantages of Wind Energy *67*
3.2.1.3 Disadvantages of Wind Energy *68*
3.2.1.4 Future Prospectives and Challenges *69*

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3.2.2 Solar Energy *70*
3.2.2.1 Applications of Solar Energy *71*
3.2.2.2 Advantages of Solar Energy *72*
3.2.2.3 Disadvantages of Solar Energy *73*
3.2.2.4 Future Prospectives and Challenges *74*
3.2.3 Biomass *75*
3.2.3.1 Applications of Biomass *75*
3.2.3.2 Benefits and Disadvantages of Biomass *78*
3.2.3.3 Future Prospectives and Challenges *79*
3.2.4 Geothermal Energy *80*
3.2.4.1 Applications and Future Prospectives *81*
3.2.5 Hydropower *82*
3.2.6 Tidal and Wave Energy *84*
3.2.6.1 Tidal Power *84*
3.2.6.2 Wave Power *84*
3.2.6.3 Benefits of Tidal and Wave Energy Systems *86*
3.2.6.4 Challenges of Tidal and Wave Energy Systems *86*
3.3 Non-Sustainable Energy Resources *86*
3.3.1 Fossil Fuels *86*
3.3.2 Atomic Energy *87*
3.4 Existing Green Energy Models *87*
3.5 Conclusions *88*
References *92*

4 Carbon-Based 2D Materials: Synthesis, Characterization, and Their Green Energy Applications *95*
Minakshi Sharma, Varsha Yadav, Prachi Diwakar, Chandra Mohan Singh Negi, and Parvez Ahmed Alvi
4.1 Introduction *95*
4.2 Synthesis of Graphene and Its Derivatives *97*
4.2.1 Graphene-Based 2D Materials *97*
4.2.2 Graphene *99*
4.2.3 Graphene Oxide *100*
4.2.4 Reduced Graphene Oxide *102*
4.2.5 Graphitic Carbon Nitride *102*
4.2.5.1 g-CN-Thin Film *104*
4.2.5.2 Graphitic Carbon Nitride (g-CN)-Powder Form *104*
4.2.5.3 Thin Film of g-CN *104*
4.3 Properties of g-CN *108*
4.3.1 Morphologvical Properties *108*
4.3.2 Band Gap *109*

10.1002/9781394243426.fmatter, Downloaded from https://onlinelibrary.wiley.com/doi/10.1002/9781394243426.fmatter by INTEGRAL UNIVERSITY, Wiley Online Library on [05/02/2025]. See the Terms and Conditions (https://onlinelibrary.wiley.com/terms-and-conditions) on Wiley Online Library for rules of use; OA articles are governed by the applicable Creative Commons License

4.3.3 Other Properties 109
4.4 Applications of g-CN 109
4.4.1 g-CN Role in Organic Solar Cells 110
4.4.2 g-CN Role in Perovskite Solar Cells 110
4.4.3 g-CN Role in Dye-Sensitized Solar Cells 111
4.4.4 g-CN Role as a Photocatalyst 111
4.4.5 g-CN-Sensing Applications 112
4.4.6 g-CN Environmental Applications 112
4.5 Conclusion 113
References 114

5 Exploring the Potential of Graphene in Sustainable Energy Solutions 119
M. Karthik, S. Allirani, G. Ilakkiya, and R. Adharsh
5.1 Introduction 119
5.2 Usage of Graphene in Various Sectors 121
5.3 Implicit Operations of Graphene in the Renewable Energy Sector 125
5.3.1 Battery Technology 125
5.3.2 Touchscreen 127
5.3.3 Integrated Circuits 128
5.3.4 Flexible Memory 129
5.3.5 Solar Power Generation 130
5.3.6 Photovoltaic Cells 131
5.3.7 Solar Cells 131
5.3.8 Lithium-Ion Batteries 131
5.3.9 Supercapacitors 132
5.3.10 Graphene Transistors 133
5.3.11 Graphene Semiconductors 135
5.3.12 Graphene Sensors 136
5.4 Catalysis 137
5.5 Renewable Energies 137
5.6 Nanotechnology 138
5.7 Conclusion 138
Bibliography 139

6 Fullerene for Green Hydrogen Energy Application 141
Manish Kumar and Sunil Kumar
6.1 Introduction 141
6.2 Green Hydrogen Energy 143
6.3 Fullerene as a Hydrogen Storage Material 145
6.4 Size Effect of Fullerene and Hydrogen Storage Efficiency 145
6.5 Functionalized Fullerene, Chemical Structure, and Its Hydrogen Storage Performance 146

10.1002/9781394243426.fmatter, Downloaded from https://onlinelibrary.wiley.com/doi/10.1002/9781394243426.fmatter by INTEGRAL UNIVERSITY, Wiley Online Library on [05/02/2025]. See the Terms and Conditions (https://onlinelibrary.wiley.com/terms-and-conditions) on Wiley Online Library for rules of use; OA articles are governed by the applicable Creative Commons License

6.5.1 Boron *147*
6.5.2 Phosphorene or Black Phosphorus *147*
6.5.3 Hexagonal Boron Nitride *148*
6.5.4 Silicene *149*
6.5.5 Carbon Nanotubes *149*
6.5.6 Graphene *151*
6.5.7 Ferrocene *151*
6.5.8 MoS_2 *152*
6.5.9 Organometallic Framework *153*
6.6 Charged Fullerene as Hydrogen Storage System *155*
6.7 Hydrogen Storage in Hydro- or Hydrogenated Fullerene *155*
6.8 Conclusions and Future Outlook *156*
Acknowledgments *156*
References *157*

7 Graphyne-Based Carbon Nanomaterials for Green Energy Applications *163*
Kulsum Hashmi, Mohammad Imran Ahmad, Saman Raza, Nidhi Mishra, Seema Joshi, and Tahmeena Khan
7.1 Introduction *163*
7.1.1 Structural Aspects of Graphyne *164*
7.2 Graphyne-Based Carbon Nanomaterials for Green Energy Applications *166*
7.2.1 Mechanisms Involved in Growth, Doping, Energy Storage, and Conversion Involving Graphyne *167*
7.3 Fuel Cells *169*
7.3.1 Oxygen Reduction Reaction (ORR) Catalyst for Hydrogen Fuel Cells or Metal-Air Batteries (MABs) *171*
7.3.2 Lithium-Ion and Lithium-Metal Batteries *172*
7.3.3 Supercapacitors *174*
7.3.4 Wind Energy *176*
7.4 Solar Energy *177*
7.5 Wastewater Treatment *181*
7.6 Perspectives and Conclusion *185*
Acknowledgments *185*
References *185*

8 Mesoporous Carbon for Green Energy Applications *199*
Vikas Jangra, Narvadeswar Kumar, Harpreet Kaur, Lal Bahadur Prasad, and Piyush Kumar Sonkar
8.1 Introduction *199*
8.2 Recent Advances in Synthetic Techniques *202*
8.2.1 Hard Template Technique *203*

10.1002/9781394243426.fmatter, Downloaded from https://onlinelibrary.wiley.com/doi/10.1002/9781394243426.fmatter by INTEGRAL UNIVERSITY, Wiley Online Library on [05/02/2025]. See the Terms and Conditions (https://onlinelibrary.wiley.com/terms-and-conditions) on Wiley Online Library for rules of use; OA articles are governed by the applicable Creative Commons License

8.2.1.1 Carbon Precursors *203*
8.2.2 Soft Template Technique *204*
8.3 Applications of Mesoporous Carbon *205*
8.3.1 Applications in Lithium Batteries *205*
8.3.2 Applications in Supercapacitors *210*
8.3.3 Applications in Fuel Cells *213*
8.4 Further Directions, Opportunities, and Challenges *217*
8.5 Conclusions *218*
References *218*

9 Green Synthesis of Carbon Dots and Its Application in Hydrogen Generation Through Water Splitting *225*
Mandakini Gupta
9.1 Introduction *225*
9.2 Carbon Dots *227*
9.3 Processes Used for Synthesis of CDs *228*
9.3.1 Bottom-Up Synthesis Processes *229*
9.3.1.1 Solvothermal/Hydrothermal Method *230*
9.3.1.2 Sol-Gel Method *230*
9.3.1.3 Microwave Irradiation *230*
9.3.1.4 Carbonization Route *231*
9.3.2 Top-Down Synthesis Processes *231*
9.3.2.1 Laser Ablation *231*
9.3.2.2 Arc Discharge *232*
9.3.2.3 Chemical and Electrochemical Oxidation Methods *232*
9.3.2.4 Ultrasonic Treatment *233*
9.4 Green Synthesis of Carbon Dots *234*
9.4.1 Biomass-Based Green Synthesis of CDs *234*
9.4.1.1 Plant Waste-Based Green Synthesis of Carbon Dots *235*
9.4.1.2 Animal Waste-Based Green Synthesis of CDs *236*
9.5 Application of CDs in Water Splitting *237*
9.5.1 Hydrogen Generation via Water Splitting (Photoreduction) *237*
9.5.2 Photocatalytic Degradation of Organic Pollutants *241*
9.6 Factors Affecting Characteristics of Nanomaterials of Carbon in Photocatalytic H_2 Production *242*
9.6.1 Doping *242*
9.6.2 Defects *242*
9.6.3 Dimensions *243*
9.7 Conclusion *243*
References *244*

10.1002/9781394243426.fmatter, Downloaded from https://onlinelibrary.wiley.com/doi/10.1002/9781394243426.fmatter by INTEGRAL UNIVERSITY, Wiley Online Library on [05/02/2025]. See the Terms and Conditions (https://onlinelibrary.wiley.com/terms-and-conditions) on Wiley Online Library for rules of use; OA articles are governed by the applicable Creative Commons License

10 Carbon-Based Nanomaterials in Energy Storage Devices: Solar Cells *255*
Seraj Ahmad, Manoj Kumar, Kahkashan Khatoon, Akram Ali, and Himanshu Arora
10.1 Introduction *255*
10.2 Carbon Nanotubes *257*
10.2.1 Synthesis Techniques Concerning Carbon Nanotubes *257*
10.2.2 Carbon Nanotube Applications in Solar Cell Technology *257*
10.2.2.1 Transparent Conductive Electrodes *258*
10.2.2.2 Charge Transport Materials *258*
10.2.2.3 Enhanced Electron Transport *258*
10.2.2.4 Improved Charge Collection *258*
10.2.2.5 Transparency and Flexibility *259*
10.2.2.6 Lightweight and Flexible Design *259*
10.2.2.7 Tunable Aspects of Optics *259*
10.2.2.8 Durability and Longevity *259*
10.2.2.9 Compatibility with Other Materials *259*
10.2.2.10 Scalability *259*
10.2.3 Recent Advancements and Challenges *260*
10.2.3.1 Recent Advancements *260*
10.2.3.2 Challenges *260*
10.3 Graphene *261*
10.3.1 Synthesis Techniques *262*
10.3.2 Utilizing Graphene in Solar Cell Applications *262*
10.3.2.1 Transparent Conductive Electrodes *262*
10.3.2.2 Charge Transport Layers *263*
10.3.2.3 Light-Harvesting Enhancements *263*
10.3.3 Recent Advancements and Challenges *263*
10.3.3.1 Recent Advancements *263*
10.3.3.2 Challenges *264*
10.4 Carbon Dots *265*
10.4.1 Synthesis Techniques *265*
10.4.2 Applications of Solar Cell Carbon Dots *266*
10.4.2.1 Light Harvesting and Sensitization *266*
10.4.2.2 Charge Separation and Transport of Electrons *266*
10.4.2.3 Energy Storage and Electrochemical Applications *267*
10.4.3 Recent Advancements and Challenges *267*
10.4.3.1 Recent Advancements *267*
10.4.3.2 Challenges *268*
10.5 The Future of Carbon-Based Nanomaterials in Solar Cell Technology *269*

10.1002/9781394243426.fmatter, Downloaded from https://onlinelibrary.wiley.com/doi/10.1002/9781394243426.fmatter by INTEGRAL UNIVERSITY, Wiley Online Library on [05/02/2025]. See the Terms and Conditions (https://onlinelibrary.wiley.com/terms-and-conditions) on Wiley Online Library for rules of use; OA articles are governed by the applicable Creative Commons License

10.5.1 Enhanced Light Harvesting and Absorption *269*
10.5.2 Improved Charge Transport and Collection *269*
10.5.3 Enhanced Stability and Durability *269*
10.5.4 Scalable Synthesis and Manufacturing *270*
10.5.5 Integration with New Advances in Solar Cell Technology *270*
10.5.6 Environmental Sustainability and Cost-Effectiveness *270*
10.6 Conclusion *270*
References *271*

11 Carbon-Based Nanomaterials in Energy Storage Devices: Fuel Cells and Biofuel Cells *275*
Ponnusamy Thillai Arasu, Arumugam Murugan, G. Kanthimathi, A. Malar Retna, S. Daphne Rebekal, Natarajan Raman, Robin Kumar Samuel, and Tola Jebssa Masho
11.1 Introduction *275*
11.2 Carbon-Based Nanomaterials' Function in Energy Storage *277*
11.3 Carbon Nanotube-Based Materials for Use in Batteries *277*
11.4 Carbon Nanotube Varieties *278*
11.4.1 Single-Walled Carbon Nanotubes (SWCNTs) *279*
11.4.2 Multi-Walled Carbon Nanotubes (MWCNTs) *279*
11.4.2.1 Chirality *279*
11.5 Carbon Nanoparticles *281*
11.5.1 Supercapacitors *281*
11.5.2 Batteries *281*
11.5.3 Fuel Cells *282*
11.5.4 Hybrid Energy Storage Systems *282*
11.5.5 Quantum Dots *283*
11.6 Carbon Nanosheets *284*
11.7 Biofuels *285*
11.7.1 Biofuel Classification *285*
11.7.1.1 Biogas *286*
11.7.2 Background of Biofuel *286*
11.8 Morphological and Evolutionary Characteristics of Enzyme-Based Biofuels *287*
11.8.1 Mediated Electron Transfer *287*
11.8.1.1 NAD^+-Dependent Enzymes *288*
11.8.2 Direct Electron Transfer *289*
11.9 Immobilization of Enzymes *290*
11.9.1 Adsorption/Carrier-Binding Method *291*
11.9.2 Covalent Bonding *293*
11.9.3 Affinity Immobilization *294*
11.9.4 Entanglement *294*
11.9.5 Ionic Binding *295*

10.1002/9781394243426.fmatter, Downloaded from https://onlinelibrary.wiley.com/doi/10.1002/9781394243426.fmatter by INTEGRAL UNIVERSITY, Wiley Online Library on [05/02/2025]. See the Terms and Conditions (https://onlinelibrary.wiley.com/terms-and-conditions) on Wiley Online Library for rules of use; OA articles are governed by the applicable Creative Commons License

11.9.6 Immobilization Associated with Metals *295*
11.10 Graphene and CNT Applications in Fuel Cells *296*
11.10.1 Comparative Performance Analysis of Existing Fuel Cell *296*
11.11 Conclusion *298*
11.12 Expected Future Application of Fuel Cells and Biofuel Cells *298*
11.13 Future Applications *298*
References *299*

12 Carbon-Based Nanomaterials in Energy Storage Devices: Supercapacitors *307*
Shikha Chander, Veerabathuni Jaya Usha Praveena, and Meenu Mangal
12.1 Introduction *307*
12.1.1 Graphene Supercapacitors as Energy Storage Devices *308*
12.2 Carbon Nanotube *311*
12.2.1 Functioning of the CNT Detectors *314*
12.3 Functionalization of Carbon Nanotubes *316*
12.3.1 Applications of Functionalized CNTs *317*
12.3.2 Precursor Features *318*
12.4 Reduced Graphene Oxide (rGO) Synthesis *318*
12.4.1 Synthesis of rGO-FCNT Hybrid *319*
12.5 Characterization *319*
12.5.1 Preparation of Electrodes and Cells *320*
12.5.2 Input Parameters for Analysis *320*
12.6 Results and Discussion *321*
12.6.1 Raman Analysis *321*
12.6.2 Powder X-Ray Diffraction (XRD) *322*
12.6.3 FTIR Analysis *323*
12.6.4 Scanning Electron Microscopy Analysis *324*
12.6.5 Transmission Electron Microscopy Analysis *325*
12.7 Applied Electrochemistry *326*
12.7.1 Galvanostatic Charge Discharge *326*
12.7.2 Electrochemical Impedance Spectroscopy (EIS) *327*
12.8 Conclusions *328*
12.9 Future Scope *328*
References *328*

13 A Review of Effective Biomass, Chemical, Recycling and Storage Processes for Electrical Energy Generations *331*
Suman Lata Tripathi, Krishan Arora, and Celestine Lwendi
13.1 Introduction *331*
13.2 Bio-Raw Materials and Utility *333*
13.3 Biomass Energy Conversion Techniques *334*
13.3.1 Thermochemical Conversion *336*
13.3.1.1 Combustion *336*

10.1002/9781394243426.fmatter, Downloaded from https://onlinelibrary.wiley.com/doi/10.1002/9781394243426.fmatter by INTEGRAL UNIVERSITY, Wiley Online Library on [05/02/2025]. See the Terms and Conditions (https://onlinelibrary.wiley.com/terms-and-conditions) on Wiley Online Library for rules of use; OA articles are governed by the applicable Creative Commons License

13.3.1.2 Biomass Pyrolysis *336*
13.3.1.3 Gasification *337*
13.3.2 Chemicval Conversion *337*
13.3.2.1 Transesterification *338*
13.3.3 Biochemical Conversion *338*
13.3.3.1 Anaerobic Digestion *339*
13.3.3.2 Fermentation *339*
13.3.4 Bioelectrochemical Conversion *340*
13.3.4.1 Microbial Fuel Cells *341*
13.3.4.2 Microbial Electrolysis Cells (MECs) *342*
13.4 Application Areas of Biomass Energy *343*
13.5 Comparative Analysis of Modern Biomass Energy Conversion Techniques *343*
13.6 Optimization Techniques for Effective Biomass Conversion and Supply Chain Management *343*
13.7 Government Policies and Marketing Strategies *345*
13.8 Applications of Biomass Energy and Biomass Products *346*
13.9 Conclusions *346*
References *347*

14 Carbon-Based Nanomaterials for Pollutants' Treatment *355*
Gaganpreet and Y. Pathania
14.1 Introduction *355*
14.2 Allotropic Forms of Carbonaceous Nanomaterials *357*
14.3 Synergistic Approaches for Carbonaceous Materials *359*
14.4 Role of Carbonaceous Materials in Environmental Remediation *362*
14.4.1 Removal of Air Pollutants *362*
14.4.2 Removal of Water Pollutants *363*
14.4.3 Soil Remediation *367*
14.5 Environmental Impact of Carbon-Based Nanomaterials *368*
14.6 Conclusions: Technological Challenges and Future Prospects *369*
Conflicts of Interest *370*
Authors' Contributions *370*
References *370*

15 Carbon Nanomaterials for Detection and Degradation of Wastewater Inorganic Pollutants: Present Status and Future Prospects *383*
Prem Rajak, Ruchika Agarwal, Sohini Goswami, Satadal Adhikary, Suchandra Bhattacharya, Abhratanu Ganguly, and Sayantani Nanda
15.1 Introduction *383*
15.2 Properties of Carbon Nanomaterials *387*

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15.3 Common Types of Carbon Nanomaterials 387
15.3.1 Carbon Nanotubes 388
15.3.2 Carbon Nanofibers 389
15.3.3 Graphitic Carbon Nitride 390
15.3.4 Activated Carbon 391
15.3.5 Nanoporous Carbons 391
15.3.6 Graphene in Wastewater Treatment 392
15.4 Elimination of Inorganic Contaminants from Wastewater 393
15.4.1 Adsorption 393
15.4.2 Catalysis 394
15.4.2.1 Photocatalysis 394
15.4.2.2 Catalytic Wet Air Oxidation 396
15.4.3 Antimicrobial and Antibiofouling Activities 397
15.4.4 Desalination 399
15.5 Carbon Nanomaterials for Sensing and Monitoring 399
15.6 Limitations 400
15.7 Conclusion 401
References 402

16 Role of Carbon-Based Nanomaterials in CO_2 Reduction and Capture Reaction Process *411*
Shyam Raj Yadav and Jai Prakash
16.1 Introduction 411
16.2 Parameters Affecting Electrocatalytic CO_2 Reduction 412
16.2.1 Onset Potential 412
16.2.2 Overpotential (η) 414
16.2.3 Current Density (j) 414
16.2.4 Faradaic Efficiency (FE) 414
16.2.5 Tafel Analysis 414
16.2.6 Turnover Frequency (TOF) and Turnover Number (TON) 415
16.3 CO_2 ECR-Derived Products 415
16.4 Plausible Mechanism for ECR of CO_2 417
16.4.1 Pathways for the Formation of C_1 Products 417
16.4.1.1 Production of Formic Acid and Formate 417
16.4.1.2 Formation of Carbon Monoxide (CO) 418
16.4.1.3 Formation of Methane (CH_4), Formaldehyde (HCHO), and Methanol (CH_3OH) 419
16.4.2 Pathways for the Production of C_{2+} Products 420
16.4.2.1 Formation of Acetaldehyde (CH_3CHO), Ethanol (C_2H_5OH), and Ethene (C_2H_4) 420
16.4.2.2 Formation of Acetic Acid (CH_3COOH) 421

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16.4.2.3 Formation of Acetone (CH_3COCH_3) and *n*-propanol ($CH_3CH_2CH_2OH$) *421*
16.5 Carbon-Based Nanomaterials in CO_2 Reduction *422*
16.5.1 Applications of Various Metal-Free Carbon-Based Nanomaterials in CO_2 Reduction *424*
16.5.1.1 Carbon Nanofibers *424*
16.5.1.2 Carbon Nanotubes *426*
16.5.1.3 Nanoporous Carbon *429*
16.5.1.4 Graphene *434*
16.5.1.5 Nanodiamond *434*
16.5.2 Applications of Various Metal-Carbon Composite Nanomaterials in CO_2 Reduction *434*
16.6 Imminent Challenges *436*
16.7 Conclusion *438*
References *439*

17 Application of Carbon Nanomaterials in CO_2 Capture and Reduction *447*
R. Sanjeevi, J. Anuradha, and Sandeep Tripathi
17.1 Introduction *447*
17.2 Different Types of Carbon Nanomaterials *448*
17.2.1 Zero-Dimensional Carbon Nanomaterials *448*
17.2.2 One-Dimensional Carbon Nanomaterials *448*
17.2.3 Two-Dimensional Carbon Nanomaterials *449*
17.2.4 Three-Dimensional Carbon Nanomaterials *449*
17.2.5 Other Carbon Nanomaterials *449*
17.2.5.1 Fullerenes: Spherical Marvels *449*
17.2.5.2 Carbon Nanotubes (CNTs): Cylindrical Wonders *450*
17.2.5.3 Graphene: The Thinnest Marvel *451*
17.2.5.4 Nanodiamonds: The Small, Shining Gems *451*
17.2.5.5 Carbon Nanohorns: Horn-Shaped Marvels *452*
17.3 Applications in CO_2 Management: Leveraging Unique Properties *452*
17.4 CO_2 Capture *453*
17.4.1 The Imperative for CO_2 Capture Technologies *453*
17.4.2 Carbon Nanomaterials: Building Blocks for Capture *453*
17.4.3 High Surface Area and Porosity: Key Features for CO_2 Adsorption *454*
17.4.4 Nanoscale Efficiency: Enhanced CO_2 Capture *454*
17.4.5 Tailoring Surface Chemistry for Enhanced CO_2 Adsorption *454*
17.4.6 Dual Functionality *455*
17.4.6.1 From Capture to Conversion *455*
17.5 Catalytic Conversion of CO_2: Nanomaterials as Agents of Change *455*

10.1002/9781394243426.fmatter, Downloaded from https://onlinelibrary.wiley.com/doi/10.1002/9781394243426.fmatter by INTEGRAL UNIVERSITY, Wiley Online Library on [05/02/2025]. See the Terms and Conditions (https://onlinelibrary.wiley.com/terms-and-conditions) on Wiley Online Library for rules of use; OA articles are governed by the applicable Creative Commons License

17.5.1 The Paradigm Shift: From Pollutant to Resource *456*
17.5.2 Carbon Nanomaterials as Catalysts: Unlocking Potential *456*
17.5.3 Electrochemical CO_2 Reduction: Harnessing Electrical Energy *456*
17.5.4 Photocatalytic CO_2 Reduction: Harvesting Solar Energy *457*
17.5.5 Metal Nanoparticles on Graphene: Catalysts for Sustainable CO_2 Conversion *457*
17.5.5.1 Tunable Catalytic Activity *457*
17.5.5.2 Enhanced Electron Transfer *458*
17.5.5.3 Stability and Durability *458*
17.5.6 Selective CO_2 Reduction: Tailoring Products for Specific Applications *458*
17.5.6.1 Methane Production *458*
17.5.6.2 Ethylene Synthesis *458*
17.5.6.3 Carbon Monoxide Generation *459*
17.5.7 Challenges and Future Directions *459*
17.5.7.1 Catalyst Efficiency *459*
17.5.7.2 Reaction Selectivity *459*
17.5.7.3 Scalability and Practical Applications *459*
17.5.7.4 Environmental Impact *460*
17.5.7.5 Cross-Disciplinary Collaboration *460*
17.6 Challenges and Future Directions *460*
17.6.1 Scalability of Production Processes *460*
17.6.2 Long-Term Stability of Nanomaterials *461*
17.6.3 Economic Viability *461*
17.7 Future Directions *461*
17.7.1 Optimization of Synthesis and Engineering *461*
17.7.2 Exploration of Novel Catalytic Mechanisms *462*
17.7.3 Fundamental Interactions between Nanomaterials and CO_2 *462*
17.7.4 Integration of Nanomaterials into Multi-Functional Systems *462*
17.7.5 Techno-Economic and Life Cycle Assessments *463*
17.7.6 Collaboration and Interdisciplinary Research *463*
17.8 Conclusion *463*
References *464*

18 Industrial Applications of Carbon Nanomaterials *469*
Y. Pathania, P. K. Ahluwalia, and Pooja Kapoor
18.1 Introduction *469*
18.2 Different Forms of Carbon-Based Nanomaterials *471*
18.3 Applications of Carbon Nanomaterials *473*
18.3.1 Biomedical Industry *473*
18.3.1.1 Biosensors *473*

10.1002/9781394243426.fmatter, Downloaded from https://onlinelibrary.wiley.com/doi/10.1002/9781394243426.fmatter by INTEGRAL UNIVERSITY, Wiley Online Library on [05/02/2025]. See the Terms and Conditions (https://onlinelibrary.wiley.com/terms-and-conditions) on Wiley Online Library for rules of use; OA articles are governed by the applicable Creative Commons License

18.3.1.2 Drug Delivery *474*
18.3.1.3 Biomedicine *475*
18.3.1.4 Imaging *475*
18.3.2 Energy Storage Industry *476*
18.3.2.1 Batteries *476*
18.3.2.2 Supercapacitors *477*
18.3.2.3 Hydrogen Storage *477*
18.3.3 Electronic Industry *478*
18.3.3.1 Field-Effect Transistors and Digital Electronics *478*
18.3.3.2 Wearable Electronics *479*
18.3.3.3 Display Technology *479*
18.3.4 Food Industry *480*
18.3.4.1 Food Processing *480*
18.3.4.2 Food Safety *481*
18.3.4.3 Food Packaging *481*
18.3.5 Aerospace Industry *481*
18.3.5.1 Spacecraft and Satellite Applications *482*
18.3.5.2 Commercial Aircraft Applications *482*
18.3.5.3 Military Aircraft Applications *483*
18.3.5.4 Rotorcraft Applications *483*
18.3.5.5 Unmanned Aerial Vehicle (UAV) Applications *483*
18.3.6 Environmental and Agricultural Sectors *484*
18.3.6.1 Environmental Applications *484*
18.3.6.2 Agricultural Applications *485*
18.3.7 Automotive Industry *486*
18.3.8 Green Energy Applications *486*
18.4 Challenges *487*
18.5 Conclusions and Future Scope *488*
Acknowledgment *489*
Declarations *489*
Funding *489*
References *489*

19 Carbon-Based Nanomaterials and Their Green Energy Applications: Carbon Nanotubes *505*
Smita Singh, Varsha Singh, Vikram Rathour, and Vellaichamy Ganesan
19.1 Introduction *505*
19.1.1 Carbon Nanomaterials *506*
19.1.2 Fullerenes (C_{60}) *506*
19.1.3 Carbon Nanotubes *507*
19.1.4 Graphene *508*

10.1002/9781394243426.fmatter, Downloaded from https://onlinelibrary.wiley.com/doi/10.1002/9781394243426.fmatter by INTEGRAL UNIVERSITY, Wiley Online Library on [05/02/2025]. See the Terms and Conditions (https://onlinelibrary.wiley.com/terms-and-conditions) on Wiley Online Library for rules of use; OA articles are governed by the applicable Creative Commons License

19.2 Synthesis of CNTs 509
19.2.1 Plasma-Based Synthesis 509
19.2.2 Thermal-Based Synthesis 510
19.3 Properties of Carbon Nanotubes 511
19.3.1 Mechanical Properties of CNTs 511
19.3.2 Electrical Properties of CNTs 511
19.3.3 Thermal Properties of CNTs 512
19.3.4 Optical Properties of CNTs 513
19.3.5 Chemical Properties of CNTs 513
19.4 Green Energy Applications of CNTs 514
19.4.1 Supercapacitors 514
19.4.2 HER 515
19.4.3 OER 518
19.4.4 ORR 521
19.4.5 Electrochemical Sensors 523
19.5 Challenges Associated with CNTs 523
19.5.1 Synthesis and Purity 524
19.5.2 Scaling Up Production 524
19.5.3 Functionalization and Dispersion 524
19.5.4 Electrode Fabrication 524
19.5.5 Chemical and Environmental Stability 524
19.6 Conclusion 524
Acknowledgments 525
References 525

20 Carbon-Based Nanoparticles as Visible-Light Photocatalysts 533
Sonam Soni
20.1 Introduction 533
20.1.1 Application of Green Energy 534
20.1.2 Importance of Photocatalytic Technique 534
20.1.3 Importance of Nanotechnology in Visible Light Photocatalysis 535
20.2 Mechanism of Photocatalysis 536
20.2.1 Oxidation Mechanism 536
20.2.2 Reductive Mechanism 537
20.3 Classification of Nanomaterials 537
20.4 Types of Carbon-Based Nanoparticles 538
20.5 Application of CNPs as Photocatalysts 538
20.5.1 Photocatalytic Splitting of Water for Hydrogen Production 539
20.5.1.1 Factors Affecting Photocatalytic Splitting of Water 541
20.5.2 Photodegradation of Organic Pollutants 542
20.5.2.1 Mechanism of Photocatalytic Degradation 544

10.1002/9781394243426.fmatter, Downloaded from https://onlinelibrary.wiley.com/doi/10.1002/9781394243426.fmatter by INTEGRAL UNIVERSITY, Wiley Online Library on [05/02/2025]. See the Terms and Conditions (https://onlinelibrary.wiley.com/terms-and-conditions) on Wiley Online Library for rules of use; OA articles are governed by the applicable Creative Commons License

20.5.2.2 Factors Influencing Degradation of Organic Pollutants by g-C_3N_4/CQDs *545*
20.6 Conclusions *548*
20.7 Future Scope *548*
References *549*

21 Carbon-Based Nanomaterials in Day-to-Day Human Life *553*

Manju Choudhary, Pooja Nain, Shivanshu Garg, and Himanshu Punetha

21.1 Introduction *553*
21.2 Utilization of CNPs in Medical Services *555*
21.2.1 Pathological Condition Detections *555*
21.2.1.1 Detection Relying on Adsorption of Metabolites *558*
21.2.1.2 Bioimaging by Photoacoustics *559*
21.2.1.3 Protection from Penetration Power of X-Rays *559*
21.2.1.4 Changing Dynamic State by Photodynamic Therapy *559*
21.2.1.5 Temperature-Induced Transformations Through Photothermal Treatment *560*
21.2.1.6 Raising Immune Responses by Vaccination *561*
21.2.1.7 Generation of Artificial Tissue Implants *561*
21.2.1.8 Engineering Tissues and Tissue Metabolites *562*
21.2.1.9 Drug Targeting and Drug Delivery Approaches *563*
21.3 Applications Pertaining to Electrical and Electronics Sectors *563*
21.3.1 Radar Waves Absorption by CNPs *563*
21.3.2 Nanoparticles Implanted on Chip *564*
21.3.3 Developing Nanosensors *564*
21.3.3.1 Gas Phase Nanosensors *565*
21.3.3.2 Optical Detection Nanosensors *565*
21.3.4 Light-Emitting Diode Screens Implanted With Nanomaterials *565*
21.3.5 Conserving Charge via Nanobatteries *565*
21.4 Applications Pertaining to Wind and Solar Energies *566*
21.4.1 The Charge Held by Nanomaterials as Supercapacitors *566*
21.4.2 Energy Conservation by Fuel Cells *567*
21.4.3 Lithium-Ion Batteries: A Run for Electric Vehicles *569*
21.5 Application Pertaining to Food Industry Sector *571*
21.5.1 Nanoencapsulation: An Approach to Increasing Shelf-Life *571*
21.5.2 Nanoemulsification: An Aid to Food Digestion *571*
21.5.3 Nanomaterial Levels in Food Packaging *571*
21.5.3.1 Type 1: Active Packaging *572*
21.5.3.2 Type 2: Intelligent and Responsive Packaging *572*
21.5.3.3 Type 3: Smart Packaging *572*
21.6 Nanoparticles Operating Within Soil *573*

10.1002/9781394243426.fmatter, Downloaded from https://onlinelibrary.wiley.com/doi/10.1002/9781394243426.fmatter by INTEGRAL UNIVERSITY, Wiley Online Library on [05/02/2025]. See the Terms and Conditions (https://onlinelibrary.wiley.com/terms-and-conditions) on Wiley Online Library for rules of use; OA articles are governed by the applicable Creative Commons License

21.6.1 Clay Particles *573*
21.6.2 Humic Substances: Humidifying Agents in Soil *573*
21.6.3 Fulvic Acids: A Response Toward Soil Salinity *574*
21.7 Agricultural Aspects of Nanomaterials *574*
21.8 Nanomaterials Bringing Out Latest Revolutions *575*
21.8.1 Fuel of Nucleotide Triphosphates (NTPs) *575*
21.8.2 Hybridization of Nanomaterials to Achieve Sustainability *575*
21.8.3 Membranous Carbon Nanotubes Role in Removing the Micro-Pollutants *575*
21.8.4 Drug Delivery Targeting to Malignant Neurons *576*
21.8.5 DNA Origami Nanoturbine and Nanomotor Revolutions *576*
21.8.5.1 Nanoturbines and Generation of Mini-Multi-Powers *576*
21.8.5.2 Induction of Power Performance of Potassium-Ion Batteries *577*
21.9 Conclusion and Future Scope *577*
References *578*

Index *587*

10.1002/9781394243426.fmatter, Downloaded from https://onlinelibrary.wiley.com/doi/10.1002/9781394243426.fmatter by INTEGRAL UNIVERSITY, Wiley Online Library on [05/02/2025]. See the Terms and Conditions (https://onlinelibrary.wiley.com/terms-and-conditions) on Wiley Online Library for rules of use; OA articles are governed by the applicable Creative Commons License

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7

Graphyne-Based Carbon Nanomaterials for Green Energy Applications

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7.1 Introduction

Carbon forms the basis of life. The atom exists in different hybridization states like sp, sp^2, and sp^3 forming diverse bonding. Carbon has several allotropes like graphene, fullerenes, carbon nanotubes (CNTs), nanorings, etc. [1, 2]. In 1987, Baughman et al. proposed the GYfamily members (GFMs) consisting of sp and sp^2 hybridized C atoms where some of the C─C bonds get substituted with C─C triple bonds, which reduces the cohesive energy. Among these, GY is the most stable and has also been associated with potential nanoelectronics and energy storage applications. GY has better electrical conductivity than graphene [3]. The presence of sp^2 and sp^3 hybridized carbon provides rich π-conjugation to graphene. It also possesses evenly distributed pores permitting water molecules to pass through it, a feature that has been useful in designing desalinators based on GY. GDY, a family member of graphene has been used in separation membranes for H_2 purification [4]. Metal-doped GYs are also found to be well-suited for H_2 storage and Li-ion batteries [5]. GYs and GDYs have been used in electronics, photovoltaics, and catalysis.

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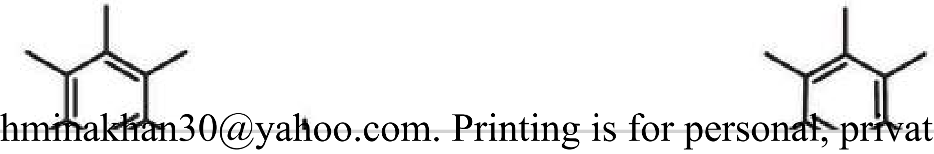
7.1.1 Structural Aspects of Graphyne

Graphene serves as the building block of several carbon-containing frameworks and holds the upper hand among all the allotropes of carbon [6]. Graphene has a high carrier mobility [7] and is used in ultrahigh-speed radiofrequency electronics [8]. However, the zero band gap holds limitations in field effect transistors (FETs) making it less useful for nanoelectronics. Therefore, the scientists worked on finding a new system having the intrinsic energy gap, which could be developed as a realistic candidate. Among 2D materials having structural similarity with graphene, GY [9] (Figures 7.1 and 7.2) and GDY [10] (Figure 7.3) were created from graphene and found to be even better in some aspects than graphene. As discussed earlier, the discovery of GY was made in the year 1987 [11] and the material got attention because of its direct band energy. It has D6h/mmm symmetry and is considered a hybrid system of graphene (sp^2C) and carbyne (*sp*C) in which the hexagonal rings are joined by the acetylenic linkage. It possesses rich optoelectronic and elastic characteristics due to these linkages [12]. GY is classified as α, β, and γ graphyne based on the number of these acetylenic linkages to the different hexagonal rings [5]. α Graphyne has 100% acetylenic bonds present in each C─C bond of graphene, while in β and γ graphyne, they are at select C─C bonds. In β-GY, two-thirds of the C─C bonds are acetylenic,whereas in γ-GY, only one-third of such acetylenic bondsare present. The γ-GY acts as a direct band gap semiconductor having a tuneable band gap in varying circumstances [13]. α and *β*-GYs are semi-metallic and have Dirac cones [14]. The directional electrical conductivity of GY makes it superior to graphene. The structure also has a higher degree of π-conjugation. GY also has mechanical stability and possesses high tensile strength and stiffness [15]. Diederich initially attempted the synthesis of GY [16]. Subsequently, the molecular fragments of GY and GDY molecular fragments were synthesized by M.M. Haley [17]. Despite the attempts, only trace amounts of GYs have been prepared in the laboratory. Large-area-multilayer GY films have been successfully synthesized [18] and also GY sheets [19]. GY has a higher degree of π-conjugation owing to *sp* as well as sp^2 hybridized C present. The carbon atoms involved in the hexagonal ring are sp^2 hybridized, whereas sp hybridized carbon atoms link the two adjacent rings. The C─C bond length in the hexagonal ring has been calculated to be 1.427 A. The px, py, and s orbitals are involved in σ bond formation between the neighboring atoms in GY, whereas the p_z orbitals are involved in π-bond formation, resulting in the π-conjugation. The bond distance between a sp^2 and sp hybridized C is 1.412 Å and is shorter than a normal *σ* bond (~1.470 Å).



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directions. *Water Resources Research* 51 (6): 4823–4839. https://doi.org/10.1002/2014WR016869.

- **140** Mehrdad, M. and Moosavi, A. (2019). An efficient graphyne membrane for water desalination. *Polymer* 175: 310–319. https://doi.org/10.1016/j.polymer.2019.05.054.
- **141** Zhang, J., Bai, Q., Bi, X. et al. (2022). Piezoelectric enhanced peroxidase-like activity of metal-free sulfur doped graphdiyne nanosheets for efficient water pollutant degradation and bacterial disinfection. *Nano Today* 43: 101429. https://doi.org/10.1016/j.nantod.2022.101429.
- **142** Zhan, S., Chen, X., Xu, B. et al. (2022). Hollow multishelled structured graphdiyne realized radioactive water safe-discharging. *Nano Today* 47: 101626. https://doi.org/10.1016/j.nantod.2022.101626.
- **143** Lin, L., Yang, H., and Xu, X. (2022). Effects of water pollution on human health and disease heterogeneity: a review. *Frontiers in Environmental Science* 10: 880246. https://doi.org/10.3389/fenvs.2022.880246.
- **144** Shindhal, T., Rakholiya, P., Varjani, S. et al. (2021). A critical review on advances in the practices and perspectives for the treatment of dye industry wastewater. *Bioengineered* 12 (1): 70–87. https://doi.org/10.1080/21655979.2020.1863034.
- **145** Ghosh, A., Orasugh, J.T., Ray, S.S., and Chattopadhyay, D. (2023). Prospects of 2D graphdiynes and their applications in desalination and wastewater remediation. *RSC Advances* 13 (27): 18568–18604. https://doi.org/10.1039/D3RA01370G.
- **146** Liu, R., Zhou, J., Gao, X. et al. (2017). Graphdiyne filter for decontaminating lead-ion-polluted water. *Advanced Electronic Materials* 3 (11): 1700122. https://doi.org/10.1002/aelm.201700122.
- **147** Xie, S., Pan, C., Yao, Y. et al. (2023). Ultra-high-efficiency capture of lead ions over acetylenic bond-rich graphdiyne adsorbent in aqueous solution. *Proceedings. National Academy of Sciences. United States of America* 120 (16): e2221002120. https://doi.org/10.1073/pnas.2221002120.
- **148** Xiao, S.X., Huang, C.S., and Li, Y.L. (2017). Carbon materials. In: *Modern Inorganic Synthetic Chemistry*, 429–462. Elsevier. https://doi.org/10.1016/B978-0-444-63591-4.00016-1.
- **149** Lasisi, K.H., Abass, O.K., Zhang, K. et al. (2023). Recent advances on graphyne and its family members as membrane materials for water purification and desalination. *Frontiers in Chemistry* 11: 1125625. https://doi.org/10.3389/fchem.2023.1125625.

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