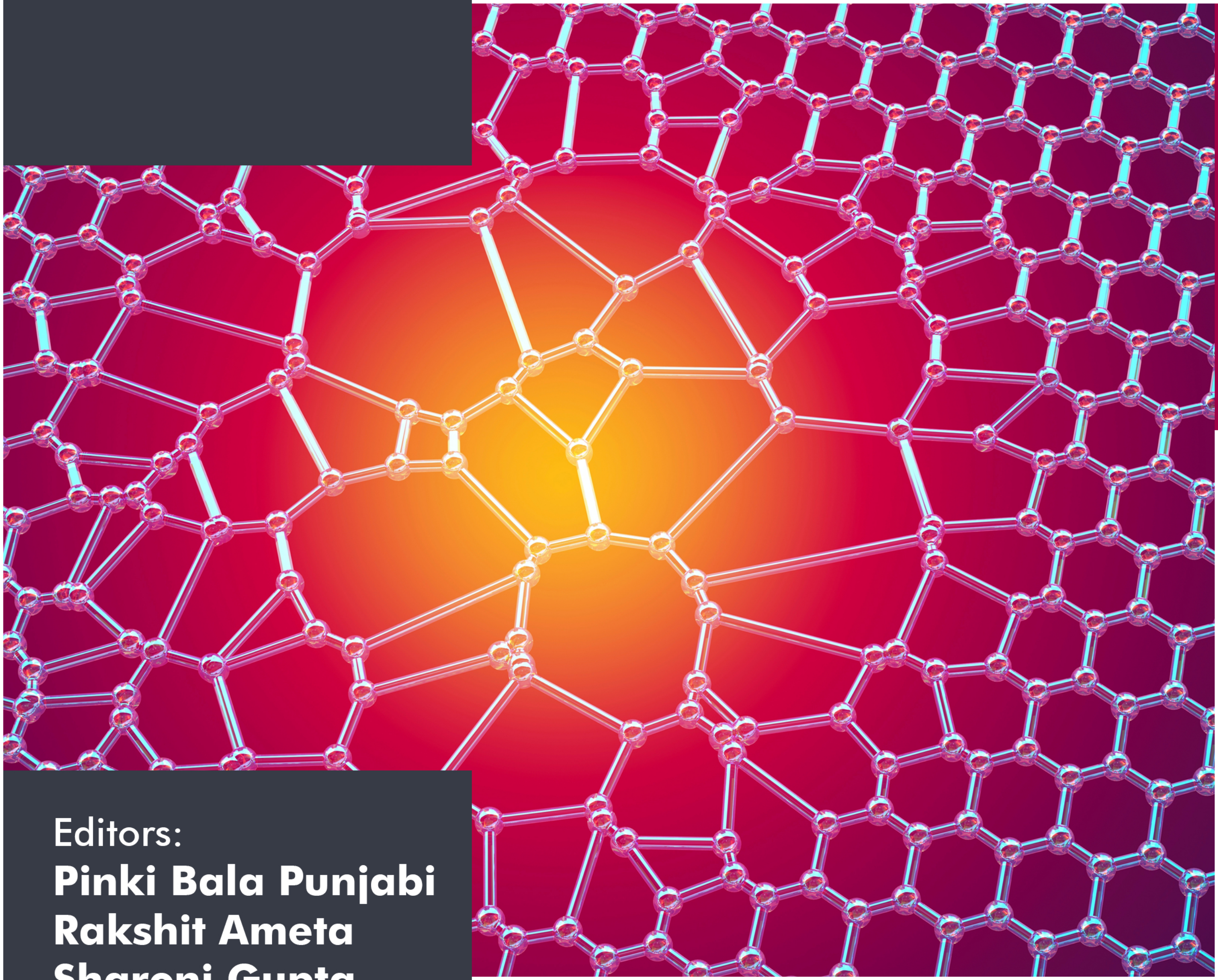
GRAPHENE-BASED CARBOCATALYSTS

SYNTHESIS, PROPERTIES AND APPLICATIONS



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Graphene-based Carbocatalysts: Synthesis, Properties and Applications

(Volume 2)

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Graphene-based Carbocatalysts:
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FOREWORD

Graphene is an allotrope of carbon, which is in the form of a thin layer with a two-dimensional honeycomb-like structure. It exhibits unique properties such as lightweight, excellent thermal and electrical conductivities, large specific surface area, easy preparation and functionalization, high intrinsic mobility, chemical stability, simple recovery, recyclability, *etc*. Therefore, it has emerged as the most successful entity with a wide range of applications in various medical, chemical and industrial processes, such as flexible electric/photonics circuits, solar cells, drug delivery, tissue engineering, bioimaging, optoelectronics, photodetectors, generation and storage of energy, biosensors, removal of contaminants, catalyst, water and sound proofing, and many more. The editors have made a very judicious choice in selecting graphene and its applications as a topic covering major fields of interest. I appreciate their efforts in compiling the different areas related to graphene and putting them all in a single arena. I not only hope but also believe that this book will get an overwhelming response from the readers.

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PREFACE

Catalysis is a fundamental and multidisciplinary phenomenon that has been ruling the energy sector and chemical industry for centuries impacting the world economy. Not only production processes but even biological and natural reactions are catalytically controlled by enzymes and other substances to maintain life on Earth. Various manufacturing units including petrochemicals, pharmaceuticals, food, polymers, materials and fine chemicals-based industries along with pollution abating firms are highly dependent on catalysts. This is because catalysts offer green means for accelerating chemical transformations *via* energy saving and atom economic pathways. Time and now, multitudes of homogeneous and heterogeneous catalysts have been explored for carrying out several conversions and enhancing the feasibility of reactions. However, the issues of catalyst recoverability and efficiency have been a cause of concern across the globe. More recently, the necessity of environmental conservation has further accentuated the search for sustainable catalysts. In such a scenario, graphene-based catalysts or carbocatalysts have emerged as a boon to meet the growing demand for efficacious, benign and inexpensive heterogeneous catalysts.

Graphene, with its distinguished opto-electronic, thermo-mechanical, surface and chemical characteristics is renowned as the most invincible nanomaterial. Ever since the path breaking discovery of graphene in 2004, the two-dimensional, honeycomb lattice-based material has enthralled the scientific community throughout the world. The exceptional conductivity, tensile strength, stability, large surface area, recoverability, recyclability and ease of functionalization of graphene materials have especially captivated the researchers working in the field of catalysis. Owing to the surge in demand for graphene-based catalysts, graphene research is being carried out at a very rapid pace. Every year new additions to the knowledge and scope of graphene carbocatalysts appear at considerably large scale. Consequently, this book is an attempt to acquaint readers with the recent advances in the field of graphene carbocatalysis.

The book encapsulates the recent developments involving the syntheses, properties, characterizations, functionalization and catalytic applications of graphene, its derivatives and composites. The book is in two volumes. The first volume is divided into ten chapters. In Chapter 1, a brief introduction of carbocatalysis has been laid out. The properties, syntheses and scope of carbocatalysts have been discussed to highlight their significance of carbocatalysts. Chapter 2 discusses the fundamental structure and properties of graphene and chemically modified graphene contributing to their applications in diverse fields. Chapter 3 describes the diverse synthetic strategies for the preparation of graphene and its derivatives. The advantages of present methods and future challenges related to industrial scale synthesis have also been outlined in this chapter. Chapter 4 focuses on the latest and most commonly employed characterization techniques used for investigating the morphological, structural and thermal properties of graphene materials. In Chapter 5, recent trends in functionalization and its role in the catalytic activity of graphene have been put forward. Chapter 6 summarizes the recent progress in the synthesis of graphene-based composites along with their properties and applications in catalytic reactions. The future prospects and challenges towards the designing and development of graphene-based nanocomposites for catalytic reactions have also been addressed in the chapter. Chapter 7 reviews the recent advances in graphene supported palladium catalysts for coupling reactions. It also underscores the synthesis of these catalysts and their mechanistic aspects spanning across a variety of cross-coupling reactions. A comparison of graphene supported catalysts with traditional catalysts has also been included in this chapter. Chapter 8 provides an in-depth review of recent applications of graphene-based catalysts in multicomponent and domino reactions. In Chapter 9, current progress made in the field of oxidation and reduction reactions of organic molecules catalyzed by graphene materials has been explored. Chapter 10 accounts for the contemporary trends in the area of graphene-based biocatalysts.

The second volume includes six chapters. Chapter 1 of second volume incorporates the most recent advances in photocatalytic applications of graphene-based materials such as graphene-based semiconductor photocatalysts for degradation of various contaminants (treatment of waste water), production of hydrogen, and photocatalytic reduction of carbon dioxide to energy rich synthetic fuels (combating against global warming and energy crisis), *etc*. Chapter 2 discusses the latest advances in electrocatalysis by graphene materials with a special focus on the electrocatalytic activities of non-metal doped graphene, graphene-2D materials heterostructures, and graphene-plasmonic nanostructures. Chapter 3 provides an overview of the recent advancement made by graphene-based materials including graphene oxide, reduced graphene oxide and graphene oxide quantum dots for hydrogen evolution from light-driven water splitting and future prospects. Chapter 4 highlights the modern trends in the fabrication of graphene-based smart energy materials for applications in various energy storage systems. The future trends and challenges have also been underlined. Chapter 5 underscores the potential utility of graphene materials in electrochemical sensing devices. Chapter 6 concludes the book and reports state-of-the-art graphene carbocatalysis with the future challenges accompanying graphene-based catalysts.

The book covers multidimensional applications of graphene-based materials cutting across various fields ranging from energy generation, chemical synthesis, electrochemical sensing to photocatalysis and much more. Hopefully, this book will serve as a reference work for all those researchers, students, industry workers and engineers who are interested in graphene research as well as its emerging applications in catalysis and beyond.

At last, we would like to thank all the authors of this book for their invaluable contribution towards enriching the content of this book. We are also extremely indebted to the managers, editors and reviewers of Bentham Science Publications for their magnanimous help throughout the creation and publication of this book. Finally, we are highly grateful to our families for their constant support and inspiration.

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DEDICATION

In fond memory of my beloved uncle Mr. Anil Kothari who taught me how to smile through difficult times.

Dr. Sharoni Gupta

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CHAPTER 1

Graphene–Based Photocatalysts

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Abstract: Graphene is a single layer of graphite with a unique two-dimensional structure with high conductivity, superior electron mobility, absorptivity, and specific surface area. The extraordinary mechanical, thermal, and electrical properties of graphene are due to long-range π conjugation. Due to these properties, graphene can be used in nanosystems and nano- devices. The photocatalytic efficiency of composites (semiconductor-based metal oxides and graphene-based photocatalysts) can be improved under visible light. Graphene behaves as an electron acceptor in these types of composite photocatalysts. Different types of graphene-based composites (graphene (G)-semiconductor, graphene oxide (GO)-semiconductor, and reduced graphene oxide (RGO)-semiconductor, where the semiconductor is TiO_2, ZnO, CdS, Zn_2SnO_4, *etc*.) can be prepared through simple mixing and/or sonication, sol-gel process, liquid-phase, hydrothermal, and solvothermal methods. This chapter includes the most recent advances in different applications of graphene-based semiconductor photocatalysts for degrading various contaminants (treatment of waste water) and producing hydrogen (fuel of future) by photosplitting water, and photo-catalytically reducing carbon dioxide to energy-rich synthetic fuels (combating against global warming and energy crisis), *etc*.

Keywords: Graphene, Graphene Oxide, Graphene Reduced Oxide, Hydrogen, Photospliting, Photocatalysis.

INTRODUCTION TO PHOTOCATALYSIS

Photocatalysis is the process by which reactions are carried out in the presence of catalyst and light. The term “photocatalysis” is derived from the combination of two Greek words; the prefix the “Photo” and the suffix “catalyst.” Thus, it is a process where light is used to activate a substance (called photocatalyst), affecting the rates of a chemical reaction without participating in the chemical transformation.

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Semiconductor photocatalysis is an emerging technology which has been applied for energy generation and environmental applications. Semiconductors are normally used as photocatalysts because there is a favourable combination of light absorption properties, electronic structure, excited-state, and a lifetime of charge transport characteristics. Various semiconductors have been used as photocatalysts (such as TiO_2, CdS, ZnO, $SrTiO_3$, *etc*.) as they absorb the light (photon) with energy that is >band gap (energy gap). As a result, an electron from the valence band (VB) is promoted (excited) to its conduction band (CB); thus, generating an electro-hole (e^--h^+) pair. Here, the hole can oxidize, while the electron reduces any substrate (Fig. **1**).

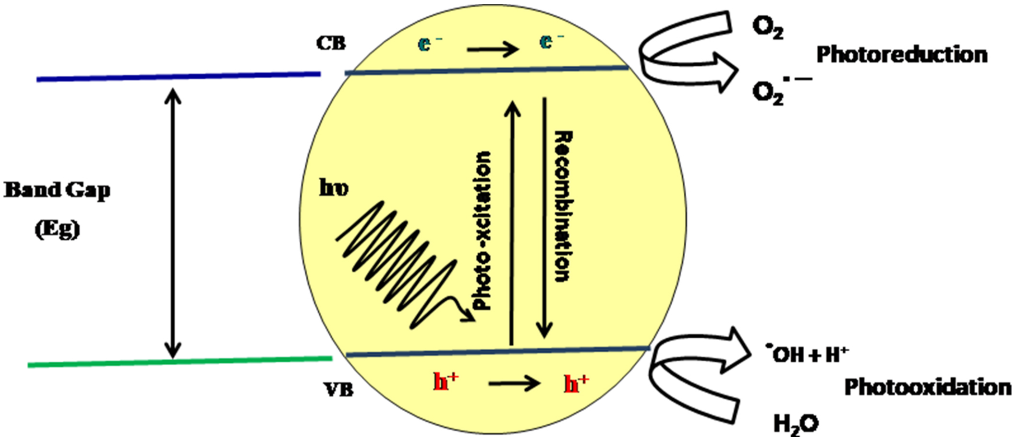

Fig. (1). Generation of an e^--h^+ pair of semiconductors exposed to light.

The major advantages of heterogeneous photocatalysis process are:

- Low cost,
- High conversation efficiency,
- High quantum yield,
- High stability, and
- High activity.

Along with this, there is a disadvantage of this process, and that is the recombination energy of e^- and h^+. In this process, energy is lost in the form of heat. The efficiency of a photocatalyst rises with an increase in the number of active sites on that surface. On the other hand, the efficiency is decreased by these three important mechanisms of recombination:

i. **Direct Recombination:** Here, photoelectron in conduction band drops directly, occupying a vacant (unoccupied) state in the valence band, and combines with the hole simply by the electrostatic attraction.
ii. **Surface Recombination:** It has selectively lower probability because surface species can utilize these photogenerated charge carriers (electron-hole) to drive the chemical reaction, and
iii. **Recombination at Recombination Centres:** It is also called volume recombination, and is highly probable. Here, the recombination centres lie at lattice sites transition within the bulk of the crystal.

To overcome this problem of recombining charge carriers, there are three common methods to modify photocatalytic surfaces by increasing the charge separation and the lifetime. These are:

i. Surface sensitization,
ii. Composite formation, and
iii. Metallized semiconductor

Composites formation is useful when the energy of the irradiated light is not sufficient enough to excite an electron in a semiconductor because of its wide band gap. It is then coupled with another semiconductor with a small band gap; thus, the composite of these two semiconductors will increase efficiency by utilizing near UV, visible light or even sunlight (Fig. **2**).

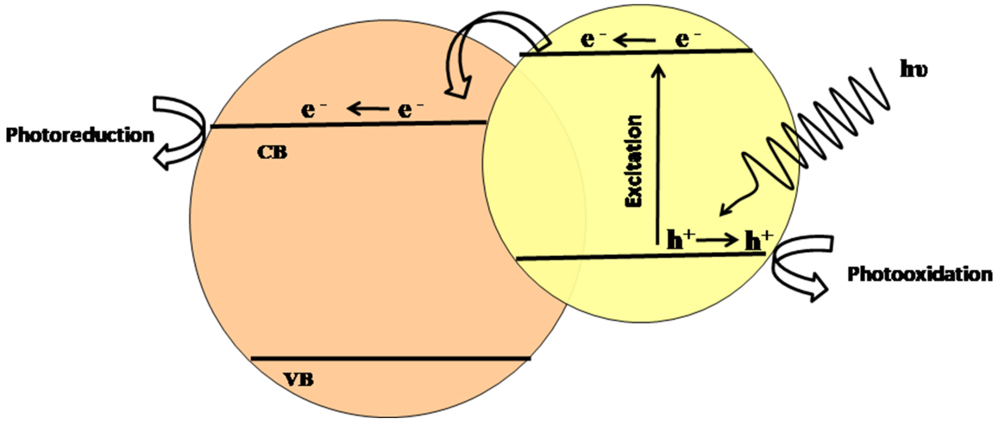

Fig. (2). Composite of semiconductors.

This composite formation has two advantages. These are:

- Increasing the response of semiconductors with a large band gap by coupling

CHAPTER 2

Electrocatalysis by Graphene Materials

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Abstract: Recently, graphene-based materials have attracted significant attention from scientific and industrial communities due to their potential applications in various electrochemical energy conversion technologies. Since pure graphene is electrochemically inert despite its outstanding versatile properties, different strategies are employed to modify the graphene to enhance its electrochemical activity. In this chapter, first, we discuss the basics of electrocatalysis and then the recent advances in electrocatalysis by graphene-based materials. Electrocatalytic activities of non-metal doped graphene, graphene-based 2D heterostructures, and graphene-plasmonic nanostructures have drawn particular attention. The challenges and future prospects of graphene-based electrocatalysts are also highlighted.

Keywords: Boron doping, Current density, Electrocatalyst, Graphene, Graphene-based 2-D heterostructures, Graphene oxide, Graphene-Plasmonic structures, Heteroatom doping, Heterostructure interface, Hydrogen evolution reaction, Hydrogen oxidation reaction, Metal doped graphene, Nitrogen doping, Oxygen evolution reaction, Oxygen reduction reaction, Overpotential, Phosphorous doping, Sulfur doping, Stability, Tafel slope.

INTRODUCTION

Today's world is in paramount need of a clean and sustainable source of energy that can substitute the decade-long reliance on traditional non-renewable energy sources [1]. The research on sustainable energy is on the top priority index and is

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tremendously progressing to address and resolve the high priority issues such as alarming fossil fuel consumption, excessive release of carbon and other deleterious gas emissions, and perennial climatic and environmental permutations. The various eco-friendly, sustainable and cost-effective catalytic technologies such as photocatalysis, electrocatalysis, sonocatalysis, *etc*., are considered to address the current energy crisis and environmental issues. But the state-of-the-art research on sustainable energy infrastructure has yet to be full-fledged for day-to-day usage. In this crucial scenario, 'electrocatalysis,' a branch of electrochemistry, is foreseen as a promising and competent technology for the production of clean energy by the scientific and technical fraternity [2].

Usually, platinum (Pt) or platinum-based metals show good electrocatalytic activity and are currently employed in various commercial electrochemical device applications. Despite their excellent electrocatalytic activity, high cost, low abundance and chemical instability are major issues that need to be addressed in Pt/ Pt-based catalysts to achieve low-cost and stable devices. Moreover, the possibility of metal dissolution often seen in pure Pt/Pt-alloys-based systems under a reactive environment limits their catalytic functionality and degrades the overall cell performance. Even though the core-shell Pt nanoparticles show better stability, platinum's high cost and low availability are still barriers [3]. Therefore, the core objective of the ongoing research is focused on developing an efficient, cost-effective and green electrocatalyst with its electrocatalytic activity in par excellence with its commercial counterparts for various industrial electrochemical applications [1, 2]. It is well-known that graphene is a fascinating pliable material. It is the most attractive material for electronic devices due to its unique properties such as electrical conductivity, large surface area, and mechanical characteristics because of its 2-D monolayer structure and multi-atomic π-π conjugation. Despite its outstanding properties, pure graphene showcases a nethermost electrocatalytic performance due to its electrochemical inertness. Since perfect graphene is electrochemically inactive, certain deliberate modifications or irregularities are essential for its chemical reactiveness [4]. Therefore, different approaches such as doping, surface modification, bandgap engineering, creating surface-active sites, strain engineering, *etc*., enhance the electrocatalytic activity of graphene. Thus, graphene-modified materials have been investigated for developing chief and stable devices [4, 5].

Therefore, in this chapter, we first discuss the principle and mechanism of electrocatalysis and then, recent developments in graphene-based materials. Further, we highlighted different strategies employed for enhancing the electrocatalytic performance of graphene. In this chapter, we primarily focus on the non-metallic doping of graphene, graphene/doped graphene-2D hetero-structures, and graphene-plasmon nanostructures to enhance electrocatalytic activity.

Principle and Mechanism of Electrocatalysis

The electrochemical process is based on heterogeneous chemical reactions, which entail converting chemical energy into electrical energy or electrical energy to chemical energy. In an electrochemical reaction, a charge transfer between the electrode-electrolyte interface results in a series of chemical changes [6]. A three-electrode cell configuration, as shown in Fig. (**1**), consisting of the working electrode, reference electrode and counter electrode, is used to quantify the electrochemical activity of an electrocatalyst (working electrode) [7]. Electrocatalysis is a special electrochemical reaction in which the electrode also acts as a catalyst [2, 6]. Electrolytic cells, fuel cells, water splitting, metal-air batteries, conversion of harmful gases, *etc*., are promising applications of electrocatalysis, which will constitute the future clean and sustainable energy infrastructure [1]. The reaction rate depends on the electrostatic potential difference generated at the electrode-electrolyte interface, and this interfacial potential also influences the activation energies of electrocatalytic reactions and the structure of the interfacial region [6].

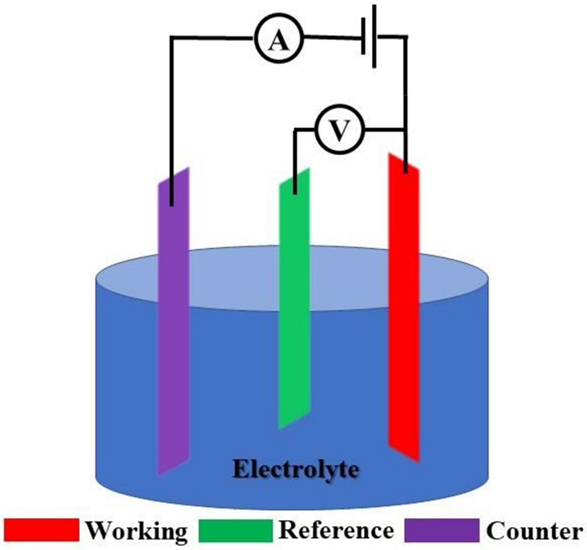

Fig. (1). Schematic of three-electrode electrochemical cell setup.

When an electrode is in contact with an electrolyte, an interfacial region consisting of opposite charge carriers is developed on the electrode and electrolyte

CHAPTER 3

Modified Graphene-Based Compound: Hydrogen Production through Water Splitting

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Abstract: Solar hydrogen production from water splitting can solve two big issues *i.e.* energy and environmental pollution. Since the discovery of graphene, its importance has been proven in many fields including light-driven hydrogen generation from water. This chapter offers a contemporary overview of the progress of graphene-based materials including graphene oxide, reduced graphene oxide and graphene oxide quantum dots for hydrogen evolution from photocatalytic water splitting. This chapter begins with a concise introduction to the current status of hydrogen energy generation from water. The chemical and physical characteristics of this extraordinary plasmonic metamaterial were also elaborated. Afterwards, the synthesis methods, various models, and associated properties of the tailored graphene oxides, reduced graphene oxide and graphene oxide quantum dots in the forms of pristine, binary and ternary compounds are discussed for their application in hydrogen production. In these modified compounds, the graphene acts as a surfactant, a charge-carrier recombination suppressor, an electron-sink and transporter, a co-catalyst, a photocatalyst, and a photosensitizer which, are elaborated . Finally, the chapter ends with a concluding remark on the challenges and future perspectives in this promising field.

Keywords: Allotropes of Carbon, Characterization of GOs, Clean Energy, Comparison of GOs with CNT, Criteria used in Determining the Effect of Reduction of GOs, Different Roles of GOs in Catalysis, Graphene Oxide, GO Quantum Dots, Brodie Method, Hummer Method and Tang–Lau Methods, Primary GOs, Reduced Graphene Oxide, Hydrogen Production, Synthesis of GO, Binary GO System, Ternary GO Systems, Water Splitting, *etc*.

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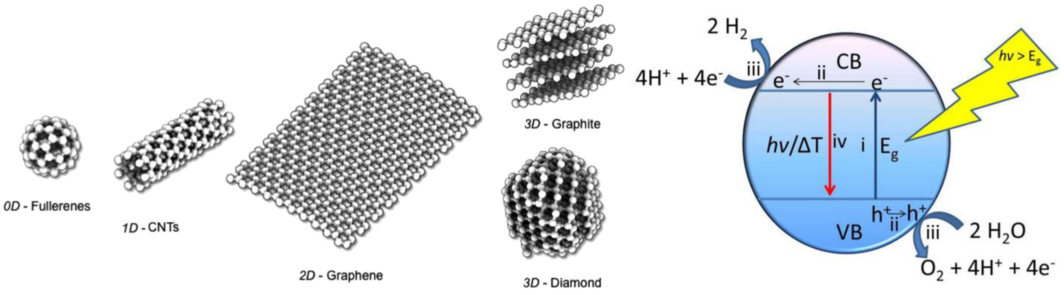
INTRODUCTION

The greatest challenge of this era is to satisfy the energy needs of the human race and animal kingdom without causing any negative impact on our environment. Day by day depleting fuel resources (conventional) lead to not only a hike in the fuel prices but also cause a bad impact on the environment in the form of the global warming and climate change. Our research community as well as industrial leadership is putting their best efforts in developing cheap, efficient and eco-friendly fuels that are based on renewable energy sources. Solar fuels, which use solar energy for making fuel, are quite interesting. Photochemical water splitting (PWS) is the one of the renewable ways to generate hydrogen, which uses solar energy and semiconducting materials for generating hydrogen fuel by splitting water. The potential of hydrogen as fuel and energy carrier is well known but currently the major source of hydrogen generation is inorganic substances. A huge number of photocatalytic materials (TiO_2, $SrTiO_3$, ZnO, $BiVO_4$, MoS_2, CdS, and graphene/CNT/ g-C_3N_4-based compounds, *etc.*) and their modified versions are available, which have been investigated since the discovery of water splitting phenomena in 1972 by Fujishima and Honda [1].



(a) (b)

Fig. (1). (a) Allotropes of carbon with different dimensions: 0D fullerenes, 1D CNT, 2D graphene, 3D graphite and 3D Diamond [2b]. **(b)** Basic steps of water splitting [3].

Graphene seems to be a winning horse in this race due to its enormous potential that is yet to be explored fully as a PWS photocatalyst for hydrogen generation. Besides its inherent goodness it has enormous potential for the fabrication of mixed-dimensional Vander Waals heterostructures that could be carried out by hybridizing graphene with 0D quantum dots or nanoparticles, 1D nanostructures such as nanowires or carbon nanotubes, or 3D bulk materials [2a, 2b]. The unmatchable properties of graphene or graphene-based materials are also suitable for microelectronics, due to their large surface-area, the strong adsorption capacity, possibility to provide charge density at certain stages of the reaction, rational design of active sites by modification of the graphene(G) sheet with metal/ metal oxides during or after the synthesis. Where, the overlapping between the d- orbitals of metal and π- orbitals of graphene results in the strong interaction between metal and graphene moieties.

In the photochemical water splitting process, sunlight, water and a semiconducting material are needed. That material should possess the apt band gap with the conduction band and valance band positions, which straddled between the reduction ($E_{H_2}O/H_2$=0.00eV) and oxidation potential($E_{H_2}O/O2$= 1.23eV) of the water, respectively [3]. In the presence of sunlight, there are four fundamental steps taken place during the photocatalytic water splitting process, as shown in Fig. (**1b**), *i.e.*

i. photo-induced charge generation,
ii. charges migration takes place,
iii. photochemical reactions proceeds, where the reduction ($E_{H_2}O/H_2$ = 0.00eV) and oxidation ($E_{H_2}O/O2$ = 1.23eV) of the water take place to produce the hydrogen and oxygen gases, at the CB and VB sides of the semiconductor.
iv. charge recombination.

Stability, efficiency, and cost are three main criteria for the selection of the photocatalytic material. The most intensively studied semiconductors for photocatalytic water splitting are transition metal oxides, (TiO_2, ZnO, WO_3) or metal chalcogenides (CdS, CdSe, and CdTe, *etc.*) or inorganic perovskites ($SrTiO_3$, *etc.*) [4]. But their low efficiency or photo corrosion prompts us to find their suitable alternatives. In this context, the graphene-based materials are attracting substitutes for above-mentioned catalysts that can be used as an additive or even as an active photocatalysts for solar light-driven fuel production. As graphene can be prepared from biomass, it is considered a renewable and ecofriendly material compared to the metal-based photocatalysts.

Moreover, graphenes can be easily processed and integrated when employed in electronic devices in the form of a thin film, which is the main advantage of this material having unique optoelectronic, mechanical and magnetic properties. Furthermore, the graphene is the thinnest, and strongest material ever known with honeycomb lattice (at atomic scale) structure made of carbon atoms. This popular 2D-allotrope, belongs to the most important class of the carbon with different dimensions, namely *i.e.* 0D-fullerene, 1D-carbon nanotube (single-walled/ multi-walled), 2D-graphene and 3D-diamond or 3D-graphite, as shown in Fig. (**1a**) [2b].

Therefore, it is expected that the complete characteristics of the GO shall become fully unraveled and universally acceptable, which will be beneficial for understanding and guiding in-depth applications. Research on the synthesis of GO

CHAPTER 4

Graphene-based Smart Energy Materials for Fuel and Solar Cell Applications

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Abstract: Energy is an incising subject matter and has had both positive and negative impacts on our society. Admittance to profuse, inexpensive, unharmed, hygienic energy is advantageous for human beings. However, the process of changing one form of energy into another, hauling and plentiful use can have negative impacts on health, the environment, and cost-cutting measures of our society. These days and at this age, the production of energy and stockpiles is one of the two main burning issues. Regrettably, conventional energy producers are not competent enough to respond to ecological transformations, whereas accustomed energy storage devices are deficient in special functionalities apart from supplying electricity. Graphene, composed of a single-layered graphite with a two-dimensional sp^2-hybridized carbon network, has recently gained tremendous research interest due to its peculiar physical and chemical properties. Gratifying from unrivalled physicochemical properties, graphene-based materials facilitate dealing with the aforesaid smoldering issues and, in recent times, have been widely studied in various energy conversion and storage applications such as supercapacitors, fuel cells, batteries, and photovoltaic devices or solar cells. In this book chapter, we summarise the recent progress reported in the synthesis and fabrication of graphene-based smart energy materials with their applications in various energy storage systems. In addition to this, the panorama and future challenges in both scalable manufacturing and more energy storage-related applications are covered in this chapter as well.

Keywords: Applications of Graphene, Dye-sensitised Solar Cell (DSSCs), Electrolyte, Electrode, Energy Materials, Fabrication, Fuel Cells, Graphene, Graphene-Based Naterials, Hybrid Materials, Membrane Fuel Cells, Modification, Organic Solar Cells (OSCs), Perovskite Solar Cells (PSCs), Polymer Electrolyte Membrane Fuel Cells (PEMFCs), Power Conversion Efficiency, Properties, Solar Cells, Synthesis, Various forms of Graphene.

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INTRODUCTION

Earth is a home for different living species and all are dependent on the environment for food, air, water, and other so many needs. Thus, the environment plays a vital role in healthy living and the existence of life on planet earth. Many human activities are directly attributed to environmental calamities. Therefore, every individual must save and protect our environment. The Intergovernmental Panel on Climate Change (IPCC) specified that the energy supply sector is the largest contributor to global greenhouse gas emissions (considering energy extraction, storage, transmission, conversion, and distribution processes that deliver final energy to the end-use sectors) [1]. At present, hydroelectric (~7%), natural gas (~22.5%), coal (~23.3%), and oil (~40%), are catering to the global energy needs [2]. With the world's population that is now about to reach eight billion people and with a prediction of even ten billion by the middle of this century, we really require the answer to the question of how mortality will be able to achieve its energy needs in the years to come. Who knows how long, most of the global electricity production has been delivered to fossil fuels which, being non-renewable, produce large amounts of carbon dioxide, the greenhouse gas that has now become a real menace to our entire ecosystem [3, 4].

The limitation of fossil fuels, the difficulty caused by energy exhaustion, and the humans' need for alternative energy sources have led to the development of fuel cells, which convert chemical energy into electrical energy *via* electrochemical reactions using oxidants and reactants [2, 5]. Sustainable evolution, environmental control, and more resourceful expertise have now become the key models for the new era. Universal energy consumption has been accelerating at an alarming rate due to the rapid industrial development and growing human population, along with the increase in energy demand [6]. In this situation, recent energy systems including solar cells [7 - 9], fuel cells [10 - 12], lithium-ion batteries [13 - 15], and super capacitors [16 - 18], have attracted much attention for use in academic world and industry alike. It is well-known that these energy devices in general possess an electrolyte layer sandwiched by two electrodes, with their overall performance intrinsically and sensitively dependent on the materials used [19].

Above all, solar energy is in prominence owing to its countless potential as an unlimited and cheap renewable energy resource. Although most of the solar cells (~90%) at present existing in the market are composed of silicone-based materials [20], the development of promising alternative solar cells, for example, organic photovoltaic cells (OPVs) [21, 22] and dye-sensitised solar cells (DSSCs) [23, 24] are getting attention due to their exceptional benefits like pliability and lucrative manufacturing processes. As an upshot of the recent progression during the last period, the Power Conversion Efficiency (PCE) of DSSCs and OPVs has been appreciably upgraded with the recently learned devices to above 15% [25] and 9% [26] respectively. It is good to know that the global recital of these solar cells strongly depends not only on the structure of the devices but also on the properties of the materials. Emerging thin-film solar cells such as dye-sensitised solar cells (DSSCs), organic solar cells (OSCs), and most recently perovskite solar cells (PSCs) have arisen as low-cost solutions for solar cell deployment [27]. Whereas comparatively simple deposition techniques and low investment expenses ensure a reduction in manufacturing cost. Power conversion efficiencies (PCEs) need to be reasonable with well-known technologies such as silicon solar cells. Recently, the PSCs technique is the focus of interest in photovoltaic research due to its impressive performance and development in only a few years of research effort [28]. The most widely used lead halide perovskite (LHP) has the potential for total productivity of 31%, according to theoretical calculations [29]. It could also reach higher PCEs if combined with other solar cell technologies to make tandem devices [30].

GRAPHENE

Carbon-based materials (Fig. **1**) such as carbon nanotubes (CNTs), buckminsterfullerene, graphene, and nanodiamonds received much attention due to their exclusive and multipurpose characteristics such as abundance, stability, processability, and relatively conservational characteristic [31 - 33]. These materials are extremely attractive for their use as electrodes in electrochemical energy devices because of their chemical stability across a wide temperature range in either basic or acidic medium [34]. Among the carbon allotropes, graphene has apprehended much interest from the research society owing to its broad prospective towards energy-related applications. It acquires high electrical and thermal conductivity, enormous mechanical strength, optical perspicuity, intrinsic elasticity, and a distinctive 2D structure. Furthermore, Graphene's carrier transfer feature stands out as its charge carrier can be tuned endlessly showing a perfect ambipolar electric field effect. It possesses prodigious surface area (~2630m^2/g), mass-less electron, extremely high mobility of charge carriers (up to 10^5 cm^2 V^{-1} s^{-1}), Quantum Hall Effects (QHE) even at room temperature, and electron wave propagation within a one atom thick layer as well [35 - 37].

The distinctive properties are noticed in their derivatives (Fig. **2**) such as graphene oxide (GO), reduced graphene oxide (rGO), graphene nanoplatelets (GNP), Few-layer graphene (FLG), graphene nano-onions or multi-layer fullerenes, and graphene nanoribbons (GNR), which show an inconsistency based on their diverse functions, for instance, flaw density, number of layers, surface chemistry, lateral dimension, configuration, purity, and nature of graphene sheets [38 - 52].

CHAPTER 5

Graphene-Based Electrodes for Electrochemical Sensors

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Abstract: Graphene-based electrodes are potential candidates and significantly participate in electrochemical reactions, providing high reactivity and selectivity. Their reaction assists in transferring electrons between the electrode and reactants and facilitates an intermediate chemical transformation described by an overall half-cell reaction. Graphene-based materials with metal/metal oxides and sulphides have been extensively applied for the fabrication of highly sensitive electrochemical sensors. They have excellent physical, chemical, electrical, and surface properties and are extensively used in the development of sensors. Graphene-based nanomaterials have also been successfully utilised for clinical diagnosis, disease treatment, and many biocompatible sensors. This chapter mainly focuses on the sensing mechanism of graphene-based electrochemical sensors *via* different approaches of potentiometry, amperometry/voltammetry, and conductometry. The electronic properties of graphene-based nanomaterials have been briefly discussed and are responsible for their outstanding sensing ability. We have also explored different forms of graphene and its derivatives with their properties and applicability in fabricating electrochemical sensors to better influence graphene for superior functioning. There is also a discussion about the general reactions (reduction/oxidation) involved within analytes and graphene materials in fabricating electrochemical sensors. Finally, a conclusion was drawn on the basis of the usage of graphene-based materials in electrochemical sensors for future electrocatalytic applications in various fields of biomedical diagnosis, environmental monitoring, food sensors, and hazardous fumes.

Keywords: Amperometric, Conductometric, Electrocatalyst, Electrochemical, Impedance, Nyquist Plot, Potentiometric, Sensors, Voltametric.

INTRODUCTION

In Electrochemical Sensors (ECS), sp^2 and sp^3 hybridization provides a connection to attach the electrodes that enhances the electro-catalytic activity of ECS. Since the 1950s, ECSs have been utilised to monitor oxygen in industries under the influence of safety and health regulations. In the Former Union of Soviet Soci-

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alist Republics' cold war in 1963, electrochemical sensors were developed to monitor water quality. Leland C. Clark proposed the concept of ECS having a two-electrode system and an oxygen permeable membrane for oxygen detection. Clark's oxygen sensor has found widespread use in medicine, the environment, and industry. Therefore, initially, ECS was applied to monitor oxygen, fumes, and other toxic gases [1, 2].

Specifically, ECS performs under a "signal transduction" mechanism for detection. Signals related to analytes are sensed. An analyte signal can be in two states: jiggling or static. Jiggling signals remain in motion and are captured and monitored. But static signals need external electrical signals to compel them to send out signals to monitor them. Jiggling or static signals are like fingerprints; they mostly remain distinguished within analytes and other external electrical signals. Distinct analyte signals are amplified through potentiometric, amperometric, voltametric, and conductometric approaches and displayed in ECS devices. ECS collectively works on the cell system that fundamentally consists of electrodes and electrolytes. ECS electrochemistry is either used to trigger the chemical reaction in the presence of a controlled electrocatalyst or to generate electricity from the reaction system as batteries. The workings of ECS are compacted into devices that perform sensing. Recent advancements in ECS are towards the fabrication and miniaturisation of devices at the micro level, known as smart micro-devices.

Components of the ECS for sensing include an analyte, a transducer, an amplifier, a detector, and are shown in Fig. (**1**). The analytes are the materials that are detected through electrochemical, colorimetric, and fluorescence sensing approaches. These materials could be elements or ions, small molecules and bulky molecules like micro-organisms, tissues, cells, organelles, nucleic acid, enzymes, pesticides, glucose, dopamine, hydroquinone, receptors and antibodies, Hg^{+2}, Pb^{+2}, NO_2 and H_2 gases, *etc* [3 - 6]. The transducers in the electrochemical sensors can be considered as the electrodes or modified electrodes. Most working electrodes are glassy carbon electrodes (GCE), disc electrodes made up of carbon, platinum working electrodes, gold working electrodes, copper working electrodes, *etc*. Working electrodes are modified with different catalytic nanomaterials. In this chapter we are focusing on discussing graphene as the electrocatalyst based modified working electrode (MWE) for sensing. The transduced signals of the analytes through MWE are amplified through various electrochemical methods, which are discussed broadly in this chapter. The amplified amplifies the transduced signal, which is then detected by the detector for display on the computer screen attached to the instrument. The parameters of the detectors include potential, scan rate, pulse width, and frequency. Scan rate is determined using cyclic voltammetry (CV) and linear sweep voltammetry (LSV), pulse width is determined using chronoamperometry (CA), differential pulse voltammetry (DPV), and frequency is determined using square wave voltammetry (SWV) [7].

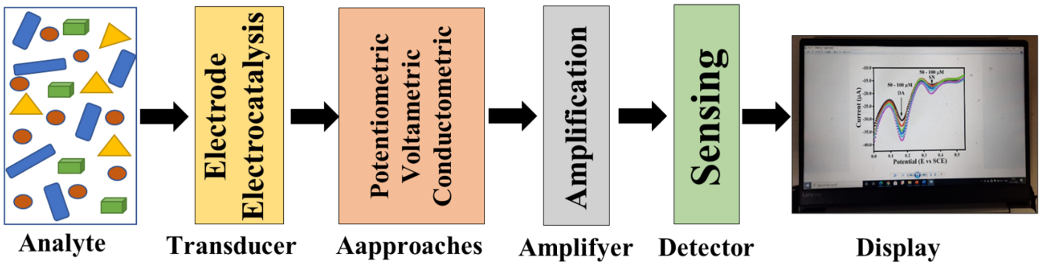

Fig. (1). Component of electrochemical sensors.

The signals derived from the presence of an analyte during the setup of electrochemical sensing are responsible for the electrochemical response. Generally, these responses are initially monitored on the basis of electric current, potential, and resistance.

Graphene

Graphene is a two-dimensional carbon allotrope, a one-atom-thick layer of nanostructured material found in the layers of graphite arranged in a hexagonal lattice as the planar conjugated structure. Graphene in itself is a remarkable substance with a multitude of astonishing properties, repeatedly titled "wonder material". It is the thinnest known material to man and, incredibly, two hundred times tougher than steel. On top of that, graphene has an admirable electric and heat conductor with light engaging ability. Truly, graphene is changing the world, with limitless potential for fabricating digital devices in most industries [8, 9].

Structures, Morphology, and Optical Properties of Graphene

Graphite in the form of a crystal structure is commonly found in pencils and batteries. By using a top-down phenomenon, graphene can be synthesized. When several sheets of graphene are stamped on one another over 30 layers, the graphene becomes graphite. The planar conjugated carbon atom of graphene covalently binds to the other three carbon atoms, making it ductile and stable enough to stretch without breaking. Indeed, the graphene flat atomic structure is accessible from both sides and creates more interaction with the environment. Although graphene carbon atoms have the capability to bind four atoms, the presence of defects attracts free atoms. which makes graphene appealing to form enhanced composite materials for electrocatalysts. Electron mobility in graphene

CHAPTER 6

State-of-the-Art Graphene Carbocatalysis and Future Challenges

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Abstract: The global surge in the demand for sustainable protocols and catalytic processes has led to an enormous rise in the research in the field of carbocatalysis. Graphene and its derivatives have surfaced as a novel category of green heterogeneous catalysts. This chapter summarizes the current trends in the synthesis, properties and applications of graphene-based carbocatalyst. The future challenges in the area of graphene-based catalysts have also been addressed.

Keywords: Graphene, Carbocatalyst, Sustainable, Composites, Electrocatalyst, Photocatalyst, Biocatalyst, Redox catalyst, Sensors.

INTRODUCTION

The discovery of graphene by Novoselov and Geim in 2004 [1] created ripples in the scientific community. With its incredibly unique thermo-electrical, optical and mechanical properties, Graphene has attracted the limelight as one of the thinnest and sturdiest known materials, and thousands of publications related to its properties, syntheses and applications have been published. Furthermore, the growing awareness of environmental preservation and sustainability also shifted the attention of the researchers and industries towards the development of renewable carbon materials such as graphene.

More than a decade of graphene research has focused on diverse applications of graphene-based materials ranging from solar cells, batteries, catalysts, circuit boards, display panels, biosensors, and supercapacitors to construction materials and fabrication of parts of vehicles, flame retardants, inks, coatings, polymers,

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additives, and so on. In the recent past, graphene-based carbocatalysis has emerged as one of the most promising fields of investigation. Carbocatalysis is a widely known catalysis, which makes use of carbon-based materials as a catalyst. From the green chemistry perspective, catalysts play a crucial role in modifying chemical reactions into energy-efficient and atom economic processes. Thus, the application of graphene, a carbon polymorph, in catalysis has paved the way for sustainable substitutes for traditional metal-based catalysts as well as acids and bases. Graphene-based materials offer remarkable characteristics, including large specific surface area, electronic properties, ease of functionalization, thermo-electrical conductivity, high tensile strength, chemical stability, recoverability and reusability, making them ideal catalytic systems for an enormous range of physical and chemical conversions.

The book highlights the broad applications of diversely fabricated and functionalized graphene carbocatalysts as heterogeneous catalysts for coupling reactions, multicomponent reactions, oxidation-reduction of organic compounds, biocatalysts, photocatalysts for removal of pollutants in the environment, electrocatalysts in hydrogen oxidation reaction (HOR), oxygen reduction reaction (ORR), hydrogen evolution reaction (HER) and oxygen evolution reaction (OER), water splitting, solar cells, fuel cells, and electrochemical sensors.

Bearing in mind the phenomenally rising interest in graphene-based carbocatalysis and the availability of several efficacious fabrication strategies such as exfoliation, unrolling or unzipping of carbon nanotubes, electric arc discharge method, laser ablation technique, oxidative exfoliation-reduction of graphene oxide, chemical vapor deposition, epitaxial growth, template synthesis, pyrolysis, substrate-free synthesis, total organic synthesis, and biological methods for synthesis of high-quality graphene and its derivatives, it is evident that graphene carbocatalysis will continue to flourish in coming days. However, some concerns regarding the industrial-scale syntheses of graphene catalysts in a cost-effective and benign manner still need to be worked upon.

Over the past few years, huge progress has been made in the field of graphene-based nanocomposites. The ever-improving knowledge of graphene surface chemistry has contributed significantly towards the functionalization and surface modification of graphene for the development of nanocomposites anchoring diverse functionalities, metal particles and non-metallic dopants. The synergistic effects between graphene and metal nanoparticles or nanomaterials in these nanocomposites do not just stabilize the composites but also result in the generation of active sites via the introduction of kinks, vacant spaces, edge or other defects. This leads to wide applications of graphene nanocomposites in various fields ranging from energy storage and generation to medicine. Different bottom-up and top-down strategies have been used for syntheses of these composites. Bottom-up processes are quite capable of manufacturing single-layered, defect-free graphene composites; however, for bulk production, these methods are unsuitable. Therefore, top-down methods have been at the forefront in the production of graphene composites as they involve simple sequential oxidation and reduction of graphitic materials in various solvents in the absence of any reducing agents offering large-scale production at low costs.

A major challenge in the synthesis of nanocomposites is the lack of methods that allow control over the size, shape, edge and thickness of graphene materials. Therefore, exploring novel approaches that would offer better control of morphological properties is the need of the hour. Further, comprehensive studies on cooperative interactions between nanomaterials and graphene surfaces are also essential for understanding the catalytic mechanisms of graphene nanocomposites.

Several techniques, including Atomic Force Microscopy (AFM), Scanning electron microscopy (SEM), Transmission electron microscopy (TEM), High-resolution transmission electron microscopy (HR-TEM), Scanning tunneling microscopy (STM), X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), Diffuse Reflectance Fourier Transform Infrared Spectroscopy (DRIFTS), X-ray absorption near edge structure (XANES) and X-ray absorption fine structure (XAFS), inductively coupled plasma mass spectrometry (ICP), thermogravimetric analysis (TGA), Brunauer-Emmett-Teller (BET), Raman, UV-Vis and FT-IR, have been the most employed characterization methods for graphene and its derivatives. These techniques have greatly helped the researchers in deciphering the atomic, surface, chemical, thermal and electronic properties of graphene-based materials. Yet, detailed investigation and identification of specific active sites on the carbon surface, an exhaustive study of structural intricacies and thermo-electronic properties of graphene-based materials driving their catalytic behaviour needs to be investigated at atomic as well as molecular levels. For this purpose, use of techniques like temperature-programmed reduction (TPR), CO chemisorption and NH_3/CO_2-temperature-programmed desorption (TPD), Solid-state nuclear magnetic resonance spectroscopy (SSNMR), Surface plasmon resonance (SPR) and Density functional theory (DFT) should be encouraged. Only a few studies have reported these techniques. These techniques can greatly help in developing advanced and thermodynamically and kinetically stable carbocatalysts.

To sum-up, it is worth noting that the industrialization and commercialization of graphene and its derivatives as catalysts can be successfully realized by probing into scalable, economically viable and benign synthetic routes. Further, to fully realize the catalytic potential of graphene materials, extensive studies related to

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Pinki Bala Punjabi

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Rakshit Ameta

Dr. Rakshit Ameta has a first-class career throughout securing the first position in the M. Sc. and was awarded a Gold Medal. He was also conferred Fateh Singh Award by Maharana Mewar Foundation, Udaipur for his meritorious performance. After completing his Ph.D., he served at Hindustan Zinc Limited, Vedanta Group for one year. He has served at M. L. Sukhadia University, Udaipur; University of Kota, Kota, PAHER University, Udaipur, and presently J. R. N. Rajasthan Vidyapeeth (Deemed to be University) Udaipur. 16 Ph.D. students have been awarded their Ph.D. degrees under his supervision in various aspects of green chemistry. He has around 150 research publications to his credit in the journals of national and international repute. He also has a patent to his credit. He is a reviewer of around 50 international journals.

Dr. Rakshit has successfully organized many national conferences at the University of Kota, Kota; PAHER University, Udaipur, and JRN Rajasthan Vidyapeeth, Udaipur. He has delivered invited lectures and chaired sessions at 20 national conferences in different parts of the country. Dr. Rakshit served as a Council Member (2011-2013 & 2020-2022) and an Associate Editor of Physical Chemistry Section (2014-16), a Scientist-in-Charge in the Industrial and Applied Chemistry Section (2014-2016) of the Indian Chemical Society, Kolkata, and an Executive Council Member (2012-2014). He was also a Zonal Secretary (2016-18) of the Indian Council of Chemists, Agra.

He has written books and chapters published by CRC Press (Taylor & Francis), UK; Academic Press, Elsevier; Nova Publishers, USA; and Trans-Tech Publications, Switzerland. In 2017, he received Prof. U.C. Pant Memorial Award instituted by the Indian Chemical Society for his significant contribution. His research specialization includes photochemistry, green chemistry, microwave-assisted reactions, environmental chemistry, waste-water treatment, nanochemistry, solar cells, bioactive and conducting polymers. Recently, he has been elected as the Vice-President of the Indian Chemical Society, India.

Sharoni Gupta

Sharoni Gupta obtained her Ph.D. degree from Mohanlal Sukhadia University, Udaipur (Raj.), India in the year 2020. She was awarded the University Gold Medal for securing the first position in M.Sc. (Chemistry) in the year 2015. She was also a recipient of the Maulana Azad National Fellowship from the University Grants Commission, New Delhi. She has contributed 10 articles and chapters to the journals and books of leading international publishers such as Apple Academic Press, CRC Press, Bentham Science, Elsevier, Springer Nature and Wiley & Sons. Her specialization fields include graphene-based chemistry, nanocatalysis, and sustainable organic synthesis.