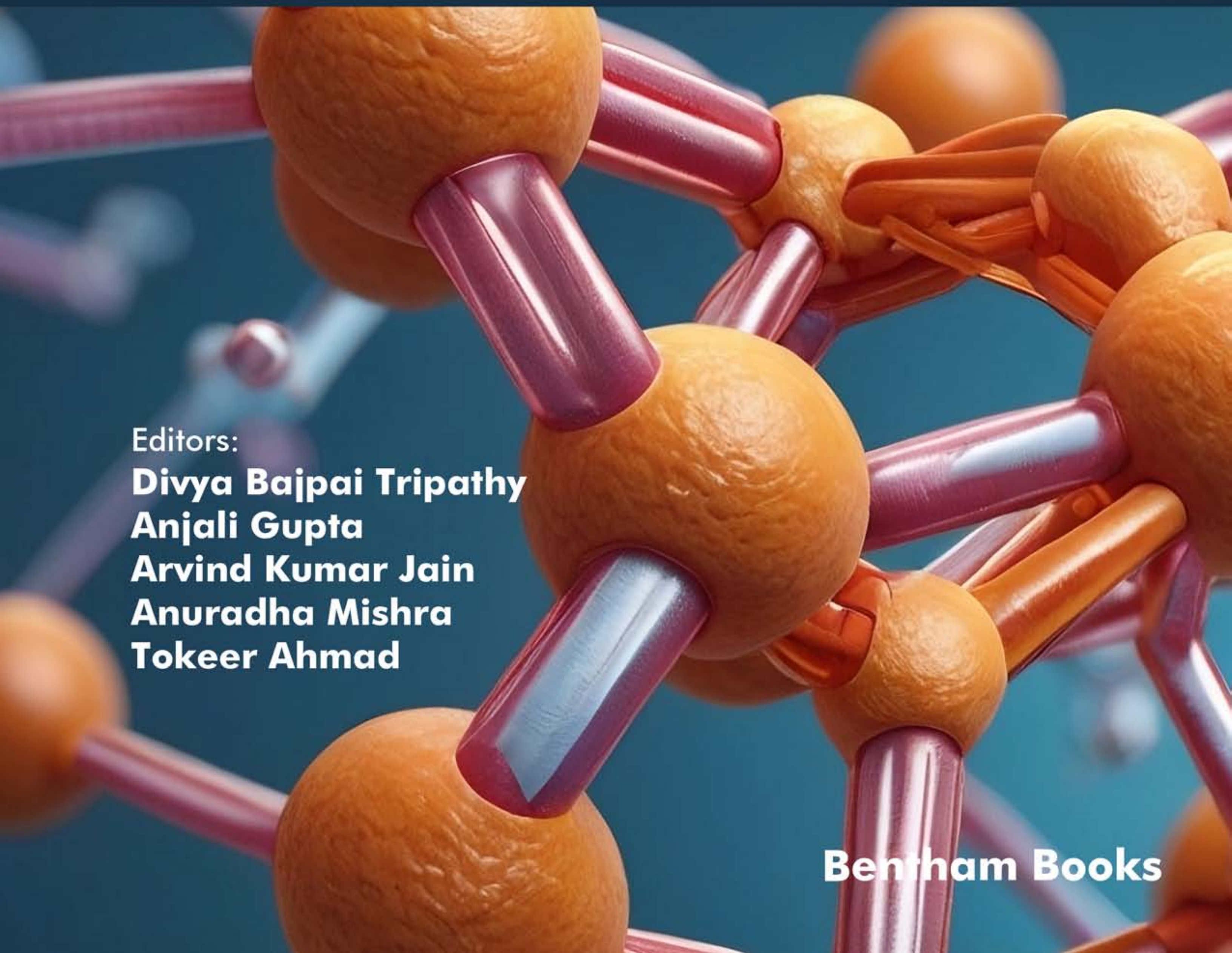
NANOTECHNOLOGY:
A QUICK GUIDE TO MATERIALS AND TECHNOLOGIES



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Nanotechnology: A Quick Guide to Materials and Technologies

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CONTENTS

PREFACE

"Nanotechnology: A Quick Guide to Materials and Technologies", is a comprehensive compendium that offers a concise yet insightful exploration of the fascinating world of nanomaterials and their diverse applications in smart devices, renewable energy, environmental sustainability, and beyond.

The rapid advancements in science and technology have revolutionized our lives, and materials play a fundamental role in driving these innovations forward. Nanomaterials, in particular, have emerged as key enablers of groundbreaking technologies due to their unique properties and versatility. This guide aims to provide a succinct overview of various nanomaterials and their remarkable applications, offering a valuable resource for both experts and newcomers seeking to understand the impact of nanotechnology on modern-day advancements.

Chapter 1 embarks on a journey through the realm of smart devices, exploring how nanomaterials are at the heart of these revolutionary technologies. From enhancing electronic components to improving energy efficiency, nanomaterials have unlocked new dimensions in the design and functionality of smart devices.

Chapter 2 delves into the world of semiconductor nanomaterials, which form the backbone of modern electronics. We investigate the unique properties of these materials, which have propelled the semiconductor industry to new heights and paved the way for quantum computing and other cutting-edge technologies.

Chapter 3 focuses on the fascinating field of photocatalysis, where nanomaterials display exceptional prowess. By harnessing the power of light, these materials can drive chemical reactions for environmental remediation, energy conversion, and much more, contributing to a cleaner and greener future.

Chapter 4 takes a closer look at polymer nanomaterials and their remarkable applications in a wide range of industries, from flexible electronics to biomedical devices, demonstrating their immense potential for shaping the technologies of tomorrow.

Chapter 5 unveils the realm of nano-catalysis, where nanomaterials act as catalytic agents with superior efficiency and selectivity, promising transformative solutions for cleaner and more sustainable chemical processes.

Chapter 6 explores the exciting world of carbon nanomaterials, such as carbon nanotubes and graphene, showcasing their extraordinary electrical, mechanical, and thermal properties that have sparked a revolution in various applications, from electronics to advanced composites.

In Chapter 7, the significance of modeling and simulation in understanding nanomaterial behaviour is discussed. The chapter provides a glimpse into the advanced techniques that underpin the design and optimization of nanotechnologies.

Chapter 8 focuses on the vital role of nanomaterials in photovoltaic applications, where they drive innovations in solar energy conversion, increasing efficiency and sustainability in our pursuit of cleaner energy sources.

Chapter 9 examines the critical role of nanomaterials in water purification, addressing the pressing global challenges of water scarcity and pollution, and offering promising solutions for access to clean and safe drinking water.

Chapter 10 explores the synergy between rare earth materials and nanotechnology, illuminating their importance in photovoltaic applications and their potential to revolutionize renewable energy technologies.

Chapter 11 showcases the fascinating realm of nanomaterials in sensing applications, enabling the creation of highly sensitive and selective sensors for monitoring environmental conditions, health parameters, and much more.

Chapter 12 unveils the innovative applications of ion beams in nanostructure development, pushing the boundaries of nanotechnology and paving the way for groundbreaking discoveries.

In Chapter 13, the realm of environmental remediation has been discussed, where nanomaterials offer ingenious solutions for mitigating pollution and addressing environmental challenges in a sustainable manner.

Chapter 14 brings us to the realm of Nano lubricants, which promise enhanced efficiency and reduced energy consumption in mechanical systems, leading to greener and more sustainable industrial practices.

This guide aims to provide readers with a concise yet comprehensive understanding of the diverse applications of nanomaterials and the significant impact they have on modern technologies. We hope that this quick guide will serve as a valuable resource for students, researchers, engineers, and anyone eager to explore the dynamic and transformative world of nanotechnology.

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CHAPTER 1

Application of Nanomaterials for Smart Devices

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Abstract: Nanomaterials have emerged as transformative agents in the realm of smart devices, enabling revolutionary advancements and applications. At the nanoscale, materials exhibit unique properties that differentiate them from their bulk counterparts, offering exceptional opportunities for enhancing the performance, functionality, and miniaturization of smart devices. The present chapter delves into the significant contributions of nanomaterials in the development of smart devices. Nanotechnology's ability to engineer materials at the atomic and molecular level has led to the creation of nanomaterials with precisely tailored properties. These nanoscale wonders have found applications in diverse fields, including electronics, healthcare, energy, and environmental monitoring. The integration of nanomaterials in smart devices has unlocked unprecedented opportunities for innovation. Nanoscale sensors with heightened sensitivity and selectivity have transformed devices into intelligent perceivers of the environment. Additionally, nanomaterials have revolutionized energy storage, enabling longer-lasting batteries and supercapacitors with higher energy density. Furthermore, nanomaterials play a pivotal role in advancing smart displays, wearable technology, and Internet of Things (IoT) devices. The seamless connectivity and improved performance offered by nanomaterials have paved the way for a more connected and efficient world. Additionally, this chapter emphasizes the immense potential of nanomaterials in shaping the future of smart devices, making them more adaptive, energy-efficient, and capable of transforming our daily lives. However, responsible implementation and safety considerations are essential for harnessing the full potential of nanomaterials and ensuring sustainable and secure technological advancements.

Keywords: Carbon, CNT, Energy storage, Flexible displays, Graphene, Metal oxide, Nanomaterials, Nanofibers, Nanoelectronics, Photocatalyst, Quantum dots, Sensors, Supercapacitors, Transistors, Wearable devices, Wireless communication.

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Divya Bajpai Tripathy, Anjali Gupta, Arvind Kumar Jain, Anuradha Mishra and Tokeer Ahmad (Eds.)

INTRODUCTION

In the ever-evolving landscape of technology, smart devices have emerged as transformative instruments that seamlessly integrate with our daily lives. From smartphones and wearable gadgets to smart home appliances and IoT-enabled systems, these devices have revolutionized the way we interact with the digital world. Over the last few decades, nanomaterials have emerged as the transformative agents driving the evolution of smart devices, ushering in a new era of technological advancements.

Nanomaterials are materials with at least one dimension in the nanoscale range, typically between 1 and 100 nanometres. At this scale, materials exhibit unique and distinctive properties that differ from their bulk counterparts. These properties arise from the high surface area-to-volume ratio and quantum confinement effects that become more pronounced at the nanoscale. Nanomaterials can be classified into different categories based on their dimensions, shapes, and structures. Some common types of nanomaterials include nanoparticles, nanotubes, nanowires, nanocomposites, and nanofilms, among others. At the nanoscale, materials exhibit extraordinary properties and behaviours that deviate from their bulk counterparts [1 - 3]. These unique characteristics, such as quantum confinement effects [4] and high surface area-to-volume ratio [5], empower nanomaterials to revolutionize the functionality and performance of smart devices. The convergence of nanotechnology and smart devices has unlocked unprecedented opportunities for innovation across various industries, reshaping how we interact with technology and enhancing our daily experiences [6]. The introduction of nanotechnology has enabled the manipulation and engineering of materials at the atomic and molecular levels, granting researchers the ability to design nanomaterials with precisely tailored properties. These nanoscale wonders have found a myriad of applications in the realm of smart devices, facilitating improvements in electronics, energy storage, sensors, and beyond [7 - 10]. Nanomaterials offer a promising avenue for addressing the miniaturization challenge in smart devices (Fig. **1**), as their nanoscale dimensions pave the way for more compact and efficient components. From quantum dots for vibrant displays to carbon nanotubes for flexible electronics, nanotechnology has unraveled a host of possibilities for smart device miniaturization and optimization [11].

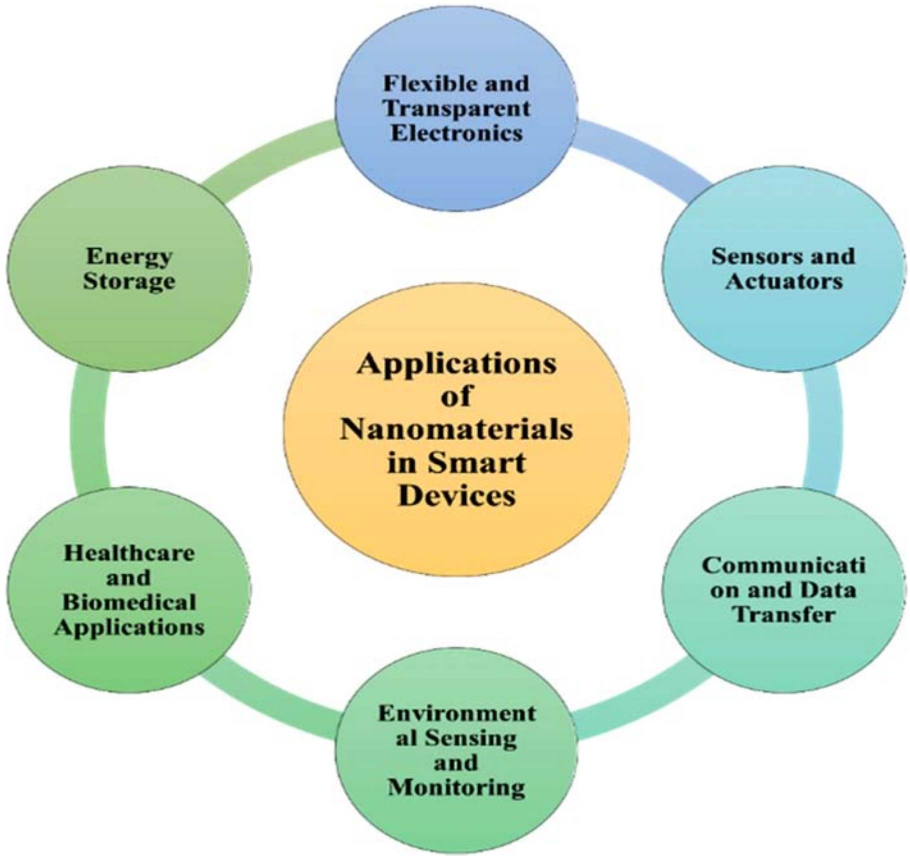

Fig. (1). Schematic representation of avenues of nanomaterials in smart devices.

One of the most significant contributions of nanomaterials in smart devices lies in their unmatched sensing capabilities. Nanoscale sensors can detect and respond to minute changes in their environment, enabling smart devices to gather real-time data and react adaptively [12]. Moreover, nanomaterials play a pivotal role in boosting the energy efficiency of smart devices. Nanostructured electrodes in batteries and supercapacitors offer higher surface area and faster ion transport, leading to improved energy storage and longer-lasting devices [13 - 15]. Additionally, nanomaterials enhance the connectivity and communication abilities of smart devices [16]. Nanoscale antennas and transceivers enable seamless wireless connectivity, enabling the Internet of Things (IoT) ecosystem and driving the interconnectedness of smart devices for a more integrated and intelligent world [17].

CHAPTER 2

Semiconductor Nanomaterials

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Abstract: The physical and chemical characteristics of semiconductor materials radically alter as their size is shrunk to the nanoscale, giving rise to unusual traits because of their enormous surface area or quantum size effect. Despite being at the research stage right now, semiconductor nanomaterials and devices hold great promise for use in a variety of sectors, including solar cells, nanoscale electronics, light-emitting nanodevices, laser technology, waveguides, pharmaceuticals, and biosensors. The semiconductors will undoubtedly experience substantial advancements as nanotechnology continues to advance. The entire mechanism is regulated with the help of band theory, which includes valence band, conduction band and an energy gap, also considered forbidden gaps. These semiconductors when converted into nano sizes are corresponded to nanoparticles, which have the potential to accommodate various functionalities due to the reduced size, which increases the surface area for better function, adsorption, efficiency, and other things as discussed in the book chapter. This chapter also focuses on some of the most important activities now underway and problems that must be solved to enhance nanostructures and nanodevices based on semiconductors.

Keywords: Light emitting nano devices, Nanomaterials, Semiconductors, Solar cells.

INTRODUCTION

Semiconductors are substances with significant capability of conversion of their electrical properties from conductors to insulators and then to conductors. Semiconductor nanoparticles were made by various techniques to get the desired shape, size, and dimension. This is done by reducing the size of semiconductors to change their physicochemical properties to generate a quantum size effect. The entire field is so widely helpful and the most promising research for their implementations as light emitting nanodevices, laser technology, waveguide, *etc.* [1]. Majorly the conductivity and optical properties of semiconductors like

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Divya Bajpai Tripathy, Anjali Gupta, Arvind Kumar Jain, Anuradha Mishra and Tokeer Ahmad (Eds.)

absorption coefficient and their refractive indices have been altered to induce nanomaterial properties. Various semiconductor nanomaterials such as Si, Si-Ge, AlInGaP, CdSe, CdS, *etc*. have been significantly used in various applications such as in computers, cell phones, CD players, satellites, traffic signals, *etc*. Semiconductors are usually generated from a variety of differently rated compounds of type II-VI, III-V, or IV-VI semiconductor nanocrystals as per the modern periodic table [1, 2]. Reduction of size affects the physical properties of semiconductors such as structure, appearance, magnetic properties, optical properties, dielectric properties, and various thermal properties. This is due to surface effects and quantum size effects. Hence, because of the extremely small size of these materials, they exhibit properties that are essentially different from the original form of semiconductors and become superior in their characteristics and other viable properties [3].

In nanomaterials generated from semiconductors, electrons are confined to regions having all one, two, or three-dimensional structures, when comparing their sizes and dimensions according to de Broglie's wavelength [4]. In the subsequent history of nanotechnology, Nanosciences is subsequently gaining a lot of potential and has an impact on various research fields. However, in the 21st century, there has been subsequent production in Nanosciences between a range of diameter of 1 to 20nm [4, 5]. According to various research works, nanosciences has opened new options and availability for drug delivery, and gene therapy. Nanomaterials are also used for various diagnostic codes in medical sciences and can be used as nanocapsules and nanodevices. Nanoparticles are so widely useful for investigation purposes in forensic sciences; the major predictable uses are in fingerprints, forensic chemistry, *etc.* [6]. For decades, carbon nanotubes have been so widely used due to their thermal conductivity being twice to that of even diamonds. These nanotubes generally carry an electric current 1000 times more than in a simple copper wire, and are thermally stable in a vacuum up to 2700°C. Carbon nanotubes can be reinforced into nanocomposites, and have a wider range of other possible uses such as in electronic devices, nanocomputers, transistors, solar cells, types of diodes, such as light emitting diodes (LED), silicon-controlled rectifiers, and digital and analog circuits, hydrogen production, synthesis of silicon semiconductors and their useful devices. Various other optoelectronic devices are wide examples of semiconductor devices.

Nanotechnology has been significantly integrated with a variety of other disciplines propagating its effective and continuous use. Examples of such integrated disciplines include nanosciences, nanobiotechnology, nanochemistry nanophysics, nano-forensics, *etc*. [7, 8]. Additionally, research into nanoparticles and nanostructures is a crucial area for developing new norms, frameworks, and methods, perhaps leading to advancements in difficult logical problems. Nanomaterials formed from nanoparticles and nanocrystals exhibit unique optical and electrical properties [9] Subsequently, these nanomaterials are classified as Zero dimensional nanomaterials, quasi-one-dimensional nanomaterials, two-dimensional nanomaterials, and three-dimensional nanomaterials. All these nanomaterials have different chemical and physical properties. These are relatively different in conductivity, resistance, and uses on the nanoscale [10].

The entire book chapter presents a thorough study of semiconductor nanomaterials, their formation, hybrids of nanomaterials, their types, functionality, and applications. [11].

NANOSCIENCES AND NANOTECHNOLOGY

Nanosciences and nanotechnology deal with the manipulation of materials at the nanoscale or nano-diameter. This manipulation has been made by scientists and nanotechnologists to make various fundamentals of life possible, to create eco-friendly and sustainable products, and to emphasize eco-friendly development [12]. Since ancient times only, various chemically synthesized nanomaterials have been significant in use. Nanomaterials in the recent world have become potentially important both to scientists, and technologists, in medical sciences and practices, diagnostic activity, drug delivery systems, *etc.* [13, 14]. These materials are evident mainly due to their physical-chemical characterization and due to these characteristics, nanomaterials open new windows towards processing of other efficient high-performance materials.

The terminology nanomaterials has been a significant part of the modest term ‘nano’ which is derived from the Greek word ‘dwarf’. Nanomaterials have been significantly classified as nanoparticles, nanoclays, and nanoemulsions. Further classification of nanoparticles is as follows: organic nanoparticles and, inorganic nanoparticles as shown in Fig. (**1**) [15].

Nanoparticles have been accepted as useful materials in mega industries incorporated by nanotechnology. Nanoparticle science is a subsequent branch of substances that are dissected with various instruments and advancements in nanoparticle science. Nanomaterials made from semiconductors are crystallined with approximate sizes of 1-100nm. The majority of semiconductors are usually explained as band hole vitality, which in in turn requires an electron to move from valence vitality into empty vitality bands [16]. These nanomaterials have very few electrons in their conduction band and have more electrons in the valence band. Major fields of research in nanotechnology are summarised in tabular form in Table **1** [16 - 20].

CHAPTER 3

Advances in Nanostructure-Induced Photocatalysis

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Abstract: As the catastrophic effects of global energy are becoming severe day by day, researchers are focusing on adapting environmental sustainability in order to restore the natural habitat of the planet. Photocatalysis is an environmentally benign approach to combating various non-sustainable operations *via* green chemistry. Photocatalysis comprises the change in the kinetics of chemical transformations by the absorption of light. Photocatalysis is the promising route of producing green hydrogen *via* overall water splitting without any toxic by-products. Verily, photocatalytic reduction of carbon dioxide is another significant sustainable operation that ascertains its sequestration and conversion into value-added chemical feedstock and fuels. These highly sought photocatalytic applications demand unique multifunctional nano catalytic systems that can effectively carry out these sustainable operations due to their advanced optoelectronic and morphological properties alongside having higher exposed active sites. Realizing the potential of nanostructures in the field of photocatalysis, we have synergistically emphasized both these topics in this book chapter under the light of the classification of nanostructures and two vital photocatalytic applications of hydrogen evolution and carbon dioxide mitigation.

Keywords: Hydrogen evolution, CO_2 reduction, Nanostructures, Photocatalysts.

INTRODUCTION

Man-made triggered natural and socio-economic calamities have mandated the establishment of sustainable activities at the scalable point so as to combat their aftermath effects. One of the most influential and multi-dimensional ways of achieving sustainability on the planet is environmental sustainability which assures the rational usage and conservation of natural resources [1]. Environmental sustainability aspires to the consideration of the environmental and socio-economic consequences of human activities. Alongside, it strives for the balance that guarantees the durable and long-lasting viability of renewable and

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non-renewable resources [2, 3]. Few fundamental principles pertaining to environmental sustainability emphasize the preservation and protection of natural reservoirs of useful land areas, freshwater bodies, clean air, and biodiversity [4, 5]. This primarily involves alleviating pollution, subduing plastic waste and safe-guarding the biospheres, ecosystems and natural wildlife habitats [6]. Another, crucial step towards environmental sustainability is making the steady transition from fossil derivative fuels to sustainable energy resources such as solar [7], wind [8], hydro [9], and geothermal power [10] that hold enough potential to deliver scalable supply. The usage of renewable energy sources (RESs) impedes the rate of emission of greenhouse gases, mitigates the extent of global warming and seasonal changes, and also reduces the dependency on limited non-sustainable energy resources [11]. Efficiency in using available resources is one vital principle of environmental sustainability that promotes the usage of resources efficiently by adopting sustainable synthetic methods and consumption practices, and by decreasing waste generation and accumulation. This comprises an efficient use of energy resources, recycling and reusing materials, and cutting down water usage. Environmental sustainability increases collective responsibility of researchers, government bodies and individuals for the development of RESs that can successfully replace conventional fuels [12, 13].

For making an adequate balance between the present and future generation demands without causing significant harm to the environment, photocatalysis has become one of an emerging candidates that ought to fulfil an eligibility to be regarded as a sustainable solution. Photocatalysis is the systematic route of exploiting light energy for driving chemical reactions to convert it into chemical energy [14]. Photocatalytic pathway basically entails the primary photocatalyst, usually semiconducting material which can effectively absorb light energy and initiate the chemical transformations [15 - 17]. Photocatalytic system conventionally functions by absorbing photons from the light source and transferring that energy into reactant species, thus accelerating the rate of the desired reaction. The most vital component of photocatalysis is the catalytic system that is generally a semiconducting material such as metal oxides [18 - 20], transition metal dichalcogenides (TMDs) [21], transition metal phosphides (TMPs) [22], gC_3N_4-based derivatives [23], perovskite derivatives [24], *etc.* These semiconducting materials have the distinguishing chemical property known as the optical band gap, which allows these compounds to absorb light in the ultraviolet (UV) or visible range of the electromagnetic spectrum [25]. When photon energy is absorbed, electrons in the photocatalyst are excited to a higher energy level, creating electron-hole pairs. Photo-excited electrons can reduce different reactant molecules by donating their energy, whereas the holes are able to oxidize several molecules by accepting electrons to undergo oxidation reaction. These redox reactions result in the formation of reactive intermediates such as hydroxyl radicals ($OH^{\cdot}$) or superoxide ions ($O_2^{\cdot-}$), which are exceptionally reactive and are capable of initiating and propagating the targeted chemical transformations [26].

Photo-generated electron and hole carriers are capable of taking part in diverse chemical reactions taking place on the surface-active sites of the catalyst such as photocatalytic overall water splitting to facilitate hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) taking place at conduction band and valence band, respectively [27]. Another important chemical reaction that transpires over a photocatalyst surface is the photo-reduction of carbon dioxide to transform it into value added chemical feedstock. Some other important chemical reactions that can take place *via* photochemical pathway are water treatment, photo-degradation of toxic dyes, removing contaminated trace metal ions from water, self-cleaning functional reactions, antifogging, self-sterilization, antibacterial and cancer treatment [28 - 31]. All these photochemical applications are significant in their respective areas to collectively fulfil the aim of environmental sustainability as photocatalysis route is utilized in wide array of fields, comprising nanoremediation, energy-related applications of generation and storage and green organic synthesis as depicted in Fig. (**1**) [32]. The functionalities of photocatalysis corroborate with thrust among researchers and actively progressed.

For effective exploitation of the active sites of catalysts, one of the most fundamental principles of photocatalysis is that it should possess a higher surface area to volume ratio, as it yields a greater number of sites available for catalysis. This is the reason that nanostructures exhibit superior catalytic efficiency as compared to their bulk counterparts. Nanostructures refer to those materials that have nanoscale dimensions, usually ranging from 1 to 100 nm. Nanostructures can occur either naturally or constructed artificially and they possess advanced properties and behaviors such as quantum mechanical effects, quantum confinement of electrons and increased surface area to volume ratio [33, 34]. Nanostructures and nanomaterials have transformed diverse fields of science and technology, enabling advancements in electronics, materials science, medicine and healthcare, energy, and several other fields. The ability to manipulate matter at the nanoscale has opened up new possibilities for designing materials with tailored properties and functionalities.

CHAPTER 4

Polymer Nanocomposites and their Applications

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Abstract: The last ten years have seen the greatest amount of research on nanomaterials due to their numerous applications. Nanomaterials are utilised in both home and industrial settings. The growing need for materials that are both lightweight and strong has led to the emergence of polymer composites as a specialty area in the field of materials research. A novel type of composite material called polymer nanocomposites uses inorganic nanoparticles scattered across an organic polymer matrix to enhance certain performance characteristics. Excellent characteristics of polymer nanocomposites include electrical characteristics, barrier resistance, and magnetic efficiency. greater rigidity, greater fire resistance, increased thermal and dimensional stability, superior optical characteristics, and improved barrier effect are the main benefits of polymer nanocomposites. A polymer serves as the matrix of polymer nanocomposites, which are mixtures of two or more components, where the dispersion phase has at least one dimension smaller than 100 nm. Due to their distinctive design feasibility and remarkable property combinations, polymer nanocomposites are employed in a variety of applications, including water treatment, gas separation, food packaging, sports equipment, the automotive industry, bio-medicine and everyday life.

Keywords: Bio-medical, Dispersion phase, Food packaging, Polymer nanocomposite, Water treatment.

INTRODUCTION

A combination of two or more phases with distinct compositions or structures, at least one of which is in the range of 10 to 100 nm, is called a nanocomposite. As it has fewer atoms per particle than bulk materials, a filler in the nanometer range may exhibit distinct characteristics and exhibit robust matrix interactions. The sequence of molecular diameters determines the separation of filler particles, which can alter the characteristics of polymers. The main objective of polymer

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Divya Bajpai Tripathy, Anjali Gupta, Arvind Kumar Jain, Anuradha Mishra and Tokeer Ahmad (Eds.)

nanocomposite research is to use molecular or nanoscale fillers to increase the strength and toughness of polymeric components. Relative to traditional composites, composites that display a change in composition and structure across a nanometer scale have demonstrated extraordinary property enhancements like large modulus, gas barrier, temperature of heat distortion, retention strength, ablative resistance, atomic oxygen resistance and resistance to small molecule penetration. It's interesting to note that these improvements in performance are obtained without raising the underlying polymer's density, sacrificing its optical properties, or reducing its recyclable nature.

Due to their small size, polymeric nanoparticles (NPs) have generated a lot of interest recently [1 - 3]. When polymers with good electrical, magnetic, mechanical, thermal, and optical properties are combined with nanoparticles in the form of nanotubes, nanofibrils, nanosheets, and polymer nanocomposites then quantum dots are created. The main goal or objective of polymer nanocomposites is to combine the properties of nanofillers with superior material and processability of the polymers in the hope of creating composite materials with noticeably improved macroscopic properties. One or more nanofillers are distributed inside a polymer matrix in these materials [4, 5]. Polymer Nanocomposites (PMCs) are hybrid materials made up of nanoparticles acting as nanofillers and polymers acting as the matrix. Because several components are incorporated into a single, compatible structure, PNCs have never-before-seen multi-functions. This makes PNCs extremely useful in a wide range of optical, magnetic, and electrical applications. There are two kinds of polymers: synthetic and natural. Natural polymers are those that can be extracted for use from their natural habitat. Water is a common constituent of natural polymers, including cellulose, silk, wool, DNA, and proteins [7]. Conversely, synthetic polymers are those that are created artificially, including epoxy, Teflon, nylon, polyester, and polyethylene. To construct a PNC with better properties tailored to a specific application, various inorganic nanofillers, such as metal-oxide nanoparticles, metal nanoparticles, carbon nanomaterials, and nanoclays, can be inserted within a polymer matrix.

Polymeric nanocomposites (PNCs) are important materials for both industrial and scientific purposes since they are widely used in electromagnetic shielding, energy, packaging, defensive systems, sensors, and catalysis [6 - 8]. Nanomaterials can be divided into natural and synthetic varieties. The typical nanomaterials used in polymer nanocomposites are nanocellulose, nanoclay, silica nanoparticles, graphene and MXene, carbon nanofibers and nanotubes, and ZnO quantum dots [9 - 11]. Among other favorable qualities, the majority are renewable, have large specific surface areas and high crystallinity, and can have surfaces that can be functionalized. Nanomaterials can play two important functions in polymer nanocomposites. Enhancing the material's many qualities, including its mechanical barrier, thermal conductivity, flame retardancy, and electrical properties, is the initial stage. Meanwhile, the second is the modification of morphology and miscibility of the polymer nanocomposites.

Polymer nanocomposites are a subset of composite materials that contain a polymer matrix and one or more nanofillers scattered throughout. The fundamental idea is to combine the processability of polymers with the superior material properties of nanofillers to produce composite materials with significantly improved macroscopic attributes [12, 13]. This chapter focuses on the different properties and applications of polymer nanocomposites.

PROPERTIES OF NANOCOMPOSITES

The nanocomposite properties are based on the characteristics of the clay, nanofiller, polymer and a combination of polymer as well as composite structure. When compared with traditional composites, the nanocomposite possesses noticeable differences in their electrical, thermal, mechanical, and barrier properties. One physical property may not be the best for the optimal structure of a nanocomposite of another physical property. This section highlights the nanocomposite properties.

Thermal Properties

Nanocomposites having thermal properties can be analyzed by DSC. The thermal stability can be calculated by weight loss on heating the nanocomposites. By several researchers, the dependence of HDT on clay content has been investigated. The heat resistance of nanocomposite on external loading can be measured from the HDT. Multiple applications such as heat sinks, thermal interface materials, connectors, printed circuit boards and thermal management of high-performance systems [14 - 17] have good thermal conductivity in the polymer nanocomposite.

Mechanical Properties

The mechanical properties of polymer nanocomposites like modulus, elongation, and tensile strength are affected by the morphology of the surface and the material which are used for production. Between the polymer and nanofiller, the mechanical properties of polymer nanocomposite improve affinity with high rigidity and high aspect ratio of nanofillers [18 - 21].

CHAPTER 5

Sustainable Nanostructured Materials for Organic Synthesis

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Abstract: Nanocatalysis represents a burgeoning field of study that is used across a wide range of catalytic organic reactions. The significance of nanotechnology is progressively growing in various industrial sectors as well as in academic research. The enhancement of catalytic selectivity and activity in nanocatalysts is observed as the size of the catalyst decreases and the surface area-to-volume ratio increases. Similarly, the morphology of particles plays a crucial role in influencing the activity and selectivity of nanocatalysts. Various types of nanocatalysts have been documented, encompassing single-metal nanocatalysts, simple/mixed metal-oxide derived nanocatalysts, and carbon-based nanocatalysts. Nanocatalysts based on noble, rare earth and transition metals have been extensively investigated in both industrial and academic areas. This is primarily due to their significant application in various chemical reactions, including carbon-heteroatom cross-coupling reactions, carbon-carbon homocoupling reactions, carbon-carbon cross-coupling reactions, esterification, C-H activation, hydrogenation, oxidation, and reduction. Currently, the analysis is centered on most recent advancements and potential applications of nanocatalysts in various chemical processes.

Keywords: Carbon Nanocatalysts, Gold-catalyzed organic conversions, Nanocatalysis.

INTRODUCTION

Modern era of organic chemistry evidences the incessant and united endeavors of numerous research groups of organic chemists and therefore it has resulted in a profusion of now known organic compounds with an extensive variety of applications in medicines and pharmaceuticals, food and textile industries, agrochemicals and most importantly as fine chemicals [1, 2]. The synthetic organic compounds with industrial and biological applications are at the center of

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Divya Bajpai Tripathy, Anjali Gupta, Arvind Kumar Jain, Anuradha Mishra and Tokeer Ahmad (Eds.)

the modern chemical industry. Thus, the current research trends in organic chemistry emphasize the advancement of synthetic processes and altering of certain existing ones. With the advent of the 21^{st} century, the concern about the perilous compounds utilized and produced during chemical processes ultimately led to the evolution of the concept of green and sustainable chemistry [3 - 5]. The rationale behind this concept is the advancement of sustainable chemical enterprises that will create innovative ways to reduce the ecological impact of hazardous chemicals and also to minimize human exposure to these substances while improving scientific growth. The recent research trends of green chemistry in the area of beneficial organic synthesis have recently adopted several ingenious scientific developments accompanied by enhanced and efficient synthetic methods that eschew the utilization of noxious reagents and reactants, harsh reaction conditions, expensive and sophisticated catalysts [6]. The evolutions of sustainable, economical, and green chemical methods are still considered as challenges in chemistry. Additionally, the conventional requirement for selective and effective catalytic reactions which will convert raw materials into beneficial pharmaceuticals, chemicals, and fuels, is that green chemistry also targets atomic potential, waste reduction and high rates of catalyst recovery [7 - 9]. During the course of ongoing research endeavors, researchers have also been intensely captivated by practicing the concepts of green chemistry in organic conversions. The significant principle of green chemistry which fascinated us is entirely devoted to the enterprise of energy efficiency that emphasizes the development of synthetic strategies demanding minimal amounts of energy to perform a precise reaction with the best productivity and the energy can be saved by employing protocols that accomplish the organic transformations at ambient temperature. Designing reaction schemes at room temperature and pressure *i.e.* under ambient conditions followed by other aspects of green chemistry is a present research area of emphasis in organic chemistry and is progressing significantly [10]. In spite of remarkable achievements in research on catalysis, the succeeding catalyst technology remains largely an art rather than a science. This account reviews recent advances in organic transformations by employing metal and carbon-based nanocatalysts. A comprehensive overview of metal-based nanostructured catalysts utilized in distinguished organic transformations including selective and total oxidations, reductions, asymmetric hydrogenations, tandem reactions, coupling reactions, esterification or acetylation reactions and many more transformations with special emphasis over oxidation and reduction reactions is presented here. With respect to the current recent trends, we focused on research related to the advancement of nanomaterials used in catalysis mainly single metal or metal oxide-based nanocatalysts, morphology and crystal-controlled metal oxide-based nanocatalysts, mixed metal oxide-based nanocatalysts and carbon-based nanocatalysts. Designing nanomaterials for the enhancement of reactivity, selectivity, and recyclability *via* dominating the size, shape, composition, and structure of catalytically active nanoparticles as per the principles of nanocatalysts design is showcased with selected examples. These principles will assist the researchers in the fabrication and design of novel multifunctional nanostructured catalysts for the advancement of sustainable and green chemical methods.

Stockholm is signified as the cradle of catalysis where, Jons Jacob Berzelius, the great Swedish chemist first employed the term "catalysis" in 1835 taken from the Greek kata-, "down", and lyein, "loosen" by analogy to the word "analysis" to correlate a group of experimental observations made by other chemists in late 18^{th} and early 19^{th} centuries such as the conversion of starch to sugar by acids, fermentation of beer and wine, synthesis of soap and sulfuric acid, alcohols oxidation to acetic acid in the presence of platinum, decomposition of hydrogen peroxide on metals and many more [11]. As the phenomenon of catalysis is defined as a method by which the reaction rate is increased by adding a small amount of such promoting agents reputed as catalysts that evidently do not experience any alteration in the course of the reaction with any change in reaction conditions. Later, some practical observations show that actual catalysts may modify in structure, selectivity, and activity with respect to time on the activation step and can deactivate rapidly. After Berzelius around 60 years later, in 1895, Ostwald postulated this phenomenon of kinetic nature and defined it as "a catalyst is a material which alters the rate of a chemical reaction without itself taking place in the products' '. Another definition in accordance with IUPAC (1976) states that, a catalyst is a material which, being present in small proportions, increases the rate of achievement of chemical equilibrium without itself undergoing chemical change. So, it can be concluded that the action of a catalyst is initiated by reducing the energy required to progress the reaction pathway that is activation energy. This activation energy Ea is the energy desired to determine how fast a reaction occurs and also to overcome the reaction barrier. The lower the activation barrier, the higher the reaction rate. It is also noted that under the action of the catalyst, the thermodynamics of reaction remains unchanged and the foremost outcome is that the catalyst affects the rate of reaction [12, 13]. The research field of solid catalysts is of colossal interest because of its numerous applications in various areas of the chemical industry. Approximately 95% of products in the chemical industry are based on catalytic methods. Almost all the methods included in chemical transformations involve catalysts. Further, organic intermediate products are promising molecules due to their diverse applications in the pharmaceuticals, polymer, cosmetic, and food industries which are procured *via* numerous catalytic strategies [14]. Environmental protection parameters for air and water remediation such as control of automobile emissions *via* gas-sensing, gas purifications that are emitted from power stations, and wastewater treatment from industrial plants would be unachievable without the utilization of

CHAPTER 6

Advances in Carbon Nanomaterials

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Abstract: Carbon, having 6 electrons, shows sp^1, sp^2 and sp^3 hybridization to produce novel allotropes. Since the recent discoveries of fullerenes in 1985, carbon nanotubes in 1991 and graphene in 2004, there is immense regard for the amazing physical and chemical properties of carbon nanomaterials, promoting the growth of techniques for large-scale manufacturing. Carbon nanomaterials have been the subject of extensive scientific study all around the world due to their important structural dimensions and excellent chemical, mechanical, electrical, optical, magnetic, catalytic and thermal properties different from bulk counterparts. The carbon nanomaterials with 0, 1, 2 and 3 dimensions (carbon black, nanodiamonds, fullerenes, carbon quantum dots, carbon nano-horns, carbon nanofibers, carbon nanotubes and graphene) have shown such built-in properties that are easily exploitable in cutting edge technology for a numerous application. Applications in technology, medicine, environment and agriculture are all part of the ever-expanding commercial use of carbon nanomaterials. In this chapter, brief history and recent advancements in carbon nanomaterials specifically fullerenes, carbon nanotubes, graphene, carbon quantum dots, and nanodiamonds have been thoroughly reviewed. Along with their methods of synthesis, future prospects and opportunities in a variety of industries have also been discussed. Significant applications of different carbon materials in important areas have been highlighted. A summary of toxic effects of carbon nanomaterials on biological systems has also been given to support wise usage and careful handling.

Keywords: Arc-discharge method, Biosensing, Bioimaging, Buckyballs, Carbon nanotubes, Carbon quantum dots, Carbon graphene dots, Chemical vapor deposition, Drug delivery, Electrochemical methods, Fullerenes, Graphene, Graphite, Heat transfer, Hydrogen storage, Laser ablation method, Nanodiamonds, Nanomaterial, Nanofluid, Photoluminescent.

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Divya Bajpai Tripathy, Anjali Gupta, Arvind Kumar Jain, Anuradha Mishra and Tokeer Ahmad (Eds.)

INTRODUCTION

Nanomaterials have become one of the most fascinating categories of materials, which are in demand for a variety of uses. A nanometer can be envisioned by lining up five atoms of silicon or 10 atoms of hydrogen (each approx. 1 nm long). If a size of a material in at least one dimension is in between 1 to 100 nm, then it is a nanomaterial [1].

Carbon, having 6 electrons, has four external shell orbitals (2s, $2p_x$, $2p_y$ and $2p_z$) and as a result, it can hybridize into sp^1, sp^2 and sp^3. According to these configurations, carbon appears as a fascinating element. Due to its allotropic qualities, it can form compounds with a variety of properties based on the positioning of carbon atoms. Graphite and diamond are thought to be two natural allotropes. Diamond exhibits sp^3 hybridization. Its bond length is 1.56 Å. On the other hand, a hexagonal (honeycomb) lattice of graphite hybridizes in sp^2 having a bond length of 1.42 Å with 3.35 Å spacing between layers [2].

Novel allotropes of 0-D fullerenes, 1-D carbon nanotubes (CNT) and 2-D graphene have recently been discovered as a result of studies. Graphene forms the structural component for various types of carbon allotropes and is seen as a mono-planar sheet of sp^2-hybridized carbon having honeycomb structure. Rolled-up graphene forms seamless cylindrical tubes of CNT, while curled up, it forms spheres of fullerenes consisting of pentagons and hexagons. CNT can be of two types: single-walled CNT (SWCNT) and multi-walled CNT (MWCNT). When compared to MWCNT, which are stacked concentric shells of SWCNT having 3.4 nm spacing, SWCNT is seen as a single graphene layer rolled up [3, 4].

Owing to their distinct dimensions and better chemical and physical properties, carbon nanomaterials have obtained much attention in recent years [5, 6]. The atomic structures and interaction of these carbon nanomaterials with other materials strongly influence the characteristics they possess [7]. Carbon nanomaterials have superior electrical, optical and mechanical properties and larger surface area to volume ratio as compared to traditional materials [8]. Owing to their novel properties that are favourable for a varied range of applications in fields, to name of a few, batteries, capacitors, electronics, membranes, wastewater treatment, catalysis, imaging, biosensing, tissue engineering and drug delivery, these materials have drawn a much interest from both scientists and industries [8, 9].

While non-carbon nanomaterials depicting fluorescence like semiconductor quantum dots, are popular, their toxicity (caused by incorporation of heavy metals) makes them unsuitable for biological applications such as biosensor, bioimaging and targeted-drug administration. Carbon quantum dots exhibit no toxicity and show an edge in comparison to other carbon nanomaterials [10]. Thus, each allotrope of carbon shows unique characteristics and has been tried in various biological applications such as biosensor, targeted-drug delivery, imaging, cancer treatment and tissue engineering [11, 12].

The dimensions, morphologies and configurations of carbon have a significant effect on the properties and uses of carbon nanomaterials. As a result, a lot of consideration is put into synthesising these materials with the desired qualities. Numerous synthesis methods have been used up to this point, including electrolysis, hydrothermal synthesis, thermolysis, epitaxial growth, chemical vapour deposition, laser ablation, arc discharge, unzipping of CNT and Hummer's approach [3, 13]. Chemical vapour deposition, laser ablation and arc discharge are the most commonly used synthesis techniques. Also, scientists have faced several challenges limiting the applications of CNT in various fields [6]. Researchers have found that nanomaterials including carbon nanotubes, fullerenes and graphene demonstrate low solubility in water and fluorescence in the visible region, on the other hand, nanodiamonds are challenging to manufacture and separate. These challenges further need to be resolved by a thorough study of synthesis method. Therefore, this chapter provides a brief discussion on various allotropes of carbon, its common methods of synthesis and a summary of its applications.

TYPES OF CARBON NANOMATERIALS

Different types of carbon nanomaterials are shown in Fig. (**1**).

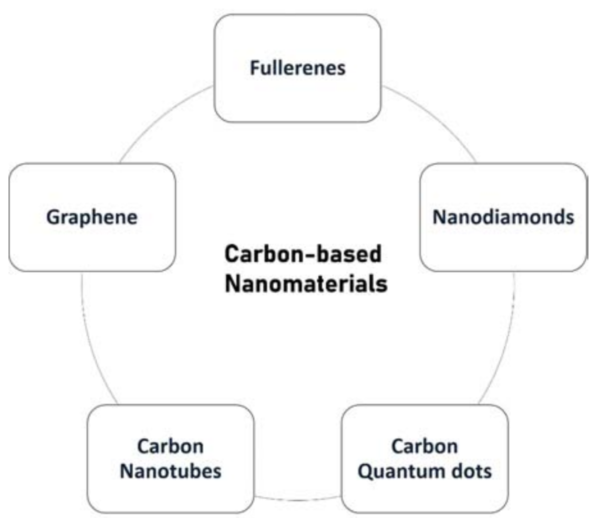

Fig. (1). Types of carbon nanomaterials.

CHAPTER 7

Modelling and Simulations of Nanomaterials

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Abstract: In view of the progression in the field of science to investigate the evolution of nanomaterial and their applications, the research seems to have been limited in providing a complete understanding of the fabrication conditions and characterizations primarily on the basis of experimental methods. The computational approaches are found to be more effective in predicting the growth conditions and the relative characterizations for the required structure. Moreover, the software counterpart for the design of structure is considered one of the most convenient approaches to estimate the process conditions in a well define way before proceeding with the complexities of the experimental trials. Another aspect of accepting the computation approach is to understand and explore the expected outcome from a structural analysis. In the present chapter, the key role of modelling and simulations in the advanced research and development at the structural level of the nanomaterial and the nanomaterial-based devices has been discussed in order to provide a guide to choose and explore a variety of software and theories for simulating or design.

Keywords: All-atom molecular dynamics Simulations (AAMD), Biomedicine, Born Oppenheimer approximation, Boundary Conditions, Coarse-grained Simulations (CG), Density Functional theory (DFT), Material Flow Analysis (MFA), Probabilistic species sensitivity distribution (PSSD), Tight Binding Approximation (TB).

INTRODUCTION

Over the past few decades, the research in the area of nanomaterials had a breakthrough in various technological sectors [1 - 28] including, smart devices for energy management, miniature electrical circuits, and biomedicine due to their distinct characteristics with size variations. Nanomaterials cover a class of particles having the critical diameter in the range of 1-100 nm, and the material could be crystalline, non-crystalline or amorphous in nature. Thus, depending on

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Divya Bajpai Tripathy, Anjali Gupta, Arvind Kumar Jain, Anuradha Mishra and Tokeer Ahmad (Eds.)

the type of the material, these can further be classified as energy storage materials, polymer nanomaterials, carbon nanomaterials *etc.* The investigation of distinct physical properties due to size effects in different fields of science has been well reported in the literature covering the advances in the deposition and characterization tools. Their ultra-small size has also advanced their use in potential applications of drug delivery [29, 30].

Nanotechnology is believed to make great contributions to medical technology, owing to its size comparable to the size of biomolecules and sub-cellular structures [31], high surface-area-to-volume ratio, and can be chemically and geometrically tuned [32]. Moreover, these materials can be modified to affect biomolecular interactions [33]. For a critical understanding of these, the three aspects of nano-bio interface interactions have been described as: a) cellular uptake; b) intracellular trafficking; and c) kinetics of nano-bio interactions [34 - 36]. Enormous research works are available focusing on molecular modelling methods as a part of computational biology, virtual experimentations for nanoparticles in drug delivery and not limited to the simulations of nanomaterials for probing their possible interactions with the cells. To understand the properties of these nano-bio interfaces between the cell membrane and the nanoparticles, a computational simulation study has been presented by Zhang *et al.* [37].

Further, at the nanoscale, the materials are much more sensitive towards environmental perturbations, therefore it is difficult to perform the repeated set of measurements *via* real-time experimentations. Computational modelling and simulation have evolved as a field of virtual experimental methods to explore the design aspects of nanomaterials and their mechanism for device applications [38]. The repetition of virtual experiments under variation of the surrounding conditions and parameters to investigate the possible outcome of the experiment is known as simulation. The simulation methods have been categorized based on the type of required investigation and the accuracy level of the results. For example, in order to examine the retardation effects with the change in size for gold nanoparticles, the methods of computational modelling have been employed [38]. A comparison has been presented for selecting different approximation methods and models for analysing these effects. These approximations are based on the boundary element method (BEM), discrete dipole method (DDM) and finite differential in time domain method (FDTD) [38]. Similarly, in one of the studies, the theoretical aspects of the behaviour of nanoparticles have been reviewed to analyse the stability conditions for growth and the practical applicability of nanoparticles in electroanalysis [39]. In 2008, Ward Jones *et al* explored the trends in the peak potential of randomly distributed nanoparticles *via* mathematical modelling [40]. The study depicts the variation in peak potential with the varying sizes of metal nanoparticles and a comparison has been made with the experimental study. Considering the electrolysis of nanoparticles, a number of theoretical studies were reported. For example, the simulation using a finite differential method for mapping the current response of nanoparticles sitting on the surface of planar electrodes has been reported [41]. To analyse the accuracy levels of the simulation technique, a distorted sphere, and hemispherical geometry have also been considered. Earlier the need for electrode modification *via* nanoparticles has also been reported [42]. The reported model simulated the voltammetric behaviour for the electron transfer at nanospheres. The observed patterns reflect the one dimensional diffusion with high coverage as there is a reduction in protons at the palladium whereas for small nanoparticles, there is low coverage and convergent diffusion has been observed.

The present chapter focuses on the terms and techniques used to model the structure of individual nano-particles and briefly outlines the basic approximation methods for modelling and simulation of these particles followed by the introduction to some of the available software for structural analysis and simulations.

Growth of Nanoparticles

The evolution of nanostructure in terms of the arrangement of atoms has been briefly discussed in order to understand the fabrication and optimized growth conditions of nanomaterials. The simplest approach to recognising the initial phases of the structure is the bottom-up approach considering the nucleation, coalescence and some intermediate phases, which form during the transition period.

In the beginning, the growth of nanoparticles starts with the appearance of a nucleating site present inside the medium. The process is known to be a physical change in terms of thermodynamically distinct phases. It can be homogeneous as well as heterogeneous. In homogeneous nucleation, the nucleating sites are activated throughout the medium whereas if nucleation takes place at the defect sites or the interface, then it is heterogeneous [43 - 45]. The temperature conditions of the surroundings play a crucial role in triggering the nucleation as homogeneous or heterogeneous. Nucleation is primarily dependent on the processes, in terms of interaction potential between the surface and the adsorbate. The adsorption of molecules is followed by the process of condensation, where a supersaturation state can be achieved. Supersaturation is the necessary condition for nucleation where the density is as high as to have short atomic separation.

The basic steps involved in the growth are thermal accommodation (Specific temperature requirements), binding of the atoms and diffusion, growth and coalescence. The primary stage of nucleation is also known as clustering. From

CHAPTER 8

Photovoltaic Applications of Carbon-Based Nanomaterials

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Abstract: The urgent need to replace fossil fuels with renewable energy sources in the twenty-first century has been driven by rising fuel prices and the escalating greenhouse effect caused by carbon dioxide emissions. Recent advancements in photovoltaic (PV) solar cell technology offer hope for meeting this demand using sustainable energy sources. Significant advancements have been achieved in the field, indicating numerous possibilities to address the ongoing global energy crisis. Carbon nanomaterials, including graphene, carbon nanotubes, and fullerene, have emerged as splendid applicants for photovoltaic solar cells. These materials are abundant on Earth, possess remarkable electrical properties, exhibit eminent optical absorption, and demonstrate paramount thermal and photostability. Graphene-based solar cells have already achieved notable breakthroughs in PV technology. However, reducing manufacturing costs through the utilization of cost-effective nanostructured materials and processes remains a crucial concern. This chapter provides a comprehensive review of various types of PV technologies using carbon-based materials.

Keywords: Carbon nanotubes, Fullerene, Graphene, Hysteresis, Morphology, Perovskite solar cells, Photovoltaic, Solar cell, Thermal stability.

INTRODUCTION

At present, the challenges confronting humanity include global warming issues, a decline in the accessibility of fossil fuels, and a persistent rise in global energy consumption. These factors are driven by the substantial emission of greenhouse

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Divya Bajpai Tripathy, Anjali Gupta, Arvind Kumar Jain, Anuradha Mishra and Tokeer Ahmad (Eds.)

gases from fossil fuels, the rapid expansion of the economy, and the substantial growth in the global population [1]. To address these issues, the development of clean and renewable energy resources has piqued the interest of both academia and industry. Sunlight, as a carbon-neutral energy source, reigns as the most plentiful and environmentally friendly form of power. Consequently, solar energy emerges as an inexhaustible and immaculate energy solution. In light of this, technologies based on solar or photovoltaic cells, capable of harnessing the sun's rays, assume immense significance. These solar cells have garnered considerable attention for their exceptional ability to efficiently convert solar energy into usable power. Solar photovoltaics can serve as a solution to both dwindling energy reserves and present climate change challenges [2 - 4]. The solar cell platform has been dominated by silicon materials since the beginning of photovoltaic technology [5]. Approximately 90% of photovoltaic (PV) cells on the market today are made of single-crystal (SC-Si) or multicrystal (poly-Si). However, the cost of SC-Si and poly-Si has risen dramatically in recent years. Solar electricity is five to ten times much costlier than traditional options due to escalating expenses of pure silicon utilized in PV cells [1]. In recent years, substantial effort has been put into the advancement of third-generation PV cells, and materials, especially based on carbon nanotubes and graphene [6 - 13]. Carbon nanomaterials such as graphene, carbon nanotubes (CNTs), and fullerene have piqued the interest of the energy world due to their promising properties such as high conductivity, mechanical flexibility, tunable energy levels, and long-term stability [14 - 17]. Furthermore, due to the advantages of carbon materials, such as their abundance, fast charge transfer rate, and ease of functionality [18, 19], they play an imperative and crucial role in a wide range of applications, including catalysis, OFETs, supercapacitor, gas separation, and electrode materials, *etc.* [20, 21]. In addition, graphene and carbon nanotubes (CNTs) are suitable candidates as electrodes, charge transport layers, and photoactive layers, which has sparked the interest of portable energy conversion devices with a wide range of applications [22 - 27]. The goal of this chapter is to showcase the latest breakthroughs in carbon nanomaterials and their ability as building blocks for organic photovoltaics (OPVs), perovskite solar cells (PSCs), and dye-sensitized solar cells (DSSCs).

CARBON NANOMATERIALS

Photovoltaics is an emerging application area for carbon nanomaterials. The elemental abundance, chemical stability, and mechanical flexibility of carbon nanomaterials present them as a distinctive candidate for photovoltaic technology. Nanostructured-carbon materials can be classified into distinct groups based on dimensionality. The first group is 0D carbon, which includes materials like fullerene, carbon dots (CDs), and graphene quantum dots (GQDs). The second group is 1D carbon, *i.e.*, carbon nanotubes (CNTs) and carbon nanofibers (CNFs). Lastly, the third group is 2D carbon, which encompasses graphene, and its derivatives. This categorization allows for a systematic understanding of the diverse carbonaceous nanomaterials and their distinct characteristics [28, 29]. Fig. (**1**) displays different types of carbon-based nanostructures. Researchers are continually exploring new ways to optimize the properties and performance of these materials to enrich the efficiency and permanence of solar cells. For example, CNTs, known for their remarkable electrical and thermal conductivity, find application in solar cells as transparent conductive electrodes, substituting typical indium tin oxide (ITO) electrodes. Moreover, CNTs possess the potential to enhance light absorption and facilitate charge carrier transport in solar cells. Another noteworthy carbon nanomaterial, graphene, has been extensively studied as a transparent electrode material for solar cells due to its flexibility, low sheet resistance, and excellent transparency. Additionally, fullerenes have proven to be effective electron transport materials in OPVs. This section will delve into the exploration of carbon nanomaterials, including graphene, CNTs, and fullerenes, which are commonly employed or investigated for their applications in solar cells.

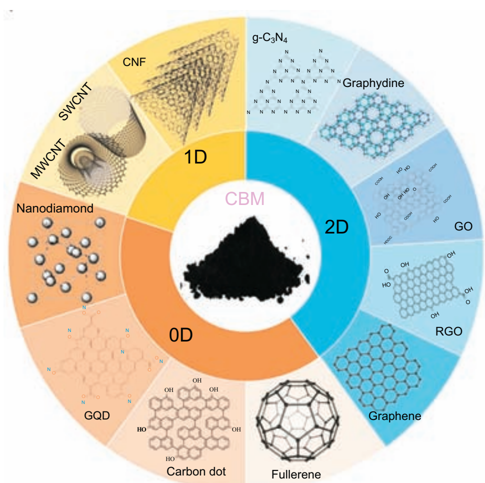

Fig. (1). Schematic representation of carbon-based nanomaterials. [Reproduced with permission [28], Copyright 2023, MDPI].

Graphene

Graphene, an extraordinary material, possesses a two-dimensional structure embodied in a sole layer of carbon atoms organized in a hexagonal lattice. This structure forms a flat monolayer composed of closely packed sp^2 hybridized carbon atoms, creating a honeycomb crystal lattice in two dimensions [30, 31]. A graphene sheet can be easily formed by exfoliating the weakly interlocking graphite layers [31].

CHAPTER 9

Application of Nanomaterials in Water Purification

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Abstract: The issue of water contamination has emerged as one of the primary problems of the current century. The discharge of hazardous contaminants, rapid industrialization, and unrestricted population rise lead to the degradation of water purity. This chapter explores the nanomaterials in water purification and aims to address the critical need for efficient and sustainable water treatment solutions. With the increasing global demand for clean water, traditional treatment methods are often limited in their ability to remove emerging contaminants and often do not meet stringent quality standards. Nanomaterials have emerged as potential candidates for improving water treatment procedures because of their special features, including high efficacy, better selectivity, good stability, high surface area, eco-friendliness, and high population growth. Adsorption, photocatalysis, membrane filtration processes, and other techniques enable the effective removal of harmful contaminants from industrial waste, groundwater, and surface water by nanomaterials. The chapter's aim is to gain comprehension of the application of nanomaterials that contain metals and metal oxides-based nanoparticles, carbon-based, composites, and dendrimers-based nanoparticles. Their use as adsorbents, photocatalysts, and membrane filters for effective and targeted removal of toxic waste has received a lot of focus at the same time. Adsorption, photocatalysis, and membrane filtration methods are discussed in detail for their usage in water purification. To illustrate the potential risks involved with nanomaterials, practical applications such as waste management and environmental effects are also taken into account. Additionally, it critically evaluates the difficulties and opportunities associated with using nanomaterials in industrial wastewater purification.

Keywords: Adsorption, Carbon-based Material, Dendrimers, Environmental Sustainability, Hazardous Contaminants, Membrane filtration, Metal oxides, Nanomaterials, Nanoparticles, Nanotechnology, Photocatalysis, Pollutants, Selectivity, Water Purification.

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Divya Bajpai Tripathy, Anjali Gupta, Arvind Kumar Jain, Anuradha Mishra and Tokeer Ahmad (Eds.)

INTRODUCTION

Water is a vital resource for life on earth and access to pure and safe water is a basic right of all living beings. However, the extensive use of hazardous substances by industries and individuals, and their subsequent release into water bodies, becomes a growing threat to both environments as well as human health [1, 2]. This results in clean water scarcity, which leads to a dangerous situation for future generations to come because the world's population is continuously increasing [3]. The World Health Organisation (WHO) announces that there are currently billions of people who do not have access to clean potable water [4].

Typically, 97% of the available water on earth is saline and hence unsuitable for human consumption. Globally, only 3% of freshwater is available out of which only one-third satisfies the standard for drinking and is considered potable. Water scarcity is a result of increasing demand for freshwater due to rapid industrialization, poor water management by authorities, and increased pollution. The lack of treatment of toxic effluents before release into water sources leads to contamination of available water on the surface, groundwater, and into soil [5]. The usage of toxic metal ions (Cr, Ni, Cu, Cd, Pb, Hg, As, *etc.*), dyes (cationic, anionic, and neutral) such as azo dyes like crystal violet (CV), methyl orange (MO), eriochrome black- T (EBT), eosin- methylene blue, giesma stain, *etc.*, pharma waste such as microbial waste, high concentration of organic matter, high salts, *etc.*, and toxic organic pollutants such as phenolic compound (polychlorinated biphenyls (PCB), 2-chlorophenol), dioxins (polychlorinated di-benzo-p-dioxins (PCDD) and di-benzofurans (PCDF)), *etc.*, are significantly increased as a result of anthropogenic activities, such as mining, pharmaceutical, agriculture, chemical production, batteries manufacturing, petroleum refining, pesticides, *etc.* [6]. The majority of hazardous chemical wastes is not biodegradable, tends to bioaccumulation, and possess considerable risks to both the environment and living organisms. In 2011, "WHO Guidelines announce limit for Drinking Water Quality", for the majority of fatal toxic metals (Pb, Cr, Cd, As, Hg, *etc.*) is 0.1 mgL-1. According to Haoyu Deng *et al.* (2022), Fig. (**1**) explains metals and their harmful impacts on existing life [7].

The considerable number of pesticides allowed in fresh drinkable water is 0.1 mg/g for single pesticides and 0.5 mg/g for combined pesticides, according to WHO regulations [8]. The maximum allowed concentration of dyes is 0.01 to 0.05 ppm and the consumption of these toxins above the permissible limits may result in disruption of the normal functioning of organs, reproductive diseases, hypertension, along with metabolic, and neurological issues [9]. This concern has led to the requirement of continual attention to the development of wastewater treatment technologies.

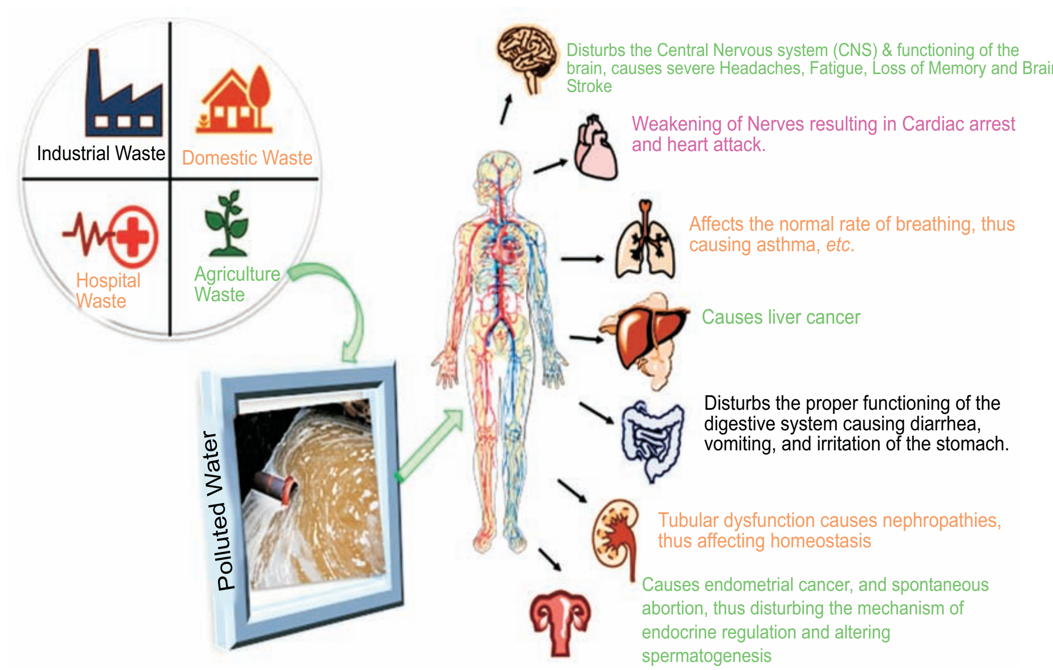

Fig. (1). Explained metals and their harmful impacts on existing life. Reproduced from reference [7].

Several research has been conducted in the past few years to identify new novel approaches that may be commercially feasible for treating wastewater. The conventional techniques for removing harmful contaminants from aquatic surroundings include coagulation, precipitation, membrane filtration, reverse osmosis, degradation of microbes, *etc*. However, the widespread utilization of these techniques has been constrained by the decrease in processing efficiency, energy demands, technical expertise, economic benefits, and infrastructure [10]. Thus, for the treatment of wastewater comprising diverse toxic effluents, photodegradation, adsorption, membrane filtration, and membrane filtration approaches have been acknowledged as promising, adaptable, easy to use, and

CHAPTER 10

Rare Earth-based Multiferroic Perovskites and Applications

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Abstract: This chapter provides an updated overview of rare-earth-based multiferroic perovskites and their diverse range of applications. Multiferroic materials exhibit simultaneous ferroelectric and ferromagnetic properties, making them highly attractive for various technological applications. The design of functional materials is challenging to tune the properties and applications. Rare earth-based perovskites, in particular, offer unique properties due to the combination of rare earth elements and the perovskite crystal structure. This chapter explores the synthesis methods, characterization techniques, and emerging applications of rare earth-based multiferroic perovskites, highlighting recent advancements in the field.

Keywords: CVD, Ferroelectricity, Ferromagnetism, Ferrotoroidicity, Perovskites, Photocatalysis, UCNP.

INTRODUCTION

Multiferroic materials are indeed remarkable due to their ability to exhibit multiple ferroic orders simultaneously. Rare earth-based multiferroic perovskites have attracted significant attention in recent years due to their unique combination of ferroic orders. These materials possess the unique property of coexisting two or more ferroic behaviors, such as ferromagnetism, ferroelectricity, ferroelasticity, and ferrotoroidicity [1]. This characteristic distinguishes them from conventional materials, which typically exhibit only a single ferroic order. The simultaneous presence of multiple ferroic orders in multiferroic materials enables them to perform multiple tasks concurrently, making them highly versatile and attractive for various applications. For instance, their ability to exhibit both ferromagnetic and ferroelectric properties simultaneously opens up possibilities for developing multifunctional memory devices that combine non-volatile data storage with electrically switchable functionality [2]. In addition, the coexistence of ferroelectricity and ferroelasticity in multiferroic materials provides opportunities for developing sensors and transducers with enhanced sensitivity and functionality. The coupling between these two orders allows for the integration of

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Divya Bajpai Tripathy, Anjali Gupta, Arvind Kumar Jain, Anuradha Mishra and Tokeer Ahmad (Eds.)

mechanical and electrical responses, enabling the design of devices that can detect, convert, and store information simultaneously. Furthermore, the presence of ferrotoroidicity in some multiferroic materials introduces a new dimension to their behavior. Ferrotoroidicity involves the presence of a spontaneous toroidal moment, which is a circulating flow of electric or magnetic dipole moments [3]. This property can be harnessed for applications in magneto-electric devices, where the toroidal moment plays a critical role in controlling and manipulating magnetic and electric properties. Multiferroic materials hold promise in various fields, including spintronics, where the coupling between ferroic orders allows for the manipulation of electron spins for information storage and processing. They also find applications in microwave and magneto-optical devices, where their multi-functionality enables the control and modulation of microwave signals and the development of efficient optoelectronic devices. In addition to that, multiferroic catalysis also gained attention recently owing to its unique properties [4 - 6].

Multiferroic Catalysis refers to the utilization of multiferroic materials for catalytic reactions under light irradiation, for instance, photoelectrocatalysis, photocatalysis, *etc.* Photocatalysis involves the use of light energy to initiate chemical reactions, typically on the surface of a catalyst material [7]. Multiferroic materials, which possess both ferroelectric and magnetic properties, offer unique opportunities for enhancing and manipulating the photocatalytic processes. The combination of ferroelectric and magnetic properties in multiferroic materials allows for the coupling between different order parameters, which can influence the photocatalytic activity [8]. The ferroelectric polarization in these materials can affect the charge separation and migration processes, while the magnetic properties can influence the spin-related phenomena during photo/electro-catalysis. By controlling these properties, multiferroic materials can offer advantages in terms of improved charge transfer efficiency, enhanced catalytic activity, and tunable selectivity [9]. One of the key advantages of using multiferroic materials in photocatalysis is the ability to manipulate the photocatalytic processes through external stimuli. For example, the ferroelectric polarization can be modulated by applying an external electric field, thereby altering the charge distribution and surface reactivity of the material. Similarly, the magnetic properties can be tuned by an external magnetic field, affecting the spin dynamics and facilitating desired chemical transformations.

Multiferroic photocatalysis has shown potential in various applications, including environmental remediation, energy conversion, and organic synthesis. In environmental remediation, multiferroic photocatalysts can be employed to degrade pollutants and contaminants in air or water through photocatalytic oxidation or reduction reactions. The enhanced charge separation and migration properties of multiferroic materials can improve the efficiency of these processes [10, 11]. In the field of energy conversion, multiferroic photo/electro-catalysis can play a crucial role in solar energy harvesting and conversion. The efficient utilization of solar energy for water splitting, carbon dioxide reduction, and hydrogen production can be achieved by utilizing multiferroic materials as photo/electro-catalysts. The ability to control charge separation and migration in these materials allows for enhanced light absorption and improved catalytic efficiency. Despite the promising potential of multiferroic photo/electro-catalysis, several challenges need to be addressed [12]. The various applications of multiferroic materials are shown in Fig. (**1**). However, it is important to note that multiferroic materials are relatively rare, and the search for new compounds that exhibit the desired combination of ferroic orders is an active area of research. Additionally, challenges such as material stability, scalability, and the development of reliable synthesis techniques need to be addressed to fully harness the potential of these materials for practical applications [13, 14].

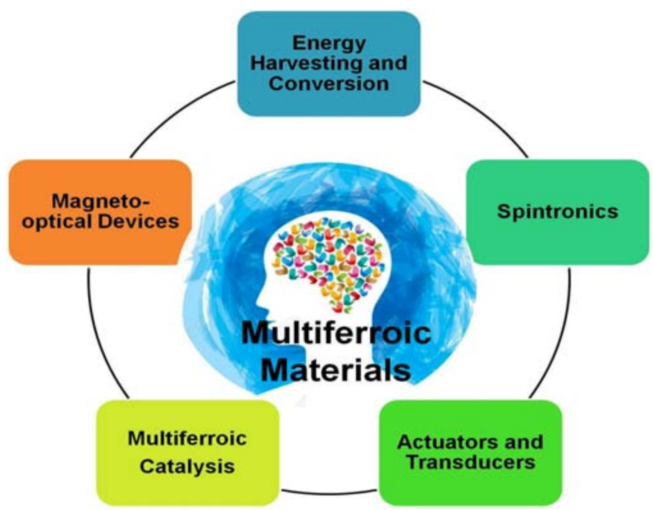

Fig. (1). Various applications of multiferroic materials.

RARE EARTH-BASED MULTIFERROIC PEROVSKITES: STRUCTURAL ASPECTS AND CLASSIFICATION

Rare earth-based multiferroic perovskites have emerged as a highly significant class of materials in the field of solid-state physics and materials science. These types of perovskites have attracted significant interest in recent years due to their unique combination of ferroelectric and magnetic properties. These materials exhibit simultaneous ferroelectric and ferromagnetic order, offering exciting opportunities for various applications in electronics, spintronics, energy

CHAPTER 11

Graphene Oxide (GO) and Reduced Graphene Oxide (rGO) Based Humidity Sensors

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Abstract: Humidity sensors are critical in a wide range of applications ranging from automotive, biomedical, chemical, and electronics industries, to scientific research laboratories. Here we discussed widely acclaimed synthesis techniques for the preparation of graphene and its derivatives. Graphene, along with its analogues GO, and rGO shows improved surface properties making it sensitive to fractional change in ambient surroundings. GO/rGO-based sensory materials owing to their distinctive physio-chemical features appeared as a competitive sensor in comparison to the widely used metal oxides. The enhancement in the merits of GO-based humidity sensors is ascribed to the various functionalized groups on the GO surface. Pristine GO is employed as a capacitive sensor, whereas reduced GO (rGO) with improved conductivity is extensively utilized as a chemiresistive humidity sensor. Similarly, Graphene quantum dots (GQDs) and 2D- layered graphene have been explored as humidity sensors due to their massive scope of manipulation in properties. The chemi-resistive humidity sensor gains an advantage over any type of available sensor owing to its cost-effective fabrication, easier integration with the CMOS platform, and efficient operation. This review aims to establish the evaluability of GO and rGO humidity sensors and their role in the progress of the next generation of flexible sensors for the Internet of Things (IoT).

Keywords: Composite, Capacitive, GO, GQD, Grotthuss mechanism, Humidity, Impedance, IoT, RGO, Resistive, Sensor.

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Divya Bajpai Tripathy, Anjali Gupta, Arvind Kumar Jain, Anuradha Mishra and Tokeer Ahmad (Eds.)

INTRODUCTION

Relative humidity (RH) measurement is an important aspect in the development of oxide-based semiconductor chemical sensors. The amount of water vapor that is present in the air can affect not only personal comfort but also various industrial processes. Thus, humidity sensors are classified as a type of chemical sensor playing a prominent role in various applications but not restricted to the production industry, agriculture sector, medical and prosthetics sector to aviation, weather and climate division, indoor air quality monitoring like HVAC, *etc*. [1 - 7]. Generally, humidity sensors work on the principle where it converts the number of water molecules present in the ambient to a measurable physical quantity, mostly an electrical signal. Humidity sensors are of various types such as capacitive, resistive, impedance, optical, QCM (Quartz Micro-balance), SAW (Surface Acoustic wave), *etc.*, depending upon their measurable physical quantity for sensory signals [4]. An ideal humidity sensor should have various properties like low power consumption, lower hysteresis, fast response, wide detection range, highly sensitive, and long stability towards relative humidity in harsh environments [1 - 10]. A large number of established works of literature show utilization of various nano- to micro materials as sensing materials such as Al_2O_3, SiO_2, and spinel compounds like $CoFe_2O_4$ [2, 3] semiconductors, such as TiO_2 [8, 9], SnO_2 [10 - 13], ZnO [14 - 18], In_2O_3, Si [19], and perovskite compounds [20 - 23]; polymers, such as polyelectrolytes [24, 25], conducting and semiconducting polymers [26], and hydrophilic polymers [27 - 30]; 2D materials, such as MoS_2 [31 - 33] WS_2 [34 - 36], and black phosphorus [37 - 40]; and carbon materials, such as porous carbon [41], carbon nanotubes [42, 43], and graphene [44, 45] towards humidity sensors. These types of humidity sensors are widely used due to their cost effectiveness, ease to handle, and reliability due to hassle-free calibration [10].

Graphene oxide (GO) is a well-known 2D material that is described as an atomically thin, and hexagonally arranged planar membrane of carbon atoms and conveyed to be of p-type material [36], which shows a decrease in electrical conduction on exposure to humidity. This distinctive atomic organization fetches unique electronic structures, and unusual physio-chemical properties, which endorse multi-functional applications of the graphene family such as in electronics, optoelectronics, spintronics, catalysts, energy generation and storage, molecular separation, other than chemical sensors [37 - 46]. GO shows an excellent property of solubility in a wide range of available solvents including water and common organic solvents like ethanol, propanol, *etc.* The main reason for excellent solubility is ascribed to the presence of various oxygen-based functional groups and their functionality to act as suitable adsorption sites towards individual analytes on the surface giving rise to marked physio-chemical properties of GO. Diverse literature [37 - 42, 46] reported that the presence of various functional groups in GO speeds up the water permeation within layers, permitting rapid water molecule diffusion during sorption and desorption of humidity based on their binding or adsorption energy towards analyte molecules [47 - 49]. Graphene oxide (GO) shows a robust hydrophilic tendency alongside improved proton conductivity due to the availability of oxygen functional groups in comparison to graphene, and reduced graphene oxide (rGO) is established as one of the ideal candidates for humidity detection. It is well-known that the energy involved is 0.044eV reflecting a weak van der Waals bond between H_2O and graphene, whereas the energy amount is 0.201eV and 0.259 eV for hydrogen bonding of H_2O with the epoxy and -OH groups, respectively [50 - 53]. Hence it can be concluded that H-bonds existing between H_2O molecules and functional groups were primarily involved in the creation of successive GO layers. In the presence of higher humidity, the water molecules dominate their binding through H-bonding and cause an increase in GO layer spacing, reducing the interlayer H-bond interactions [54, 55] for faster detection of humidity level change in the ambient. Hence for improvement of selectivity of sensors towards particular analytes, controlling the concentration of specific functional groups is highly justified. In terms of economic feasibility, it has already been reported that GO-based resistive humidity sensors are well-deployed owing to their cheaper fabrication, enduring stability, and compatibility with available semiconductor fabrication technology [25, 26, 28, 29, 56]. Various studies have reported the progress made in graphene and graphene-based materials potentiality as chemical (gas and humidity) sensors due to their ultrahigh specific surface areas, exceptional high electron mobility at working temperature, and low electrical noise due to their crystal lattice and very high electrical conductivity [1 - 7, 44, 45, 57 - 67]. Still, there is no specific literature available on the progress of graphene-based humidity sensors with proper validation of humidity sensing mechanisms. This chapter emphasizes the advancements in GO/rGO-based humidity sensors divided into three main parts: (i) synthesis and properties of graphene-based materials, (ii) plausible sensing mechanism, and (iii) progress in the GO/rGO based humidity sensors. Keeping the readers' perspective in mind before proceeding to material-specific aspects of humidity sensing, a dedicated segment narrating the basics related to chemical sensing in terms of response, sensitivity, response/recovery time, the limit of detection, *etc.* was discussed as a prerequisite.

CHAPTER 12

Role of Ion Beam in Nanomaterials: Synthesis, Morphology Control, and Applications

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Abstract: The exceptional performance of nanomaterials, as a result of their size and unique morphology, has attracted a lot of researchers. The structure and constituents of materials have been modified using a variety of techniques. The ion beam techniques have so far been widely employed to modify the performance of different nanomaterials. The surface configuration and chemical composition of nanomaterials can be altered by energetic ion beams. The ion beam techniques approach is purely physical in comparison to conventional methods. These techniques exhibit outstanding control and reproducibility without adding any impurities to the target materials. Here, current developments in surface modification of nanomaterials employing ion beam methods are thoroughly reviewed.

Keywords: Focused ion beam, Ion irradiation, Ion implantation, Morphology control, Nanomaterials, Nonvolatile memory, Photodetector, Resistive switching, Surface modifications, Transistors.

INTRODUCTION

In recent years, nanomaterials have emerged as a remarkable class of materials, capturing widespread interest and garnering considerable attention. These innovative materials, characterized by their distinct structure at the nanoscale, offer a range of exceptional properties that distinguish them from conventional bulk materials [1 - 6]. Typically ranging in size from 1 to 100 nanometers,

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Divya Bajpai Tripathy, Anjali Gupta, Arvind Kumar Jain, Anuradha Mishra and Tokeer Ahmad (Eds.)

nanomaterials exhibit fascinating and unique characteristics that make them highly appealing for various applications [7 - 14]. When a material approaches a nanometer range, the properties of the materials take a great shift due to the quantum size effect, along with surface, and boundary effects. This uniqueness has enormous potential for a variety of applications in numerous different fields. Nowadays, nanomaterials are extremely useful in several fields, including electronics, energy, environmental remediation, catalysis, and pollution detection because of their improved mechanical, magnetic, electrical, and optical properties [15 - 18]. Nanomaterials offer high-efficiency electronic devices, lightweight, durable materials for aerospace applications, high detection limits for toxicity detection, and tailored medication delivery in the biomedical field [16 - 18]. Therefore, with an ongoing increase in demand, researchers aspire to design and develop such nanomaterials with superior properties. Numerous strategies, such as doping, surface smoothing /modification, nanoparticle embedding, and so on, have been applied to enrich the properties of nanomaterials [19, 20]. Ion implantation, ion irradiation, and focused ion beam are all examples of the advanced technique referred to as ion beam. Ion implantation and ion irradiation have paved the way for new opportunities for a wide range of applications, including biomedical, energy, sensors, and semiconductor manufacturing [21, 22]. This approach enables the controlled introduction of dopants, modifying their electrical, mechanical, and optical properties with exceptional precision, by carefully driving materials with ions. As a result of their exceptional precision, these techniques are often used for altering the features of nanomaterials. In an ion beam, energetic ions interact with the material, altering its properties. If the energetic ions possess sufficient energy, they can displace the atoms within the target material, resulting in the creation of defects at the atomic scale [21, 22]. Alternatively, after dissipating their kinetic energy, these incoming ions can remain within the material as dopants. The ion beam technique encompasses two distinct terms: ion implantation and ion irradiation, which possess subtle differences. Ion irradiation is commonly employed when the primary focus of the study revolves around defect formation. Ion beam irradiation is a useful technique to investigate the damaging effects of radioactive waste immobilization in nuclear materials [21]. Conversely, ion implantation is used when the main objective is to introduce dopants into the functioning material [22]. Ion beam techniques hold great promise for doping and surface modification applications. The ion implantation strategy, which employs semiconductors such as silicon and germanium, as well as compounds such as ZnO, GaN, and SiC, opens up new possibilities for the fabrication of the devices like solar cells, photodetectors, and transistors [23].

In comparison to growth and diffusion-based doping methods, ion implantation offers better control and reproducibility. Additionally, ion implantation serves as an effective means to embed nanoclusters within host materials. Furthermore, ion irradiation/implantation serves as an effective technique for modulating the morphology and surface structure of various materials. Ion implantation has been broadly applied for the modification of nanostructures. Interestingly, existing methods of introduction of the dopants in the semiconductors for doping have been replaced by ion implantation. As an approach of industry, it is highly accurate and reproducible. In contrast to other doping techniques, ion implantation does not introduce additional impurity elements. Furthermore, ion implantation/irradiation is not constrained by the solid solubility of constituents in the materials.

MATERIAL MODIFICATION: ION BEAM TECHNOLOGY

Ion beam technology can be classified into several categories, which are as follows:

I. Low-energy ion implantation/irradiation: It has been extensively employed in the modification of two-dimensional materials. It is possible to selectively doping and modify the surface morphology with low-energy ions below one keV. In addition, the defect engineering of two-dimensional materials can be proficiently achieved by ion implantation upon energy tens of keV [23].
II. Medium-energy ion implantation: It can be applied to modify the micro/nanostructure and element doping in different types of thin-film electrode materials [24, 25]. Nowadays, cutting-edge material surfaces and interfaces have been produced and altered by employing energies ranging from tens of keV to a few MeV [26, 27].
III. Swift heavy ion irradiation: Typically, a heavy ion has an energy greater than one meV [28 - 30]. For highly energetic ions, the electronic energy loss phenomena predominate and cause rapid local ionization, which is the main factor in track development, damage production, and damage recovery. These features facilitate the conversion of energy loss into the creation of defects within the material [25]. Because of the enormous amount of energy that is transmitted to the target atom, a huge number of imperfections can be created at a very low fluence to alter the morphology and engineer the defects [31 - 34].
IV. Focused ion beam (FIB): FIB is an impressive technique to develop micro- and nano-systems [35]. Among the plethora of fabrication techniques, FIB nanofabrication stands out as a highly promising and well-suited method across numerous fields, including nanotechnology, material science, and the microelectronic industry [36]. The growing demands from both industry and research have elevated its status as an essential approach to creating intricate 3D nanostructures and devices [37].

CHAPTER 13

Role of Nanomaterials in Remediating Environmental Pollutants

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Abstract: The rapid urbanization and industrialization have resulted in the environmental pollution, which is the biggest challenge faced by the society. Remediation is mainly associated with the environment. Environmental remediation is the process of removing pollutants or contaminants from the environment such as soil, air, and groundwater for the safeguard of human health and the environment. There are various technologies involved in remediation such as physical remediation involving processes like filtration, extraction, etc; chemical remediation involving chemical reactions, photocatalysis, *etc* and biological remediation involving microorganisms and plants. The use of nanomaterials for remediation is called nanoremediation. Nanomaterials reveal better performance in environmental remediation than other techniques used because of their high surface area and the associated high reactivity. Different nanomaterials in various shapes, function as adsorbents, catalysts and sensors for detection and removal of gases, contaminants and organic pollutants. This chapter provides an overview of different kinds of remediation techniques and a detailed discussion on different types of nanomaterials used for environmental remediation.

Keywords: Adsorption, Bimettalic nanomaterials, Carbonaceous nanomaterials, Catalyst, Environmental pollutants, Environmental remediation, Metal nanoparticles, Nanoremediation, Nanotechnology, Nanomaterials, Polymer-based nanomaterials, Photocatalysis.

INTRODUCTION

Environmental pollution is a growing global threat due to urbanization, industrialization, and changes in people's lifestyles. Given this, it is a difficult effort to provide people with clean environments, clean air, and pure water. A rise in industrial installations and production is the result of expanding consumer demands and a growing population. But the environment suffers as a result of

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Divya Bajpai Tripathy, Anjali Gupta, Arvind Kumar Jain, Anuradha Mishra and Tokeer Ahmad (Eds.)

these developments. The release of harmful pollutants into the environment by diverse anthropogenic sources is a serious issue that needs to be addressed right away. The health of people and animals, plants and trees, as well as the environment as a whole, are all being negatively impacted by pollution. It is also upsetting the marine life in lakes and streams, which leads to the extinction of native flora and fauna [1, 2]. Waste products *e.g.* atmospheric pollutants toxic gases (sulfur oxides, carbon oxides, nitrogen oxides, ozone, *etc.*) and other contaminants can include organic chemicals (*i.e.* phenols, hydrocarbons, *etc.*), heavy metals (arsenic, cadmium, lead, mercury, *etc.*), and microbial organisms are released into the environment in various forms. Since these pollutants can enter the human body through inhalation, inhalation or inhalation, they will adversely affect human health [3, 4]. In addition, some of these toxic substances are often found in food, such as the bioaccumulation of heavy metals and persistent organic pollutants (POPs) in biota and fish, providing great luck for humans and wildlife [5 - 10]. Therefore, it is necessary to develop effective, economical and environmentally friendly technologies for the monitoring and control of environmental pollution [11]. Degradation of these pollutants is frequently required for pollution control. Different physical, chemical, or physicochemical methods can be used to degrade contaminants. Due to the inefficiency of these approaches, biological methods were first developed. The process of employing bacteria, fungi, plants, algae, *etc.* to break down a variety of environmental toxins, is known as bioremediation. One such technology that has attracted a lot of attention in recent years is nano-bioremediation. Nanoparticles have higher chemical and biological reactivity because they have a huge surface area compared to their volumes. Nano-bioremediation attempts to simultaneously lessen the effects on the environment and reduce the contaminant concentrations to low risk-based thresholds. It combines the advantages of bioremediation and nanotechnology to create more effective, faster and better treatments [12]. To prevent the spread of harmful pollutants in the environment, nanotechnology provides a number of affordable and effective techniques. One of the most recent advancements in this area is the use of nanoparticles for environmental clean-up [13]. Nanotechnology promises to facilitate the development of clean, efficient technologies with significant environmental and health benefits [14]. Despite a number of benefits, toxicological concerns over the use of nanoparticles in the environment are being taken seriously. In its current form, this chapter emphasizes how important nanoparticles are for cleaning up environmental toxins. It seeks to inform readers of the latest developments in the effective use of various nanoparticles and nanoscale materials for environmental clean-up. There has been a brief discussion of the toxicological effects of these nanoparticles on environmental living things. By offering some suggested solutions, efforts have been made to allay the worry about the damaging impact of nanoparticles on the environment [15]. The term “nanotechnology” refers to a group of technologies designed to work at the nanoscale (*i.e.* in the 1 to 100 nm range) to create materials, devices, and systems with new properties and functions by controlling the size and shape of nanoparticles [16, 17]. The process is one of the best ways to update the environmental purification process. Due to the potential applications of nanotechnology in a wide range of industries (for example medical, the food industry, energy, and pollution treatment), it is expected to overtake and revolutionise conventional remediation technologies in the near future [18 - 20]. Over the past 20 years, nanoremediation has been developed and assessed. However, there are worries about how it will affect both people and the environment. To minimise or reduce any potential environmental or ecological risks, proper review must be conducted given the rapid growth of nanoremediation technology. Nanotechnology improves our daily lives by improving the functionality of ordinary objects. Clean air, water and renewable energy ensure a better future for all. Trade and resource use increase as people use the natural world. While we do not regret the disadvantages of existing methods (such as Fenton, coagulation, adsorption, advanced oxidation, *etc.*, and their combination), pollution that is not good for the earth urgently needs to be eliminated. Nanoparticles seem to work at both small and large levels, which could provide a better and more effective way to tackle this serious problem. Various types of nanoparticles can be used to remove certain pollutants in the natural environment, such as sewage and soil [21 - 27]. Nanotechnology techniques are being explored for their potential to provide solutions for pollution control and mitigation as well as improving the performance of conventional environmental remediation methods [13]. Nanotechnology can help the environment by reducing energy consumption in production and production paths, the possibility of recycling products after use, and the possibility of developing and using environmentally friendly materials [11]. Nanotechnology currently holds great promise in addressing sustainability issues, but at the same time, harm to the environment and human health must also be considered. Various types of nanomaterials have been prepared by various techniques such as deposition-deposition (DP), photocatalytic deposition (PD), chemical solution separation (CSD), chemical vapor decomposition (CVD), wet chemical, sol-gel bonding, ultrasonic radiation, thermal and hydrothermal processes, *etc*. [28]. These materials have special qualities that set them apart from their bulk counterparts. Due to their unique properties, including thermal, optical, mechanical, electromagnetic, structural and morphological, they can be used as nanoadsorbents, nanosensors, nanomembranes and antibiotics [29]. Additionally, it has been claimed that numerous attempts have been made to synthesise more complex nanostructures (such as nanorods, nanobelts, nanowires, and nanofibers, *etc.*) in an effort to increase the adaptability of nanomaterials and remove all

CHAPTER 14

Nano Lubricants and their Applications

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Abstract: In the current growing demand for lubricants, there is a need for the improvement in their lubricating property. This chapter presents an extensive review of Nano lubricants as well as their applications in a variety of business sectors. Nowadays, the additives of the nanoparticles are coming in trend to increase the lubricating property of any lubricant for use in various applications, for this purpose the additives are dispersed in the base oil which forms the stable lubricating fluid. The addition of nanoparticles in the lubrication provides several benefits as compared with the ordinary lubricant such as reduced friction wear and tear, increased load-carrying capacity, and enhanced thermal stability. Continued research and development in the field of nanotechnology are unlocking the potential pertaining to Nano lubricants resulting in applications in high temperatures, high pressures, and corrosive environments where ordinary lubricants cannot work properly. Additionally, they are being explored for their uses in microdevices, electronics, and advanced materials. When seen from the perspective of the future, the future of Nano lubricants presents many exciting potentials. The current focus of research is on the investigation of innovative nanoparticles, the enhancement of dispersion techniques, and the customization of lubricant compositions for particular applications. The potential of Nano lubricants will be further explored as nanotechnology, tribology, and material science make further strides forward. This will allow for an expansion of their use in developing industries and the creation of lubricating solutions that are more environmentally friendly and efficient in terms of energy use.

Keywords: Energy generation, Friction reduction, Fuel efficiency, Heat dissipation, Load carrying capacity, Nano lubricants, Nanoparticles, Synthesis of nano lubricants.

1. INTRODUCTION

Lubrication is extremely important in many different fields since it ensures a smooth operation, reduces the amount of friction that occurs, lessens the amount of wear that occurs, and lengthens the lifespan of mechanical components. These functions have been fulfilled by conventional lubricants for a considerable amount

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Divya Bajpai Tripathy, Anjali Gupta, Arvind Kumar Jain, Anuradha Mishra and Tokeer Ahmad (Eds.)

of time, but developments in nanotechnology have made it possible to explore new avenues for enhancing the effectiveness and functionality of lubrication. The world has always struggled with the problem of energy being wasted as a result of friction and wear. The presence of friction and wear may be seen virtually everywhere, from manufacturing equipment to common home items. It has been calculated that friction and wear account for around 30 percent of the total energy that is lost.

Nanoparticles used in nano lubricants are typically between 1 and 100 nanometers in size and made of a variety of substances, including metals, metal oxides, ceramics, or substances derived from carbon. Nanoparticles made of titanium dioxide, alumina, zinc oxide, tungsten disulfide, and carbon nanotubes are a few examples of regularly utilized nanoparticles. It is important to keep in mind that there are still problems to solve in the development and application of nano lubricants as shown in Fig. (**1**). These difficulties include regulating the potential aggregation or settling of nanoparticles over time, achieving uniform dispersion and stability of nanoparticles in lubricant formulations, and assuring compatibility with current lubricating systems. Here's an overview of the current research status of nano lubricants (Table **1**).

Table 1. Overview of the current research status of nano lubricants.

Research Area	Current Status	References
Nanoparticle Selection	Ongoing research on identifying optimal nanoparticles based on specific lubrication requirements and compatibility with lubricant matrices.	[1]
Dispersion Techniques	Active research on developing effective dispersion methods to ensure uniform distribution of nanoparticles in lubricant formulations, including sonication, surfactant-assisted dispersion, and functionalization techniques.	[2]
Stability and Aggregation	Ongoing investigations on controlling the stability of nanoparticles in lubricants to prevent aggregation and settling, through surface modification and formulation optimization.	[3]
Tribological Performance	Extensive research on evaluating the tribological properties of nano lubricants, including friction reduction, wear resistance, load-carrying capacity, and extreme pressure performance, using various testing methods and equipment.	[4]
Thermal Conductivity	Ongoing studies on exploring the thermal conductivity enhancement potential of nano lubricants and optimizing nanoparticle content to improve heat dissipation and thermal management in lubricated systems.	[5]

(Table 1) cont.....

Research Area	Current Status	References
Compatibility	Active research on investigating the compatibility of nano lubricants with different materials and lubrication systems, including seals, gaskets, elastomers, and other components, to ensure no adverse effects or degradation.	[6]
Environmental Impact	Growing focus on assessing the environmental impact of nano lubricants, including nanoparticle release, potential toxicity, and biodegradability, to ensure their safe and sustainable use in various applications.	[7]

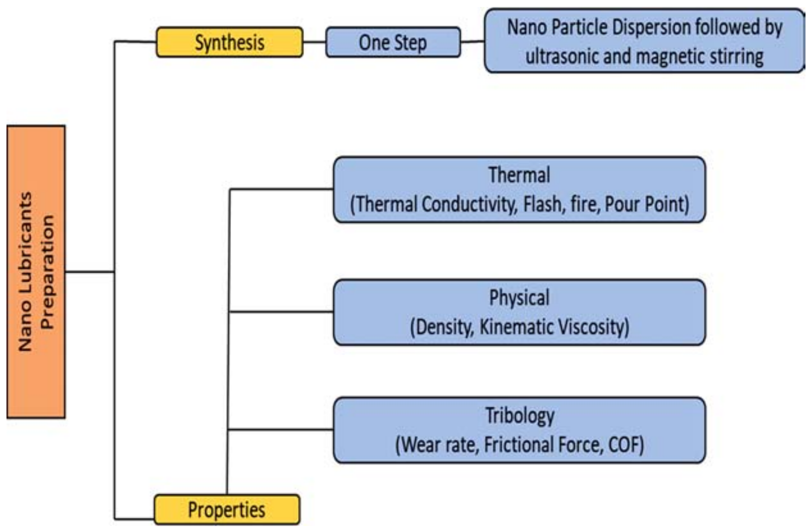

Fig. (1). Nano lubricants' basic properties and synthesis [8].

2. SYNTHESIS OF NANO LUBRICANTS

The technique of integrating nanoparticles into a lubricant matrix to produce a specialized lubricant with improved qualities is known as the synthesis of nano lubricants.

- The first step is to choose the correct nanoparticles depending on the properties and use of the nanolubricants that are wanted. The nanoparticles' size, shape, composition, and surface properties are taken into account.
- Several procedures, including chemical precipitation, sol-gel synthesis, mechanical milling, and aerosol treatments, are used to create or obtain the nanoparticles. This stage makes sure that nanoparticles are produced that have the correct size, shape, and surface characteristics [9].
- To optimize the dispersion of nanoparticles, their stability, or their compatibility with the matrix of the lubricant, it may be required in some instances to modify

SUBJECT INDEX

A

B

C

Divya Bajpai Tripathy, Anjali Gupta, Arvind Kumar Jain, Anuradha Mishra and Tokeer Ahmad (Eds.)

D

E

F

G

H

I

L

M

N

O

P

R

S

T

V

W

X

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