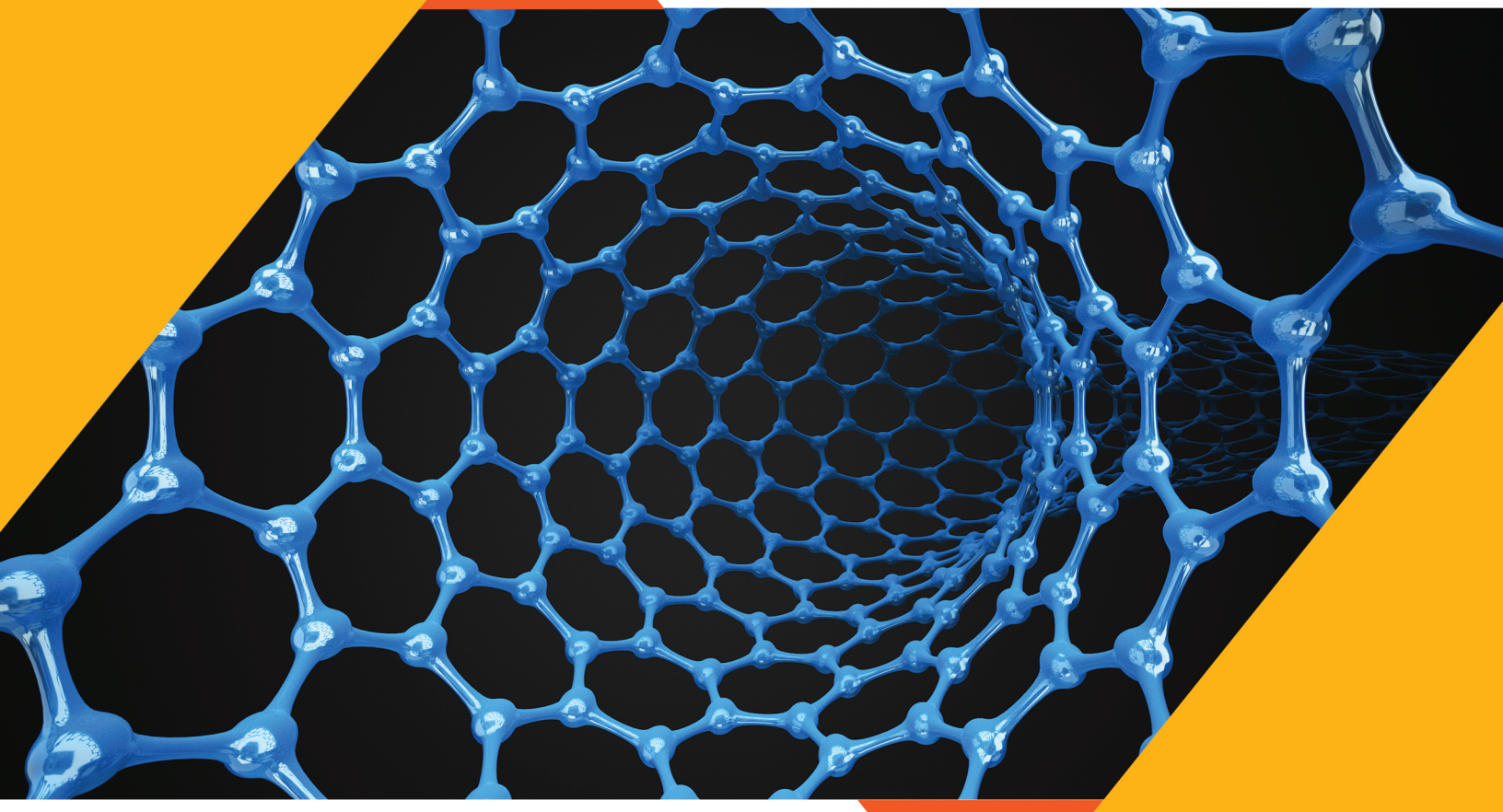
ADVANCED MATERIALS AND NANO SYSTEMS:

THEORY AND EXPERIMENT - PART-1



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Advanced Materials and Nano Systems: Theory and Experiment-Part 1

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Advanced Materials and Nano Systems: Theory and Experiment

(Part 1)

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FOREWORD

The editor **Dr. Dibya Prakash Rai** has requested me to read the first edition of the book "*Advanced Materials and Nanosystems: Theory and Experiment*". I am fortunate and delighted to have the opportunity to read and review this book before it is officially published. I'm particularly pleased to learn that this book will be published by one of the reputed publishers, "**Bentham Science**" which has published over 150 articles, books, and other works in multidisciplinary fields. Not only that, it has a large number of followers, readers, and subscribers worldwide. The book's title looks very attractive, broad, trendy, and interdisciplinary in the rapidly growing research areas. All the chapters and their titles are very much within the scope of the book as proposed.

This book's collection provides brief and comprehensive information on current advanced materials and nanosystems research. All the contributing authors are experts in their respective fields, such as in Physical Sciences, Chemical Sciences, Material Sciences, Nano Sciences, BioSciences, and Engineering Sciences. Awareness of Nanotechnology is a strategic aim in today's situation to meet the significant objectives of energy harvesting, generation, usage, and storage, along with water treatment, waste management, medical sciences and more.

This book is written and visualized as an instrumental material that intends to offer information for technology progress to students, scholars, scientists, engineers, and professors. The present phases of nanotechnology and the creation of novel energy materials are highlighted in this book, defined by the integration of fundamental knowledge, the fabrication of nanostructure samples, and analysis using standard theory and computing. Nanotechnology is crucial both in terms of experiment and theory to tame and utilize material energy in devices. There has been a worldwide scientific revolution concerning the preparation and integration for the development and uses of new technologies. The current novel discoveries, findings, and results from diverse experimental methodologies and theoretical calculations were discussed in several chapters of this book. Many new topics are covered, including wastewater treatment using nanomaterials, nanoparticles in medical research (targeted drugs, pharmaceutics, dental implants), nanomaterial for air purification, nanomaterials for food preservation, nano-sensors, cosmetics, *etc*. This book contributes to the present trend by bringing together numerous current and foreseen scopes on various themes. It also presents a broad range of viewpoints and opinions on the current state of the art and future prospectus. Whether the readers are novices or experts in the subject, they will start a thought-provoking exploration of contemporary advances in Material Sciences.

My best wishes to **Dr. Dibya Prakash Rai**, for collecting beautiful chapters, compilation, and publication of the first edition of this edited book in **Bentham Science**. I know Dr. Rai for the last ten years as a dynamic and hardworking researcher. I believe he will continue his leadership role in advancing computational material sciences and advanced materials with this book.

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PREFACE

In the present scenario, the research in materials sciences are devoted to enslaving the solid-state materials and utilising their properties in devices to perform desired applications from nanotechnology. The introduction of new materials and manipulation of their exotic properties in device fabrication for advancing technology is crucial, which has urged me to think for this title, "**Advanced Materials and Nanosystems: Theory and Experiment**". Nanomaterials and Nanoscience have taken this development in science and engineering to a new height for the well-being of humankind. This topic covers all sectors of research field like Physics, Chemistry, Engineering, Biosciences, *etc*. This will only be the possible book covering maximum relevant and latest topics both from a theory and the experimental point of view. The present compilation would help many students, scholars, teachers, scientists, *etc*., in their curriculum development and research work. This book highlighted the latest development and the significant role of different new materials in future technology.

In **Chapter 1**, Thakur *et al*., elucidated the theoretical progress of the emergent materials like Carbon and boron nitride nanostructures for hydrogen storage applications from the first-principles simulations. They discussed phenomenological models and explore the essential chemical and physical properties for integration into the applied sciences. The direct combinations of theory and model provide concise pictures in understanding the diverse phenomena of 2D nanomaterials for potential H_2-storage capability, they can thoroughly clarify the critical mechanisms in pristine subsystems and even the composite systems. Interestingly, there exist a lot of theoretical predictions on the stationary ion transport. However, how to develop a unified theoretical framework suitable for the very complicated and active chemical environments in ion-related batteries remains to be urgently solved during the near-future studies. The close relations between the optimal current density and the vanishing/slight/great asymmetries of crystal structures are expected to be a studying focus.

Chapter 2, discusses the prospective future nanomaterials for retinal implant technique. From a medical science point of view, this work would be of great interest in which the authors have discussed the artificial vision for blind patients suffering from retinal diseases with the help of advancement in CMOS technology. The materials such as titanium nitride (TiN), iridium oxide (IrOx), platinum grey, and carbon nanotube (CNT) were employed in recent years in many retinal prosthetic projects. This chapter discusses the important and desired physical properties of nanomaterials viz. conductivity, tensile strength, absorption of photons, and adsorption of water molecules for the subretinal implant technique.

Chapter 3, this chapter talks about the advancement of electrode materials for rechargeable batteries. The demand for high-performance batteries has exploded like never before. To meet such a prospect massive amount of research endeavours in the design and development of high-performance rechargeable batteries are being taken. Starting with such critical analysis, they discuss the fundamental principle that governs the performance of electrochemical devices. They reviewed the state-of-the-art advancement of various types of materials used in the fabrication of electrodes including a description of their structures and storage mechanisms.

Chapter 4, Kumar *et al*. reported the production of ammonia from Nitrogen Reduction Reaction (NRR) adopting an eco-friendly approach. They design cost-effective catalysts holding on a substrate for the nitrogen reduction reaction. As an alternative, the direct conversion of nitrogen has been carried out by photocatalysis and electrocatalysis. This chap-

ter discusses the challenges faced by researchers to formulate righteous catalysts for the sustainable reduction of nitrogen by studying each of these types with a few examples.

Chapter 5 discusses the nanoparticles in environmental remediation. Nanocomposites offer an exclusive advantage over bulk materials in terms of efficiency on account of their greater surface area, higher reactivity, ease of modification, good dispersion and hence, multi-faceted applications. The various forms of nanocomposites derived from low-cost resources, especially carbon-based materials are of unique interest. Activated carbons offer a unique advantage as the matrix for nanocomposites synthesis, large surface area and porosity offer vivid applications in various fields such as environmental remediation as adsorbents, suitable sorbents in analytical determination of organics, targeted drug delivery, diagnostic agents, fuel cells and sensors, to name a few. The role of nanocomposites as sensors and environmental remediation tools includes adsorption, nano-catalysis, membrane filtration, *etc*., for pollutants ranging from inorganic ions, heavy metals, pesticides, dyes, anti-bacterial, oil spills and many more.

Chapter 6 reveals the concentration-dependent optical properties of aqueous, ethanol and toluene binary solutions, the refractometry method was used. The direct relation between the chemical bonds of the molecules and their chemical structure is discussed.

Chapter 7 overviews a description of the Nanotechnology-Based Nanomaterials focusing on the developments and challenges of Metal Oxide Nanoparticles such as chromium oxide (Cr_2O_3) nanoparticles, indium oxide nanoparticles (In_2O_3), and magnesium oxide (MgO) nanoparticles. These materials are considered novel materials for biological and smart applications such as antimicrobial, drug delivery systems and cancer therapy. The mechanism of anti-microbial activities of metal oxide nanoparticles is discussed here in detail.

Chapter 8 describes the analysis of the effect of load direction on the stress distribution in orthopaedic implants. Characteristics of implant materials such as rigidity, corrosion, biocompatibility, surface morphology, tissue receptivity, and stability are the key factors that influence the choice of the implant material. The mechanical properties of the implants are one of the significant factors for bone substitution. In this study, 3-dimensional modelling of implant and simulation using the finite element analysis software were incorporated to investigate the effect of load direction on the stress distribution in different orthopaedic implant materials.

Chapter 9 accentuates the latest breakthrough in the catalysis, sensing and wastewater treatment applications of advanced and smart materials. The number of catalytic and sensing operations of advanced and smart materials is discussed in detail. Catalysis and sensing phenomena involve the conversion of obtained signals into a readable format and advanced materials with their exemplary optical, semiconducting or physical properties are studied widely. With the advancement in the latest synthesis and functionalization methods, these advanced materials are becoming nanohybrid systems. It covers the implementation of these nanohybrid systems for catalysis, wastewater treatment and sensing.

Chapter 10 discusses the recent advancement of topological materials. Topological materials are characterized by a unique band topology that is prominently distinct from ordinary metals and insulators. This new type of quantum material exhibits insulating bulk and conducting surface states that are robust against time-reversal invariant perturbations. Bi_2Se_3, Sb_2Te_3 and Bi_2Te_3 were predicted as 3D Topological insulators (TIs) with a single Dirac cone at the surface state. For application purposes, however, bulk conductivity due to Se vacancy in Bi_2Se_3 or anti-site defects in Bi_2Te_3 has been a challenging issue. To achieve an enhanced surface conductivity over the bulk, nanomaterials are irreplaceable. Nanostructures' high

surface to volume ratio provides a good platform for investigating the topological existence of surface states.

Chapter 11 is a final chapter that provides information about the hollow nanostructure materials, the most studied topics in current nanoscience research. These hollow structures can be in the form of nanospheres, nanocages, nanorods, nano boxes, single-layered, multi-layered, *etc*. All these variations in hollow structures like carbon buckyball, nanotubes, *etc*. open up several applications in various fields of research from biomedicines to optoelectronics. The observed properties of a material in a hollow shape, like better conductivity, trapping capacity, and catalytic effect, *etc*. This chapter covers the basic information about different kinds of hollow structures like carbon buckyball, variations in their properties along with recent developments, and their applications. Also, includes detailed research about buckyball structures of ZnO, ZnS, and Al-doped ZnO using simulations, with their comparative study and future applications.

Guest Editor:

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CHAPTER 1

Carbon and Boron Nitride Nanostructures for Hydrogen Storage Applications; A Theoretical Perspective

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Abstract: We present the recent progress in hydrogen storage in carbon and boron nitride nanostructures. Carbon and boron nitride nanostructures are considered advantageous in this prospect due to their lightweight and high surface area. Many researchers highlight the demerits of pristine structures to hold hydrogen molecules for mobile applications. In such cases, weak van der Waals interaction comes into account. Hence, the hydrogen molecules make weak bonds with the host materials and, therefore, weak adsorption energy and low hydrogen molecules uptake. So, to tune the adsorption energy and overall kinetics, methods such as doping, light alkali-alkaline earth metals decoration, vacancy, functionalization, pressure variation, application of external electric field, and biaxial strain have been adopted by many researchers. Physisorption with atoms decoration is promising for hydrogen storage applications. Under this condition, the host materials have high storage capacity, average adsorption energy and feasible adsorption/desorption kinetics.

Keywords: Adsorption energy, Boron nitride, Carbon nanotube, Chemisorption, Density Functional Theory, Desorption temperature, Graphene, Hydrogen storage, Physisorption, Pressure, Temperature.

INTRODUCTION

Population increase and rapid population surge in different parts of the world, accompanied by the need for a sustainable and better quality of life, resulted in

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Dibya Prakash Rai (Ed.)

a significant increase in energy demands [1]. Currently, fossil fuels are the primary and dominant energy source due to their established infrastructure, ease of delivery, and cost competitiveness compared to other energy sources. Fossil fuels are known to cause serious harm to the environment due to the emission of harmful pollutants by their use in different industries. The need for renewable energy sources to mitigate these environmental challenges and the secure energy future due to the limited availability of fossil fuels is excellent. The transition to a clean, renewable energy source is essential due to the various drawbacks of fossil fuels.

Lithium-ion (Li-ion) batteries in Unmanned Aerial Vehicles (UAVs) have limitations in their operating range due to low energy density. As hydrogen has a very high mass and volume-specific energy value, it can provide a significant range improvement over Li-ion batteries. Hence, efforts are ongoing to investigate the potential of hydrogen-fueled power plants for small UAVs [2]. The use of hydrogen fuel cell electric vehicles (HFCEVs) produces zero tailpipe pollutant emissions and is more traditional than gasoline-based internal combustion engine vehicles (ICEVs). Study shows that an HFCEV, even fueled by hydrogen from a fossil-based production pathway, uses 5%–33% less WTW fossil energy and has 15%–45% lower WTW greenhouse gas emissions than a conventional gasoline ICEV [3].

Hydrogen is abundant in nature but not in a free state. It can be utilized as an energy carrier because it does not have any harmful by-products during combustion (by-product is water) and has a high energy density compared to other elements [4, 5]. Even though hydrogen has many advantages over other energy sources, the problem lies in its storage. As per the United States Department of Energy, the benchmark hydrogen uptake capacity should be above 6.5wt%. Different means of storing hydrogen have been explored, such as compressed gas, liquid organic hydrogen carriers, inorganic systems, *etc* [6 - 8]. The average adsorption energy benchmark is set to 0.2-0.8 eV per H_2 molecule at ambient conditions. However, considering the recent progress made in hydrogen storage materials, they lack at achieving all the benchmark criteria. Also, the current experimental storage methods are not cost-effective and have safety concerns.

High-pressure storage is the most accomplished and easiest method to store hydrogen. But the main obstacle to this method of storing hydrogen is the high manufacturing and development costs. For vehicle application, hydrogen storage needs to be at extremely high pressure of 700-1000 bar. The consumed power is 10% of the gas energy content at the mentioned hydrogen storage pressure range [9 - 11]. Liquid hydrogen storage is another method of hydrogen storage that shows significant storage density and safety benefits compared with pressure

storage. The total power consumption in this method is about 35% of the energy content of the stored hydrogen, which is relatively higher than other hydrogen storage techniques. The liquid hydrogen storage method is quite popular for space and flight applications as high volumetric and gravimetric energy storage density is required regardless of its high energy consumption [12, 13]. In the cryo-compress method, optimized temperature and pressure values for hydrogen storage enhance the storage density compared to the pressure storage method. The power consumption value reduces to 25% compared to the liquid hydrogen storage method [13].

Recently, many researchers have focused on material-based hydrogen storage techniques. The materials used for storing hydrogen in such techniques should have specific characteristics such as good reversibility, affordable price, high storage capacity at operating temperature, and pressure. The possibility of hydrogen storage on nanomaterials like silicene, TMDs, carbon nitrides, silicon carbides, boron carbides, metal hydrides, magnesium-based hydrides, metal nitrides/amides/imides, polymers, clathrate hydrates, zeolites, metal-organic frameworks (MOFs) has been studied. Most of these materials have a storage capacity in the desired range, but the hydrogen molecules are mostly chemically absorbed by the host materials. In such cases, the materials are not considered fit for onboard applications. At present, researcher's interest is in MOFs, which under doping show a favorable response with better adsorption/desorption kinetics towards hydrogen storage [7, 8, 9 - 16, 17, 18]. Due to the high porosity, one-dimensional nanostructures have become an attractive prospect for hydrogen storage applications. Kumar *et al.* theoretically investigated magnesium functionalized on the boron clusters for hydrogen energy storage application. Boron clusters (six boron atoms) with two magnesium atoms decoration have a gravimetric density of 8.10 wt% [26]. Magnesium oxide($Mg_{12}O_{12}$) nanotube showed a higher possibility of surface adsorption of 12 - 24 hydrogen atoms. The adsorption of hydrogen on Mg and O sites decreased the work function of the nanotube [27]. When functionalized with transition metals, silicon carbide nanocages and nanotubes shows favorable responses towards hydrogen molecule adsorption [28, 29].

Carbon nitride nanostructures where the bonding between carbon and nitrogen atoms is sp^2-type and similar to graphene have also garnered interest from researchers. The hydrogen adsorption possibility on such nanostructures has garnered interest due to its lightweight and high surface area. Wang *et al.* also highlighted the possibility of lithium and calcium co-doped g-CN nanostructures for hydrogen storage applications. They reported that the hydrogen molecules adsorb on the host material with an adsorption energy of 0.26 eV/H_2 and a gravimetric density of 9.17 wt%. The adsorption mechanism is through

CHAPTER 2

Suitable Nanomaterials for Retinal Implant Technique and Future Trends

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Abstract: Artificial vision for blind patients suffering from retinal diseases has shown promising results in the last two decades, especially after the advancement in CMOS technology. In the modern era, two types of retinal implant techniques are very popular, one is the epiretinal implant and the other is the subretinal implant technique. Even though the method of data processing is different in the above-mentioned techniques, utilization of appropriate nanomaterial for the durability of the implant has always been a major concern. Materials such as titanium nitride (TiN), iridium oxide (IrOx), platinum grey, and carbon nanotube (CNT) were employed in recent years in many retinal prosthetic projects. Manufacturing of stimulating electrodes and coating of electronic devices to avoid infiltrations are the two important applications where nanomaterials are utilized in the retinal implant system. This chapter discusses the important and desired physical properties of nanomaterials viz. conductivity, tensile strength, absorption of photons, and adsorption of water molecules for the subretinal implant technique. Since the implant is located inside the retina, the isolated and corrosive environment is the main challenge. This study is based on the first-principles of density functional theory (DFT). Considering the recent advancements, the materials are comparatively analyzed, and new nanomaterial is also suggested.

Keywords: Absorption, Adsorption, Artificial vision, Conductivity, CMOS, Corrosive, Density Functional Theory, Electrode, Nanomaterial, Retinal implant, Tensile strength.

INTRODUCTION

The visual prosthesis is the art of substituting the damaged retinal cells with some electronic aid causing the electrical elicitation resulting in vision.

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Dibya Prakash Rai (Ed.)

The damage in retinal cells is mainly caused by the diseases like retinitis pigmentosa and age-related macular degeneration [1]. The researchers across the globe initially targeted the identification of the phosphene area including its behaviour, mapping of retinal tissues, and methods of processing the image data. Different combinations of electrode were utilized in the past to generate visual sensations. Microphotodiodes, charged-coupled-devices (CCD), and now CMOS image sensors are frequently utilized for retinal implant applications. Before going into the details further, it is important to understand the functioning of an eye [2].

The neuroepithelium sensor, which is present in the retina, processes the tremendous complex information received through the excellent neuroprocessor called the retina that results in vision. In the retinal implant technique the damaged retinal cells (rods and cones) are electrically stimulated through elicitation of nerves resulting in artificial vision. The 130 million photoreceptor cells with 1.2 million retinal ganglion cells (RGC) convert the chromatic and achromatic color images into a chemical and electrical signal. This conversion results in spatial and temporal resolution of the images. After this, the electrical form of the information is carried towards the cortex of the brain through geniculation muscles and humans see the image [1].

The categories of the visual prosthesis are:

Visual Cortical Implant

This is one of the conventional approaches of retinal implant and the largest number of blind patients were treated using this approach. The diseased visual pathways, glaucoma, and diabetic retinopathy responsible for damaging the inner structure of the retina are bypassed in this approach (Fig. **1**). It bypasses all diseased visual pathways, glaucoma, and diabetic retinopathy which can damage the inner retina. Despite these advantages, the visual cortical implant has a very high safety threshold than the other approaches of the visual prosthesis. Due to this high threshold, sometimes the patients face an unhealthy environment leading to death. Moreover, in this approach, the signal is processed outside the retina through signal processing devices; hence its efficacy and placement of electrodes inside the visual cortex are the other significant challenges of this approach [1].

Optic Nerve Implant

The Optic nerve implants, on the other hand, have the advantages of higher density resolution and compact size. It is safer than the visual cortical implant and

the invasiveness of this approach is lesser too. As shown in Fig. (**2**), the optic nerve is responsible to carry the information to the brain; hence, in this approach the rehabilitation becomes viable. However, the adaptability of this approach is discouraged due to the blur vision perception, size, and position of the implant to capture images. In comparison to the retinal implant technique, this approach is more challenging and dangerous because of its position. The elicitation of visual spikes resulting in vision rebuilding is still a matter of discussion [1].

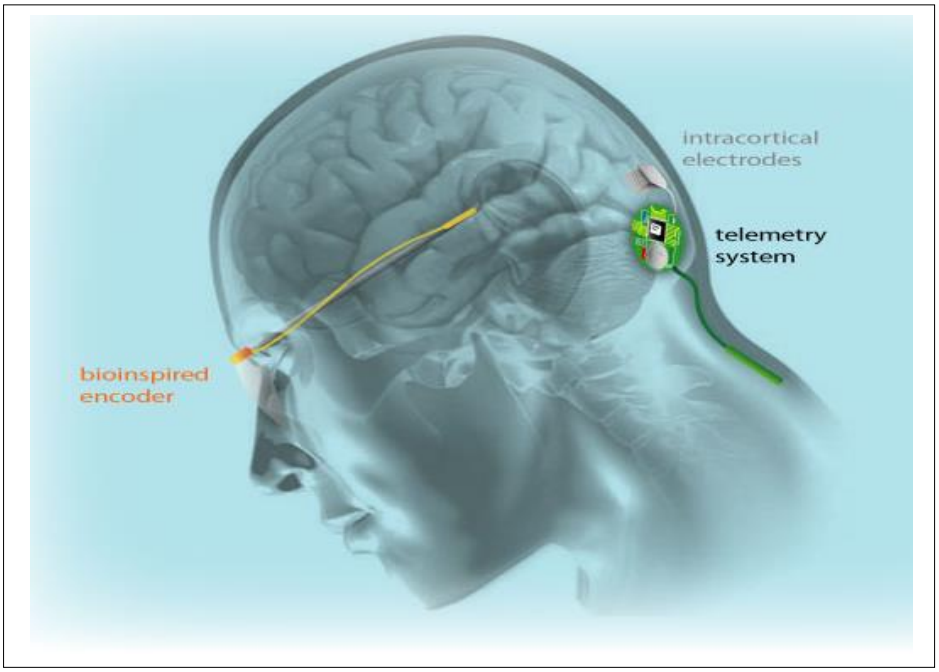

Fig. (1). Visual cortex implants position with intracortical electrodes.

Retinal Implant (Epiretinal and Subretinal Implant)

The distinguished approach of epiretinal and subretinal implant is depicted in Fig. (**3**). In epiretinal implants, the device is placed over the retinal tissues and image data is processed via external devices whereas in subretinal implants, the damaged retinal tissues are itself replaced with the implanting device such as CMOS image sensor. Both the techniques have their own advantages and disadvantages, such as in epiretinal implant it is easier to produce the high resolutions and surgical requirements are minimal. The major challenge is to provoke the inner retinal through the outer signal excitation [3]. The subretinal implant has the advantages of less mechanical fixation and decreased stimulation current. Isolated environment generating the heating effect and placement of implanting device

CHAPTER 3

Recent Advancements in the Design of Electrode Materials for Rechargeable Batteries

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Abstract: As the world progresses towards sustainable energy and concomitant decarbonization of its electrical supply, modern civilization is approaching the fourth industrial revolution with a boom of digital devices and innovative technologies. As a result, the demand for high-performance batteries has skyrocketed, and many research initiatives for the design and development of high-performance rechargeable batteries are being taken. With the incremental standardization of battery designs, enhancement in their performance mainly relies on technical advancement in key electrode materials (cathode and anode materials). This chapters reviews the state-of-the-art materials used in fabricating electrodes, including a description of their structures and storage mechanisms and modification of commonly used materials for electrode working either in the solid-state or in the solution for aqueous or non-aqueous electrolytes. Based on the appropriate metrics such as operating voltage, specific energy, capacity, cyclic stability and life cycle, the performance of different electrodes has also been assessed. Along with the recent advancement, pertaining limitations are briefly covered and analyzed with some viable solutions in the pursuit of cathode and anode materials with fast kinetics, high voltage, and long cycle life.

Keywords: Electrode materials, Life cycle, Operating voltage, Rechargeable batteries, Specific energy, Sustainable energy.

INTRODUCTION

Lithium-ion batteries (LIBs) is one of the most promising secondary sources for portable electronic devices such as laptops, mobile, camera, *etc* [1]. LIBs got

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commercialized in 1992 as the first rechargeable battery to be used in future electronic devices [2]. Its components included carbon as the negative electrode, a non-aqueous electrolyte, and lithium cobaltate ($LiCoO_2$) as the positive electrode [3]. Recently rechargeable batteries have gained tremendous attention for application in hybrid electric vehicles [4]. With the increase in demand, the need for advanced battery technology is accelerating at a rapid pace. Batteries that could give high power density, high energy density and are safe have become a requirement in the present scenario [5]. The better performance of the battery is limited by expensive positive electrodes; which is one of the key element of the battery [6, 7]. Since 1980, Goodenough has devoted enormous efforts to formulate oxides based on transition metal elements with a particular emphasis on those materials whose structure supports higher mobility of Li^+ ions [6]. The journey of discovery of electrode materials started with the layered structure of $LiCoO_2$ in 1980 marked by two important milestones: one in 1986 with the discovery of $LiMn_2O_4$ spinel structure and the other in 1997 for the $LiMPO_4$ (M = Fe, Mn, etc.) olivine family [2]. For systems with high energy density, mainly layered structure cathodes are employed, whereas spinel and olivine families are preferred ones for Li-ion batteries with high-power density [7]. High specific capacity, safety, good chemical stability, environment friendliness, and cost-effectiveness are some of the specific properties of the lithium compounds required for suitable insertion of lithium-ions [8]. This chapter primarily focuses on the pros and cons of cathode and anode materials used in LIBs such as $LiCoO_2$ (LCO), layered $LiNiO_2$ (LNO), layered NCA, spinel $LiMn_2O_4$ (LMO), olivine $LiFePO_4$ (LFP), hard carbon, soft carbon, carbon nanotubes (CNTs) and graphene. By keeping some very important physical parameters in mind, comparative study of these materials as the active electrochemical element is discussed in this chapter. From the perspective of transportation of Li-ion in these lattices, it is our goal to address different types of electrode materials, their structural and synthesis challenges, efficiency, electrochemical stability window and safety issues [9].

MECHANISMS OF ENERGY STORAGE IN LI-ION BATTERIES

There are three main components in a battery: one positive electrode (cathode), one negative electrode (anode) and an ion-conducting medium in between the electrodes called the electrolyte. When a battery charges cations like Na^+, Li^+, H^+ from one electrode migrate *via* the electrolyte and are inserted or absorbed on another electrode causing the electrochemical system to polarise [1]. The discharge is a reversible depolarization process in which ions desorb or get extracted from one electrode and are transferred to the other. Electricity is produced as electrons are generated due to the movement of ions passing *via* an external circuit. In LIBs, lithium ions leave the cathode material and go to the

anode through the electrolyte and separator. At an anode, lithium ions penetrate the anode material structure by different mechanisms resulting in the storage of energy between the electrodes [1]. Lithium ions from the anode flow through the electrolyte to the cathode during LIB discharging, generating energy to power the batteries. While charging and discharging, electrons generated are forced to flow through the external circuit in the direction opposite to that of Li-ion. Ions flowing oppositely through the electrolyte and electrons flowing through the external circuit are related processes, which implies that if one stops, the other automatically will get abandoned. To put it another way, if ions can't go through the electrolyte because the battery is completely discharged, electrons can't move through the outside circuit either, and the battery can't power the device. This is the complete energy storage mechanism in lithium-ion batteries (Fig. **1**) [10].

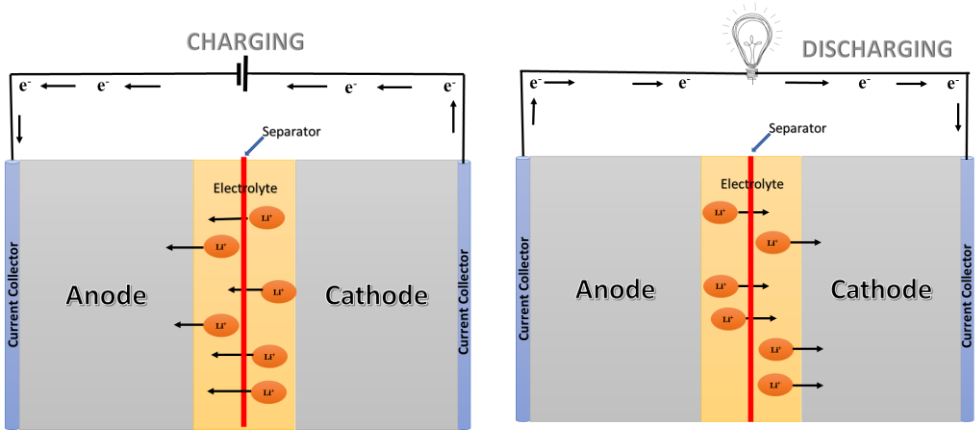

Fig. (1). Mechanism of charging and discharging of Li-ion battery.

The performance of LIB is highly governed by anode and cathode material. Any rechargeable cell relies on reversible chemical processes at the electrodes. A membrane that is permeable to electrolytes physically separates the anode and cathode. The role of electrolyte is also important as it mainly decides the ionic conductivity and electrochemical window of a battery. Electrolytes could either be liquid or solid. Typically solid electrolytes are coupled with liquid or gaseous electrodes. Solid electrodes and solid electrolyte is hardly used together because of the challenging solid-solid interface. Electrolytes must not allow electrons to pass through them such that electrons are forced to move *via* an external circuit to power an electronic device [1].

CHAPTER 4

Design of Supported Catalysts for Nitrogen Reduction Reaction: A Continuous Challenge

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Abstract: The production of ammonia is facilitated by the nitrogen reduction reaction (NRR), where the inert di-nitrogen molecule is converted to ammonia. Along with being a major carrier of hydrogen, ammonia holds authority in the fertilizer realm. Therefore, it is inevitable to develop a viable and eco-friendly method of production that is cost-effective and resource-efficient. The primary challenge of nitrogen reduction is the cleavage of the particularly stable nitrogen bond. The most popular Haber-Bosch process for ammonia production, although efficient, is highly energy-intensive, and the need for maintaining exceptionally high temperature and pressure conditions is an environmental concern. As an alternative, the direct conversion of nitrogen has been carried out by photocatalysis and electrocatalysis. However, this strategy falls short of achieving superior conversion efficiencies. Consequently, it is conceivable that a fitting catalyst can be the solution for the difficulties associated with NRR. Over the years, several attempts have been made at formulating the best catalyst, including chromium oxynitride nanoparticles, niobium dioxide, various metal (Ru, Al, Rh, Ga) clusters, single-atom catalysts supported on different surfaces, and double-atom catalysts. Recently, perovskites have emerged into the spotlight as excellent catalysts for NRR. In this chapter, we discuss the challenges faced by researchers to formulate righteous catalysts for the sustainable reduction of nitrogen by studying each of these types with a few examples. We also review the recent advancements in the experimental domain of NRR using different electrochemical cells.

Keywords: Ammonia, Density functional theory, Double-atom catalysts, Haber-Bosch process, Heterogeneous catalysis, Nitrogen reduction reaction, Perovskites, Single-atom catalyst.

INTRODUCTION

The major obstacle concerning nitrogen reduction reaction (NRR) is the weakening of the dinitrogen bond due to its high N≡N bond energy (940.95

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kJ/mol) [1], electron affinity (-1.9 eV), and the large gap between its HOMO and LUMO (10.82eV) [2, 3], which make electron transfer difficult. Furthermore, the bond length associated with a molecule of nitrogen is very short, 1.09Å [4], indicating that the cleavage would be strenuous. The resulting product of interest from NRR, ammonia, is crucial in various ways. While ammonia is primarily known for its significance in the synthesis of fertilizers, it has several other roles; a few of which are: (i) ecological energy carrier, (ii) transportation fuel, (iii) in agriculture, pharmaceutical, plastic, and textile industries. There are three well-known paths formulated for the synthesis of ammonia; biological nitrogen fixation by *Azotobacter*, the Haber-Bosch process, and electrochemical catalysis. However, the common drawback shared by these methods is the low rate of reaction. *Azotobacter*, Gram-negative aerobic bacteria, reside in the soil. They use the nitrogen available in the atmosphere to synthesize cellular proteins, which are subsequently mineralized upon the death of the bacteria, thereby contributing to the availability of nitrogen in the soil. The Haber-Bosch process has been employed for the synthesis of ammonia since its invention. The typical conditions necessary to carry out the reaction in the presence of Fe/Ru catalysts are temperatures ranging from 300°C-500°C, and pressures ranging from 150-200 atm [4]. In addition to requiring extreme temperature and pressure conditions, the reaction also contributes to global warming by emitting 300 million metric tons of CO_2 every year [4]. Therefore, it is obvious that a clean and sustainable strategy for nitrogen reduction is inevitable. In this regard, electrochemical catalytic methods have gained popularity in the recent years. Although Hydrogen Evolution Reaction (HER), Oxygen Reduction Reaction (ORR), Oxygen Evolution Reaction (OER), and CO_2 Reduction Reaction (CO_2RR) are extensively studied, the electrochemical catalytic reduction reaction of nitrogen to yield ammonia using dinitrogen and water is not thoroughly investigated.

Electrocatalysts can be categorized based on whether they are associated with (i) noble metals, (ii) non-noble metals, or are (iii) metal-free. The activity of the catalyst depends on its properties, including morphology, electronic structure, active sites, and crystallinity. A few ways to augment the catalytic activity are introducing structural defects, doping, increasing the available surface area, and revealing more active sites. Let us look at some of the catalysts that have been explored.

i. Noble metals: Noble metals such as Au, Pt, Ru, Rh have been studied for their catalytic activity in NRR. Yan *et al.* used a binary surfactant mixture to develop tetrahedral Au nanorods and found that the yield of ammonia was low [5]. The low yield was accredited to the surfactant synthesis molecules staying

on the catalytic surface and arresting the active sites. Lan *et al.* [6] reported Pt anchored on carbon black for the synthesis of ammonia from air and water under a moderate environment. The yield was found to be 69.8 μg/h/cm^2. However, Ru catalysts are known to favour the adsorption of hydrogen, which inhibits NRR. Ultimately, the cost involved with noble metal-based processes is too high to be normalized.

ii. Non-noble metals: These are mainly transition metals and are cost-effective. Sun *et al.* [7] proposed an array of MoS_2 nanosheets on carbon cloth for the production of ammonia. The yield was found to be 4.94 μg/h/cm^2. The key factor involved in the activation of nitrogen is the positive charge present around Mo. The charge is shifted from nitrogen to the edges of Mo, leading to the development of N-Mo bonds and thus, weakening the N≡N. As with several other examples, the drawback here is, the edges of MoS_2 nanosheets are active sites for HER.

iii. Metal-free: Although transition metals are cost-effective, their binding to nitrogen is weak and often fails at activating the molecule. Additionally, their d-orbitals tend to form bonds with hydrogen, which brings on HER. Main group elements, unlike transition metals, do not possess the combination of free and occupied orbitals. Yu *et al.* [8] reported graphene doped with Boron; the positive B atoms preferred nitrogen adsorption and, therefore, ammonia production. The yield was found to be 9.8 μg/h/cm^2.

Theoretically, the electrochemical reduction reaction of nitrogen giving ammonia as the product is feasible at room temperature and atmospheric pressure, provided that abundant voltage is applied externally. However, practically, very few catalysts can offer high yields.

NITROGEN REDUCTION REACTION – THE MECHANISM

The pathway of electrochemical reduction of nitrogen to ammonia can be outlined as [4]:

$$N_2 + 6H^+ + + 6e^- - \leftrightarrow 2NH_3(g)\ E° = 0.148V\ vs.RHE \quad \textbf{(1)}$$

$$2H^+ + + 2e^- \leftrightarrow H_2\ E° = 0V\ vs.SHE \quad \textbf{(2)}$$

$$N_2 + 6H_2O + 6e^- \leftrightarrow 2NH_3 + 6OH^-\ E° = -0.763V\ vs.SHE\ at\ pH\ 14 \quad \textbf{(3)}$$

$$2H_2O(l) + 2e^- \leftrightarrow H_2(g) + 2OH^-\ E° = -0.828V\ vs.SHE\ at\ pH\ 14 \quad \textbf{(4)}$$

CHAPTER 5

Role of Nanocomposites in Environmental Remediation: Recent Advances and Challenges

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Abstract: Nanocomposites offer an exclusive advantage over bulk materials in terms of efficiency on account of their greater surface area, higher reactivity, ease of modification, good dispersion, and hence, multi-faceted applications. The various forms of nanocomposites derived from low-cost resources, especially carbon-based materials, are of unique interest. Activated carbons offer the unique advantage as the matrix for nanocomposites synthesis due to their graphite structure, thereby providing strength and the ease of modification on the surface of nanocomposites while introducing desired functional groups. Apart from this, they are widely popular for their large surface area and porosity. Therefore, carbon-based nanocomposites offer vivid applications in various fields, such as environmental remediation as adsorbents, suitable sorbents in the analytical determination of organics, targeted drug delivery, diagnostic agents, fuel cells and sensors, to name a few. Amongst these, the role of nanocomposites as sensors and environmental remediation tools has been studied extensively. The varied modes of action include adsorption, nano-catalysis, membrane filtration, *etc* ., for pollutants ranging from inorganic ions, heavy metals, pesticides, dyes, anti-bacterials, oil spills, and many more. However, there are constraints in their stability, cost, storage and disposal triggered by varying environmental conditions.This chapter presents a review of the synthesis, application and challenges of nanostructured composite materials in environmental remediation.

Keywords: Carbon nanotubes, Environmental decontamination, Nanocomposites, Synthesis.

INTRODUCTION

Composite materials are prepared by the amalgamation of two or more raw materials embedded in a matrix, each having its own unique properties, to create a new material having characteristic features of greater advantage. These are

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broadly categorized into polymer matrix-based composites, carbon matrix-based composites, metal matrix-based composites, and ceramic matrix-based composites. When the size dimensions are reduced to a nanometric scale, they are known as nanocomposites. Nanocomposites are those entities that exist in the nanometric-sized phase, *i.e.*, those particles having a diameter in the range of 10^{-9} m. The reduced size and greater surface area thereof provide them an edge over other conventional microcomposites. Reported as the material of the 21st century, nanocomposites find versatile applications in an array of studies. The very first advent of nanocomposites is believed to have started with clay/polymer composite. In 1990, Toyota company used clay and nylon-6 nanocomposites to manufacture timing belt covers in cars. Ever since then, the application of nanocomposites has proliferated in every sector. Reportedly, around 13420 papers have been published on nanocomposites in the last several years, specifically between the years 1988-2008.

Today, the application of nanocomposites is found in every field, starting from fuel cells, aerospace engineering, biomedical applications, sensors, environmental remediation tools, and many more (Fig. **1**). The reduction in size or the change in the size of the particle size induces a change in the behavior of the particle properties. In a review study [1], the "critical size" or the feature size at which such changes in properties are expected to occur in the nanocomposites has been enlisted (Table **1**).

Table 1. Critical size limits in nanocomposites beyond which changes in properties occur [1].

Properties	Reported Critical Size (nm)
Catalytic activity	<5
Hard magnetic materials turn soft	<20
Change in Refractive Index	<50
Super paramagnetism observed	<100
Change in strength and toughness	<100
Change in hardness and plasticity	<100

The ceramic matrix nanocomposites (CMNC) mainly have aluminium oxide (Al_2O_3) and silicon dioxide (SiO_2) as the matrix (examples include Al_2O_3/SiO_2, Al_2O_3/TiO_2, Al_2O_3/SiC, and Al_2O_3/CNT) and as the reinforcing material. The CMNC find applications in aerospace designing, engine exhausts, hypersonic vehicles, nuclear power industry, *etc* ., owing to their high thermal resistance, creep resistance, and inertness properties, to name a few.

The metal matrix nanocomposites (MMNC) consist of an alloy matrix in which nanosized materials are reinforced (examples include Fe-Cr/Al_2O_3, Ni/Al_2O_3, Co/Cr, Fe/MgO, Mg/CNT, and Al/CNT). The MMNCs have good ductility, elastic modulus, fracture toughness and strength imbibed from the metal and ceramic constituents, and they find great applications in high-strength structured materials in aerospace and automobile material manufacturing. One of the drawbacks of MMNCs is the high surface area which leads to agglomeration of nanoparticles on the surface, thereby reducing the strengthening capacity of the nanocomposites. However, this nanocomposite is a newly developed material, and more research studies are focusing on overcoming this challenge by modifying preparation routes.

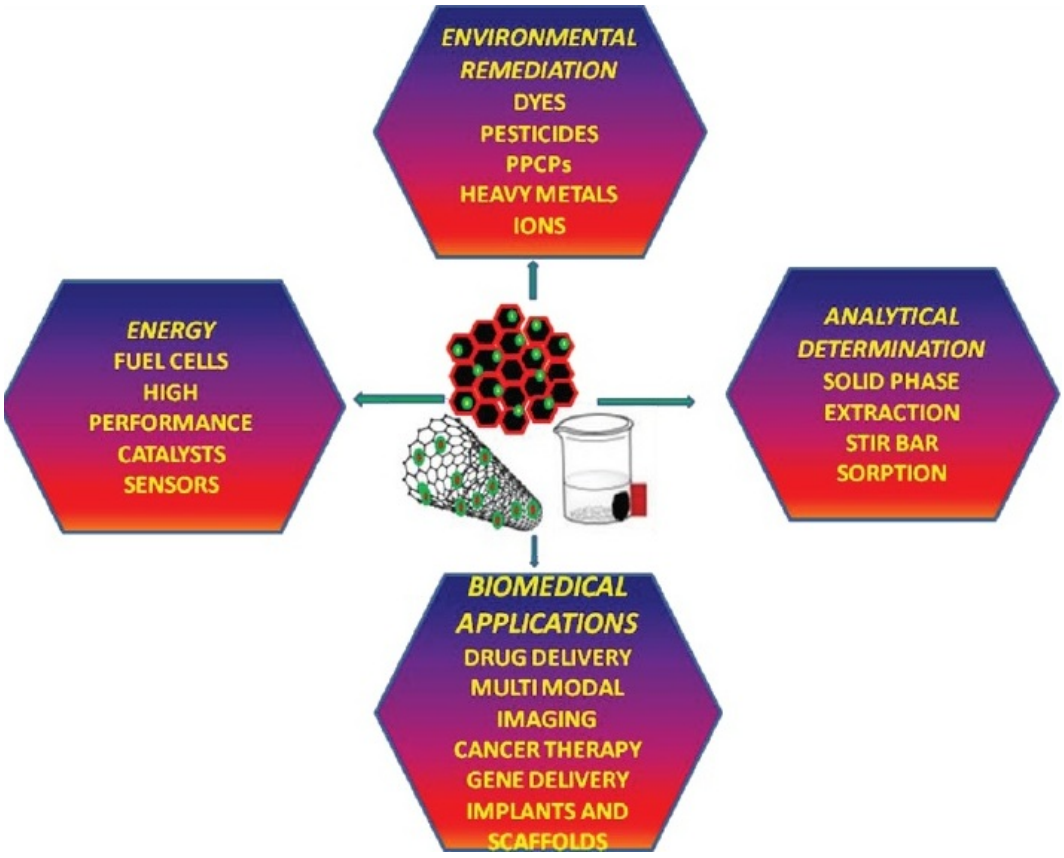

Fig. (1). Functional perspectives of nanocomposites.

The Polymer Matrix Nanocomposites **(**PMNC) consist of the polymeric matrix such as the thermostat or thermoplastic embedded with nanosized particles. Another classification based on the number of nanoscale dimensions they have is

CHAPTER 6

The Excess Refractive Indices of Some Organic and Inorganic Components

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Abstract: To reveal the concentration-dependent optical properties of aqueous, ethanol and toluene binary solutions, the refractometry method was used. The peak of refractive indices corresponds to formed heteromolecular complexes with a certain concentration. The bonds between the molecules formed in mixtures are also directly related to their chemical structure. The bonds that form between polar and non-polar compounds and also between polar protic and polar aprotic compounds are different. All solutions were measured in the concentration range ~0÷1 mole fraction at room temperature. In our work, we have shown that, along with Infrared and Raman spectroscopy, the refractometric method is effective for the determination of formed structures in mixtures.

Keywords: Binary solutions, Dipole-dipole interaction, Excess refractive indices, Hydrogen bonds, Intermolecular interactions, Organic and inorganic mixtures, The refractometric method.

INTRODUCTION

Wide usage of mixed solvents in various nanotechnological processes necessitates establishing the relationship of physical and chemical properties of individual components with the structure and composition of their binary and multicomponent systems. The application of mixed organic systems is due to the possibility of a different variation of their physicochemical features in multicomponent solutions to create a system with predetermined characteristics. It

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is known that in polar solvents and their solutions, reactions are accompanied by complex formation and associations of molecules due to the presence of a dipole moment in molecules characterized by a complex set of intermolecular interactions. To establish the formed structures of the associates in solvents and in their binary solutions, as well as to study the role of hydrogen bonds in the formation of various types of associates, the concentration features of the optical characteristics of solutions were studied by the refractometry method. Refractometry is one of the methods that allows to obtaining information about the nature of the interaction between the components and the structure of characteristics of the system. In this chapter, we present experimental measurements of refractive indices of some organic and inorganic mixtures.

Experimental Setup

All pure components presented in this work and their mixture of water, toluene and ethanol were measured using high-sensitivity digital refractometer PAL-BX/RI (ATAGO, Japan). To analyze the refractive index, mixtures were carried out five times over the entire concentration range at a fixed temperature of 25±0.05 °C. The average value has been chosen. To calculate the excess refractive index n^E , the measured refractive indices were used in equation 1 [1]:

$$n^E = n_{solutions} - (xn_1 + (1-x)n_2) \quad \textbf{(1)}$$

Refractive Indices of Pure Component

The refractive index is used to determine optical density of the material and calculated excess refractive index can show change in the molecular structure of mixed liquids, and to study physicochemical properties of the solutions. An advantage of the refractometric method quickly and accurately analyze and orient whether the organic/inorganic liquid under study contains impure compounds and whether the liquids obtained are pure for the experiment. Organic liquids are used in many such fields, including the synthesis and optoelectronic properties of sulvanite nanocrystals [2, 3]. Refractive indices of several organic and inorganic compounds used in our experiments are illustreted further in Table **1** to compare with our results.

Table 1. Experimental refractive indices (*n*) values of several pure liquids at the temperature 298 K.

S.NO	Liquid	Molecular Formula	Refractive Index, *n*), at T=298K	Literature
1.	Dimethylformamide	C_3H_7NO	1.4279	[4]
2.	Water	H_2O	1.3610	[4]

(Table 1) cont.....

S.NO	Liquid	Molecular Formula	Refractive Index, *n*), at T=298K	Literature
3.	Ethanol	C_2H_6O	1.3324	[4]
4.	Tetrahydrofuran	C_4H_8O	1.4045	[4]
5.	Acetic acid	$C_2H_4O_2$	1.3699	[5]
6.	Toluene	C_7H_8	1.4908	[7]
9.	Acetonitrile	CH_3CN	1.3402	[8]
10.	Cyclohexane	C_6H_{12}	1.4237	[9]
11.	Benzene	C_6H_6	1.4898	[10]
12.	Hexane	C_6H_{14}	1.3437	[11]

Refractive Indicies of Some Binary Solutions

Aqueous Solutions

Refractive indices of freshly prepared water solutions of ethanol, acetic acid, tetrahydrofuran, and dimethylformamide (DMF) are measured and plots of the changes of the absolute values of the excess refractive index of this solutions are shown in Fig. (**1**) . It can be seen that maximum values of refractive indices are achieved at component concentrations of *C* ~0.2÷0.3 mole fraction. A non-polar hydrophobic part and a polar hydrophilic group of ethanol and acetic acid molecules participate in interactions with water molecules.

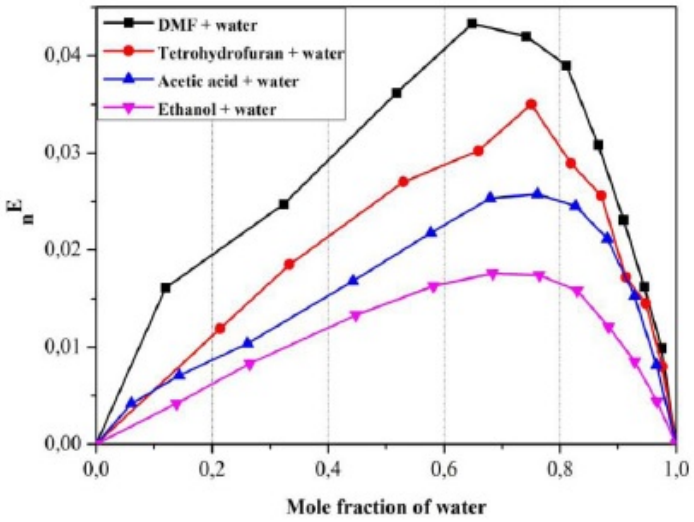

Fig. (1). Changes of the absolute values of excess refractive index of aqueous solutions of ethanol (pink triangle), acetic acid (blue triangle), tetrahydrofuran (red circle) and DMF (black square).

CHAPTER 7

The Fundamental Concepts of Nanotechnology-Based Nanomaterials: Recent Developments and Challenges of Metal Oxide Nanoparticles

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Abstract: Nanotechnology is one of the most promising new technologies in the recent decade, which involves structures, devices, and systems with novel properties and functions due to their atomic arrangement on scales of 1–100 nm. In general, the materials at the nanoscale have unique physical, mechanical, chemical, and biological properties compared to their bulk materials. Thus, these properties lead to a new novelty and variety of technological applications in the different fields (physics, science and engineering, electrical and computer science, materials, chemistry, biology, and medicine). This chapter provides a brief introduction of nanotechnology, nanomaterials, and their applications while discussing structural, optical, and magnetic properties as well as antibacterial activities. This chapter overviews the current research being carried out on the properties and application of metal oxide nanoparticles, especially chromium oxide (Cr_2O_3) nanoparticles, indium oxide nanoparticles (In_2O_3), and magnesium oxide (MgO) nanoparticles. These materials are considered novel materials for biological and smart applications, such as antimicrobial, drug delivery systems, and cancer therapy. Multi-drug and antibiotic resistance are among the great challenges that confront researchers in designing and developing efficient antimicrobial and biomedical agents. Inspired by the remarkable developments in nanoparticles in recent times, antibacterial metal oxide nanoparticles have been discovered as potential antibiotics to restrict infectious diseases. Thus, the mechanism of anti-microbial activities of metal oxide nanoparticles is discussed here in detail. In this chapter, a brief literature survey related to the present study is also performed. By the end of the chapter, the concluding remarks with views on the recent progress and future challenges of metal oxide nanoparticles are appended.

Keywords: Antimicrobial activities, Chromium oxide, Indium oxide, Metal oxide nanoparticles, Magnesium oxide nanoparticles, Magnetic properties, Nanotechnology, Optical properties.

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INTRODUCTION TO NANOSCIENCE AND NANOTECHNOLOGY

Nanoscience and nanotechnology are progressive studies to create and use structures in the form of very advantageous functional materials, devices, and systems possessing novel properties and functions within the dimensions of less than 100 nanometers (one billionth of a meter) length scale [1]. Nanotechnology is the capability to study and manipulate the behavior and properties of the materials at atomic, molecular, and supramolecular levels and organize them systematically. It implies the creation and utilization of different systems as chemical, physical, biological, and others with structural characteristics between molecules or single atoms to submicron size particles, encompassing consequent nanosize structures to larger units [2, 3]. Nanoscale's uprising in technology and different fields endures many reasons for being significant marvelously, some of which have been listed below [4].

1. Nanosystems possess a high-density texture, in addition to its enhanced conducting behavior of electricity which may create new devices of electronics with advanced functions, developed circuits (smaller and faster), and greatly reduce the energy consumption simultaneously through controlling the interactions and complication of nanostructure [5].
2. Improvement in the surface area to volume ratio at the nanoscale provides the effect of a new quantum mechanical potential. Therefore, the reduction of particles size leads to the significant change in the electronic properties of materials. By manipulating the nanoscale design of materials, there is a possibility for changing their properties, like macroscopic and microscopic, magnetization, charge capacity, and melting temperatures, without altering their chemical composition [6].
3. Chemical properties of nanoscale provide features for catalysis, according to the chemistry of interfaces and surfaces and the large ratios of surface area to volume [7]. Nanostructures are idyllic for energy storage, composite materials, catalysis, and target drug delivery. Additionally, it can be used in medicine due to numerous properties, like increased erosion resistance and the probability of inhibiting bacterial growth.
4. Research and nanotechnology involve the development of engineered particles, and molecular structures orman-made nanoscale objects. When nanoscale objects are incorporated with biotechnology components, nanotechnology becomes significant with large potential applications such as biological sensors, new pharmaceuticals, diagnostic devices, medical imaging, and others [8]. As well as, this technology contributed the possibility to examine the matter macrostructure and microstructure by using molecular self-assembly [9].

There are two principal factors of nanomaterials that cause significant differences in properties and behavior of nanomaterials from the other bulk material:

a. Surface area (the fraction of atoms at the surface and typical smoothly scaling properties due to surface effects). The drastic increase in the ratio of surface area/volume is linked to the protuberances on the surface.
b. Quantum effect known as "Quantum confinement effect" which exhibits discontinuous behavior, according to completion of shells on systems with delocalized electrons.

Both of these factors have an effect on the nanomaterial's properties such as mechanical, optical, structural, electrical, transport, and magnetic properties, also affect the chemical reactivity of materials [10]. Over the last few decades, the development has been particularly cleared in the three areas where size effects are important, *i.e*., metals (Ag, Au, *etc*.), semiconductors (Ag_2S, CdSe, *etc*.), and magnetic materials (Fe, CO, Ni, *etc*.) [11]. The size of particles affects the materials properties, which is associated with the confinement of electrons in different dimensions (quantum confinement effects). Thus, the properties of nanomaterials differ from their bulk material. The quantum confinement of excitons (electron-hole pairs) describes the electrons in the terms of energy levels, whereas the confinement means to restrict the random motion of the electron which is moving to the particular levels of energy. When the particle's materials have a dimension in nanoscale, the confinement dimensions lead to discrete energy levels, resulting in a broad energy band gap [12]. In the terms of bulk metals, between the valence and conduction bands, there is no band gap (bands overlap). So, the bulk metals differ from nanostructures of metal, whereas in the metal nanostructures two bands are separated by an energy gap. A diagram of the electronic bands in bulk metals, semiconductors, semiconducting nanoparticles and insulators is shown in Fig. (**1**)**.**

Nanotechnology has attracted increasing attention from researchers and scientists to synthesize materials that have extraordinary magnetic, optical, photocatalytic, electrical, and chemical properties. Nanotechnology is contributing to changing the world around us which possesses widespread and pervasive applications across various sectors. Since previous years, nanotechnology has touched the everyday life of people in various forms with myriad applications. Nanotechnology has greatly and decisively contributed to the development and production of innovative materials and processes in numerous fields. Nanotechnology has an extensive range of applications such as biotechnology, biomedical & drug delivery, optical engineering & communication, cosmetics & plants, agriculture & food, textile, defense & security, metallurgy & materials,

CHAPTER 8

Analysis of the Effect of Load Direction on the Stress Distribution in Orthopaedic Implants

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Abstract: Orthopaedic implant materials have an important role in the field of medical science. Characteristics of implant materials such as rigidity, corrosion, biocompatibility, surface morphology, tissue receptivity, and stability are the key factors that influence the choice of the implant material. The mechanical properties of the implants are one of the significant factors for bone substitution. To understand the mechanical properties of these solid substitutes, the use of solid mechanics, which is intended for general structural analysis of 2-dimensional and 3-dimensional bodies is vital. In this study, 3-dimensional modelling of implant and simulation using the finite element analysis software were incorporated to investigate the effect of load direction on the stress distribution in different orthopaedic implant materials.

Keywords: Finite element analysis, Load-bearing capacity, Load direction, Mechanical properties, Metal alloys, Orthopedic implant, Simulation, Solid mechanics, Stress distribution, Volume displacement, Von Mises stress distribution.

INTRODUCTION

Orthopaedic implants have developed critically through the years. Its sole purpose remains the same – to replace bone or articulating surfaces of a joint [1] so that patients can regain full range of motion. In 1965, Brånemark in Sweden conceptualised orthopaedic implants while supervising and leading a research project at the University of Gothenburg [2]. The original research of Brånemark was based on the microcirculation of blood flow in rabbit tibias. For this investigation, a small titanium optical chamber was inserted in a bone to investigate the rabbit's blood supply. Later, Brånemark found it impossibly difficult to remove the blood chamber as it was now integrated into the bone [2], leading to Brånemark evidently realising that the integration between these and

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particular metals and the bone is possible, eventually leading to the concept of orthopaedic implants. Today, dental implants are extremely beneficial; for example, the osseointegration of implants provides great benefits and advantages to the patient when compared to removable prosthesis dentures; it gives better support to the denture [3], and improves aesthetics. However, the decision to use an orthopaedic implant must be made while considering an analysis of the biological conditions of the patient, in order to avoid potentially harmful complications that may occur to worsen the condition.

This paper focuses on the effectiveness of various possible implant materials by analysing to find the one that adheres most to an ideal bone substitution material. Several implant material characteristics (rigidity, corrosion, biocompatibility, surface morphology, tissue receptivity, and stability) are vital to ensure it is an ideal candidate for bone substitution. The mechanical properties of the material are critical to confirm it has the intended load-bearing capacity to structural support the surrounding bones, without causing much volume displacement of the pre-existing bone and tissue around the implant and relatively uniform stress distribution. It is imperative that the material used for the orthopaedic implant has the required mechanical and structural properties to support the load so that the patient has no difficulty moving.

The implant material will be the independent variable in this investigation, differentiating between various alloys. The five possible orthopaedic materials are Ti-6Al-4V, Nitinol, CoCrMo, CoCr, and 316L. There are multiple deciding factors when it comes to the properties of these alloys, some of which are used to simulate, for example, Young's modulus, Poisson ratio and Density. The 3-dimensional modelling of the implant consists of two cylinders at the top and bottom, with the orthopaedic implant being the smaller cylinder in the middle. The upper and lower bone is kept to be the same throughout the simulations and structural analysis, only changing the implant material with a different alloy each time. A load was applied tangentially to a specific side of the upper bone, Fig. (**4**), with the constraint of keeping the base, Fig. (**3**), fixed (immobile) the model was analysed to see the stress distribution across it and its volume displacement. Force distributions, bending moment, torque and flexural rigidity are determined by structural analysis of the osseointegrated implant system using finite element analysis (FEA) [4].

The finite element analysis (FEA) is largely known to be used for damage evaluation [5], material characterisation [6], and biomechanical applications [7] for many years. It is also used to predict biomechanical occurrences on the bone-implant interface [8].

In this study, we analyse the effects of external loading applied tangentially and its stress distribution on different implant materials using 3D FEA. This study can further be used to evaluate and analyse the consequences of forces applied on osseointegrated implants and also understand how the properties of implant materials affect its behaviour and its biocompatibility with surrounding tissue and bone.

Geometrical Model

The three-dimensional geometrical model of the bone-implant structure, Fig. (**3**), is analysed using the finite element methodology. The upper and lower big cylindrical structures, Fig. (**1**), are modelled to be bone. The upper cylinder was given the dimensions: 1cm radius, 3 cm height and the position coordinates (0,0,4). The lower cylinder was given the dimensions: 1cm radius, 3 cm height and the position coordinates (0,0,0). The implant is presented as a smaller cylinder in between the bone, Fig. (**2**), with the dimensions: 0.5cm radius, 3cm height and the position coordinates (0,0,2).

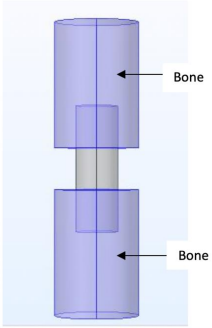

Fig. (1). Bone structures indicated by purple.

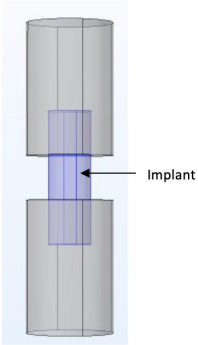

Fig. (2). Orthopaedic implant indicated by purple.

CHAPTER 9

Advanced Materials and Nanosystems for Catalysis, Sensing and Wastewater Treatment

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Abstract: This chapter accentuates the latest breakthrough in the advanced and intelligent materials' catalysis, sensing and wastewater treatment applications. The various engineered materials are securing the interest of researchers for optimized technical utilizations. This chapter discusses the number of catalytic and sensing operations of advanced and intelligent materials in detail. Catalysis and sensing phenomena involve the conversion of obtained signals into a readable format, and advanced materials with their superior optical, semiconducting or physical properties are studied widely. However, wastewater treatment needs adsorption and advanced oxidation of the different types of contaminants by the advanced materials. The list of advanced materials includes many organic/inorganic and natural/synthetic platforms with desired properties. These advanced materials have high biocompatibility and easy biodegradable characteristics. With the latest synthesis and functionalization methods, these advanced materials are becoming nanohybrid systems. This chapter covers implementing these nanohybrid systems for catalysis, wastewater treatment and sensing. The first half of the chapter focuses on introducing the basic catalytic, sensing and wastewater processes based on the application of advanced materials. However, the second half includes introducing various advanced materials in the techniques mentioned above.

Keywords: Advanced Oxidation, Carbon Dot, Carbon Nanotube, Ferrite, Gold Nanoparticles, Metal and Metal Oxides, Nanomaterial, Photocatalysts, Semiconductor, Wastewater Treatment, Water Splitting.

INTRODUCTION

Material science and nanotechnology advancements are currently resulting in novel materials for improving in situ remediations of the most ubiquitous and persistent contaminants, as well as providing accessible sensing techniques. The earth faces two significant threats: rapid consumption of non-sustainable energy resources and an extended increase in pollution concentrations in the ecosystem.

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Recently, numerous studies on alternative energy conservation and generation methods have been accepted and studied in laboratories to fulfill the need for energy [1, 2]. Nowadays, with the increase in population and pollution every moment, the obligation of researchers has also been raised to develop new materials with extra unequivocal features like quick recovery, excellent reusability, facile degradation, immediate resolution, easy processing, and less processing expensive, desired dimensions along with others. For the last few decades, nanotechnology has been catering to all these needs of researchers and levering the expansion in material science domains. Nano ranged dimensions of these particles have resulted in compelling transition due to their peculiarity in analogy to similar bulk components. Generally, nano dimensional particles can be formed by following two methods: Top-Bottom or Bottom-Up, where the first one includes breakdown and grinding like methods, and the second one incorporates proportionate mixing of precursors [3]. Some of the commonly used nanoparticle synthesis techniques are listed in Fig. (**1**). Nanoparticles have high surface reactivity compared to bulk materials, and their size and shape depend on the preparation technique. Nowadays, plant-based green synthesis methods provide cost-effective and chemical-free techniques for nanoparticle synthesis.

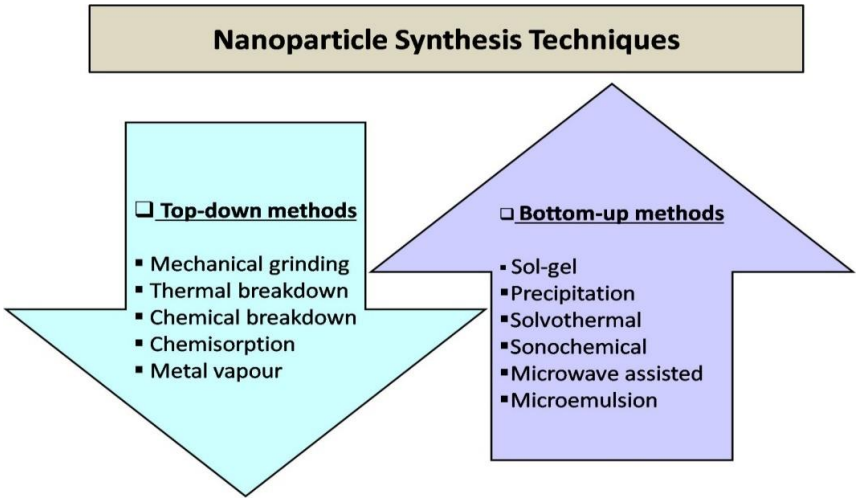

Fig. (1). Nanoparticle synthesis techniques.

Catalytic reactions necessitate the involvement of a fascinating material named a catalyst to expedite a chemical process without leaving any perpetual transition in the material. For the last few decades, catalytic reactions and advanced engineered catalysts have been investigated in detail and prepared by chemical and bio-inspired synthesis techniques. Green synthesis techniques have elaborated ingenious strategies to establish solar light-driven systems for afferent energy

production [4]. Catalytic processes effectively perform their role in supportable ecological systems and energy sources for forthcoming centuries, as depicted in fuel cells and catalytic converters [5]. Many nano ranged functionalized substances are used as a substrate for catalytic studies and have also been found to increase the efficacy of the reaction immensely. Various types of homogeneous and heterogeneous catalytic materials, including photocatalysts, Gold nanocatalysts, metal and metal oxide-based nanocatalysts, nanoclusters, carbon-based catalysts, etc. are engineered by combining catalysis studies with material and surface science [6, 7]. Many nano ranged functionalized substances are used as a substrate for catalytic studies and have also been found to increase the efficacy of the reaction immensely. Various types of homogeneous and heterogeneous catalytic materials, including photocatalysts, gold nanocatalysts, metal and metal oxide-based nanocatalysts, nanoclusters, carbon-based catalysts, etc. are engineered by combining catalysis studies with material and surface science [8].

This chapter includes a brief discussion about advanced innovational materials such as nano catalytic systems, sensing probes and wastewater treatment. Nanoparticles have a common characteristic of heterogeneity as different sizes and shapes of these nanoparticles impart different catalytic activity rates to each particle [9, 10]. Catalytic reactions are also found to play an essential role in sensing and wastewater treatments. The sensing mechanism involves stimuli-responsive systems attached to a signal converter, whereas wastewater treatment includes the degradation of toxic, harmful, organic, or inorganic materials by certain substances using various mechanisms. An efficient sensor should have high selectivity and sensitivity with an easy manufacturing process. Nanoparticles have facile characteristics, due to which they can be easily employed in the sensing field. They have nano ranged dimensions which come in the close range of visible light wavelength and can show electron collective motion known as SPR. SPR phenomena lead to the development of the real-time and label-free sensing of different targets, including harmful gases, pesticides and bio-organisms. SPR sensors include the collective electron excitation by incident photons on the surface. The resonance frequency of SPR oscillations depends on the refractive index of the surface, type and morphology of the nanoparticles [11]. As we are quite aware, the availability of potable water is a primary concern of human beings nowadays. Due to the mass industrialization required for human lives, surfaces and groundwater resources are getting polluted daily. Various remediation techniques based on different mechanisms are used to remove contaminants. Naturally, minerals provide a low-cost way to remove toxic and harmful contaminants from the wastewater, but with advancements in scientific processes, new low-cost methods are developed using advanced nanomaterials [12]. All wastewater treatment methods are categorized into conventional and

CHAPTER 10

Advancement of Topological Nanostructures for Various Applications

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Abstract: Topological materials are characterized by a unique band topology that is prominently distinct from ordinary metals and insulators. This new type of quantum material exhibits insulating bulk and conducting surface states that are robust against time-reversal invariant perturbations. In 2009, Bi_2Se_3, Sb_2Te_3 and Bi_2Te_3 were predicted as 3D Topological insulators (TIs) with a single Dirac cone at the surface state. For application purposes, however, bulk conductivity due to Se vacancy in Bi_2Se_3 or anti-site defects in Bi_2Te_3 has been a challenging issue. In order to achieve an enhanced surface conductivity over the bulk, nanomaterials are irreplaceable. Nanostructures' high surface to volume ratio provides a good platform for investigating the topological existence of surface states. By tuning the position of Fermi level through field effect gating, it is also possible to terminate the bulk residual carriers. Moreover, the synthesis of nanomaterials allows for morphological, electronic, and chemical regulation, resulting in the ability to design structures with desired TI properties at the nanoscale. In this article, we review various technological applications of nanostructured topological insulators. We also survey the implementation of topological nanomaterials in the field of optoelectronic devices, p-n junction, superconducting materials, field effect transistor, memory device and spintronics, ultrafast photodetection, and quantum computations.

Keywords: Band topology, Dirac cone, Quantum computations, Quantum material, Topological nanostructure.

INTRODUCTION

Topological insulators, the recent discovery in condensed matter physics, contains insulating bulk and spin helical surface state with a unique band topology. The surface states are protected by time–reversal symmetry and caused by the inversion of the bulk bandgap, occurring by the strong spin–orbit coupling of the heavy (high Z) material. Fig. (**1**) manifests the 1D helical edge state and 2D helical surface states of 2D and 3D topological insulators. The exceptional electr-

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onic nature of the TI surface states assures spintronics devices and quantum computing, as well as guarantees applications in energy conversion such as thermoelectrics. Presently, the investigation of topological materials also includes Weyl semimetal(WSMs), Dirac semimetal(DSMs), and Nodal line semimetal (NDSMs) with different degeneracy and distribution of band crossings. Among them, the band crossing of Dirac semimetal possesses 4-fold degeneracy near the Fermi energy. When those Dirac points split into Weyl points with the breaking of either time reversal or inversion symmetry, Weyl semimetal comes into picture. The Weyl points always come into pairs with opposite chirality. Type 1 WSMs have point-like Fermi surfaces, whereas tilted Weyl cones that appear at the contact of electron pockets and hole pockets are Type 2 WSMs. For NLSMs, band crossings make closed loops instead of discrete points in the Brillouin zone.

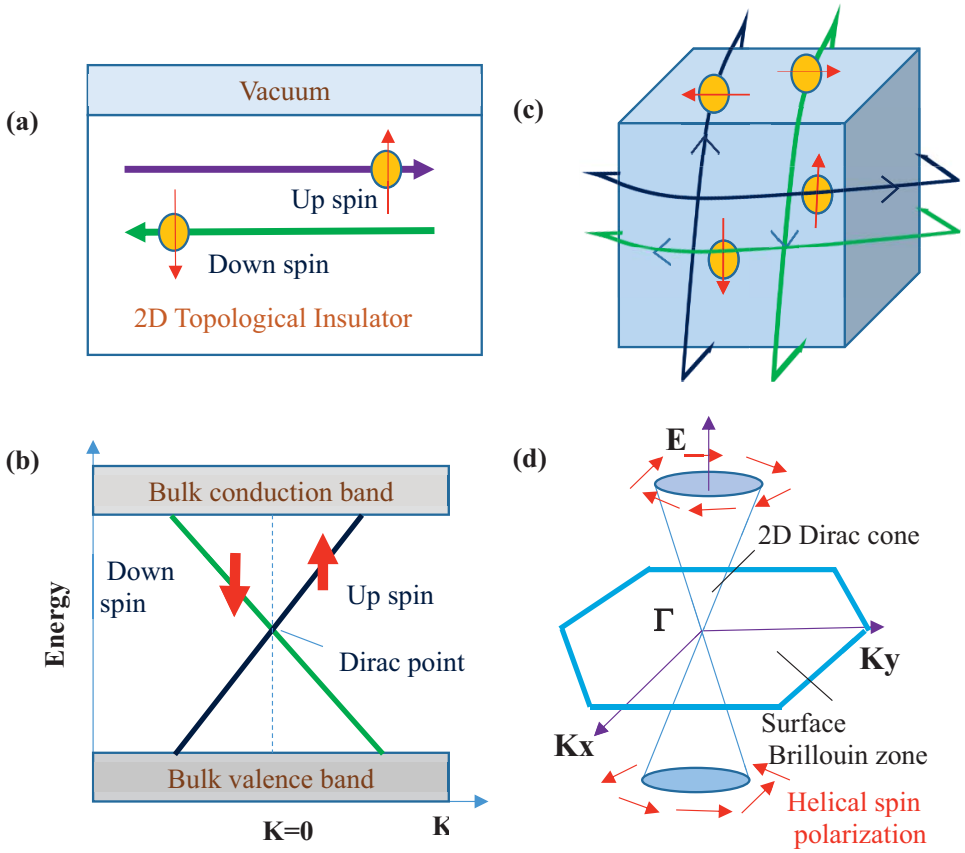

Fig. (1). (Modified from [9]. Edge and surface states of topological insulator with Dirac dispersions. **(a)** The 1D helical edge state of a 2D TI is shown schematically, **(b)** Energy dispersion of a 2D TI's spin non-degenerate edge state forming a 1D Dirac cone, **(c)** The 2D helical surface state of a 3D TI is shown schematically, **(d)** Energy dispersion of a 3D TI's spin non-degenerate surface state forming a 2D Dirac cone.

Fig. (**2**) represents the schematic diagram of normal metal and three types of topological semimetals. In this review, we will discuss the ongoing progress of nanostructured topological insulators and their implementations in future directions. The experimentally realized first predicted 2D TI was HgTe/CdTe quantum wells. Later $Bi_{1-x}Sb_x$ alloy was confirmed as 3D TI with a complex surface state; however, the A_2B_3 type of materials with a single Dirac cone signature was proved as 3D TI with simpler surface states.

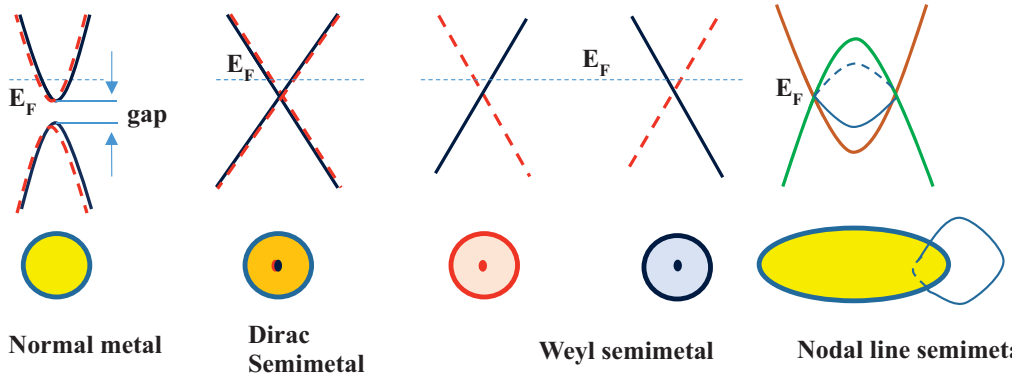

Fig. (2). Modified from [10]. Schematic diagram of Fermi surface and band structure for normal metal and three kinds of topological semimetals, The close path (blue thin circle) interlocked with the nodal ring (thick circle) is also shown.

Although the theoretical aspects of topological insulator materials are adequately recognized, there are numerous difficulties and ongoing efforts in solving the experimental challenges. One of the foremost experimental problems faced by the researchers associated with the synthesis of those materials in the bulk forms is unnecessary bulk residual carriers due to intrinsic defects. The benefit of nanostructured topological surface states is that they reduce the effect of unwanted bulk electronic states in transport measurements as much as possible, thus increasing the surface-to-volume ratio to facilitate the contribution of topological surface or edge states. Therefore, material dimensions are crucial in the surface-dominant transport regime with a view to take advantage of the surface electrons' invaluable properties. One more advantage of the nanostructured materials is the easy modulation of Fermi level *via* field effect gating (FEG) which is difficult in the case of bulk crystal because of the large volume. Together with the sizeable surface to volume ratio in nano TI, FEG ensures surface dominated electron transport. Additionally, the extraordinary morphology of TI nanomaterials provides control over the topological surface states in reduced dimensions such as nanoribbons [1, 2], nanoplates [3], nanorods [4], nanowires [5], nanotubes [6], nonorings [1] and quantum dots [7]. Bi_2Te_3

CHAPTER 11

The Advancement in Research and Technology with New Kinds of Hollow Structures

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Abstract: Hollow structures are one of the most highlighted topics of research in nanotechnology. These hollow structures can be in the form of nanospheres, nanocages, nanorods, nano boxes, *etc*. They can be single-layered or multi-layered, with different kinds of doping. All these variations in hollow structures open up various fields of research, from biomedicines to optoelectronics. With the discovery of hollow structures like carbon buckyball, nanotubes, *etc*., several application-based -research was carried out, both theoretically as well as experimentally. Modifications are observed in the properties of a material when formed in a hollow shape like better conductivity, trapping capacity, catalytic effect, *etc*. These properties were the highlight of the studies. This field is still under investigation, and there is a lot of scope for new possibilities in the future. This chapter covers the basic information about different kinds of hollow structures like carbon buckyball, variations in their properties, along with recent developments and their applications. This chapter also includes detailed research about buckyball structures of ZnO, ZnS, and Al-doped ZnO using simulations with their comparative study and future applications.

Keywords: Al-doped ZnO, Buckyball, Hollow structures, Nanocages, ZnO, ZnS.

INTRODUCTION

Hollow structures came into the limelight due to their wide range of applications. These structures have a huge number of applications because of their configurable pore size, high value of the specific surface area, and large surface-to-volume ratio [1]. For example, in the green and sustainable energy conversion system with better efficiency and minimum cost, hollow nanostructures have proven to be excellent electrocatalysts [2]. In the field of biomedicines, spherical hollow

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structures are at the top. Due to their desired shape, they can be used as a drug delivery tool or in biosensors and bioimaging devices [3]. They also have several other applications in the areas of optoelectronic devices, water treatment, armoury, energy storage devices, sensors, *etc*.

Hollow structures can be in various shapes like spherical cages, square boxes, cylindrical rods, *etc*. Each kind of hollow structure has its own advantages and application. For example, nano boxes are used in the fields like fuel cells, batteries, *etc*., while nanowires are majorly used in Field-Effect Transistors, photocatalysis, *etc* [2].

Hollow structures of different elements have different properties of their own, which imply specifications in their applications. Among hollow structures of different elements present in nature, carbon is one of its kind, with a huge range of applications. Carbon nanomaterials have some very interesting and important qualities like good mechanical and chemical stability, a large value of electrical conductivity, *etc* [4]. These properties grab the attention of researchers to explore more. Different kinds of hollow structures made up of carbon atoms are known as Fullerenes. It can be a hollow-sphere or a hollow-tube, *etc*. The study of fullerene is very vast due to the presence of a huge range of possible structures and isomers. Two different carbon hollow structures, carbon nanotube and carbon buckyball, are shown below in Fig. (**1**).

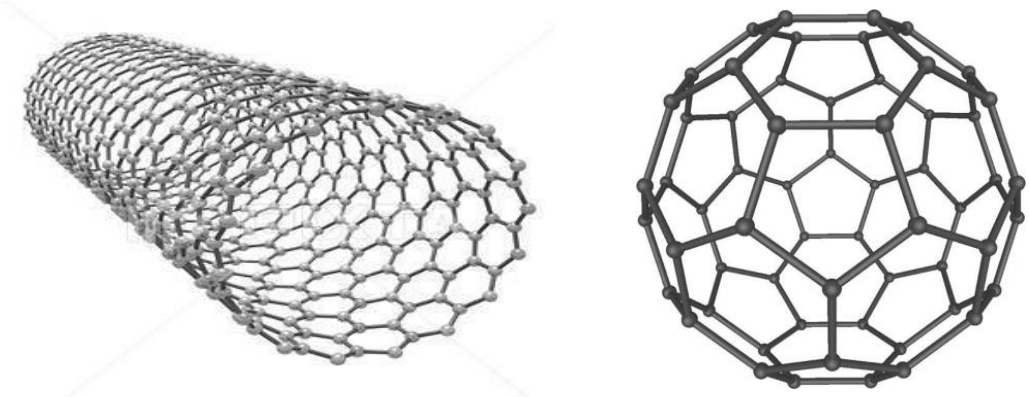

Fig. (1). (a) Hollow cylindrical structure of carbon nanotube [Photos by: PIXTA "Carbon nanotubes molecular 3d structure", Eugene Sergeev/ PIXTA, Copyright: PIXTA]. (b) Hollow spherical structure of carbon buckyball [Photos created by Michael Ströck (mstroeck), "A 3D model of a C-60 molecule", on 6th of February, 2006, by using iMol for Mac OS X and Photoshop CS2].

Among different kinds of Fullerenes, Buckminsterfullerene with 60 carbon atoms (Buckyball) is one of a special kind. This structure has mesmerized researchers from around the world since its discovery [4, 5]. The carbon buckyball structure

(C_{60}) is made up of carbon atoms arranged in six-fold rings, where few are replaced by some five-fold rings in the hollow-cage-like structure. There are 20 hexagons and 12 pentagons in this structure, where no two pentagons share a vertex [6]. The Swiss mathematician Leonhard Euler showed that a geodesic structure must have 12 pentagons to form a spheroid, where the number of hexagons may vary. This outcome in the 18th century led to some specifications in the fullerene structures. The fullerene structures are represented by 'C_n' where $n \geq 20$, with 12 pentagonal faces, 3 connected vertices, and 3n/2 number of edges. With this formula, it could be verified that C_{60} has 20 hexagonal faces while C_{70} has 25 [4]. The Isolated Pentagon Rule (IPR) is followed for the formation of stable fullerenes. This rule states that *only when the pentagons at the surface are separated, a non-reactive and stable fullerene is formed*. There are several reported works on buckyball structures with different numbers of carbon atoms. As we know, the buckminsterfullerene structure consists of 60 carbon atoms. Thus, C_{60} with only one isomer is the smallest stable fullerene structure. Other than that, C_{20}, C_{26}, C_{28}, C_{70}, C_{74}, C_{90}, *etc*., are also present. The difference in their stability and symmetry are discussed in various publications [7]. Fullerenes like C_{20} or C_{36} have formed already, but due to their high reactivity, the study is possible only under some special environment [8].

Other advances in the field of fullerene include variations like fullerene dendrimers, fullerene-substituted acetylenic polymers, endohedral metallo-fullerenes, *etc*. These variations have applications like tumour treatment, chromatographic purification, *etc* [9].

There are some previously reported works on the buckyball structures with not only carbon atoms but others as well. In some cases, one of the atoms of carbon is replaced by another atom, and in other cases, more than one is replaced. Later, a whole bunch of buckyballs with different elemental atoms were formed. For example, Boron Buckyball structure. Before Boron, some other elements were also visualized as buckyballs like Uranium, Silicon, Molybdenum disulfide, Gold, Tin, *etc* [10]. However, these structures were not that close to the resemblance of Carbon Buckyball. The Boron buckyball structure with 80 boron atoms resembles the most to C_{60}. Theoretical discovery of B_{80} was done in 2007, and after seven years of this discovery, experimental evidence of its existence came to light. This particular structure showed its application in hydrogen storage systems. Buckyball structures of multi-walled Boron Nitride were also reported earlier [11].

The hollow microspheres of Triple-shelled $ZnO/ZnFe_2O_4$ were recently explored due to their sensing capacity of acetone vapour. The unique heterojunction of ZnO and $ZnFe_2O_4$ with high specific surface area proved to be superior sensors for acetone vapour [12].

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Dibya Prakash Rai

Dr. Dibya Prakash Rai, is currently working as an assistant professor in the department of Physics, Pachhunga University College Campus (constituent of Mizoram University). He completed his PhD degree from Mizoram University (2013) and Post doctorate from Computational Science Research Centre (CSRC), Beijing China (2014). Dr. Rai is a dynamic researcher, he has published more than 200 papers in national/international peer reviewed journals (Elsevier, Springer, Wiley, Taylor & Francis, RSC, ACS, etc). He has also provided his service in reviewing a number of articles from journals of reputed publishers like Elsevier, Springer, Wiley, Taylor & Francis, RSC, ACS, etc. He has received 4 major projects from DST-India and UGC-India. Out of the four projects two are international major projects in collaboration with the scientists from Institute of Microelectronics Technology High Purity Materials Russian Academy of Sciences Moscow and National University of Uzbekistan, Tashkent Uzbekistan. Dr. Rai has expertise in Density Functional Theory (DFT) and he can efficiently use some of the DFT-based computational codes like WIEN2K, SIESTA, CRYSTAL17, VASP, Quantum Espresso, SPR-KKR, FPLO etc. Currently, he is supervising 4 PhD scholars working with DFT in analyzing and predicting different functional properties of computationally efficient materials. He is the editorial board member of Current Chinese Nanotechnology (Bentham Science) and associate editor of SENHRI, a multi-disciplinary journal of Pachhunga University College, India.