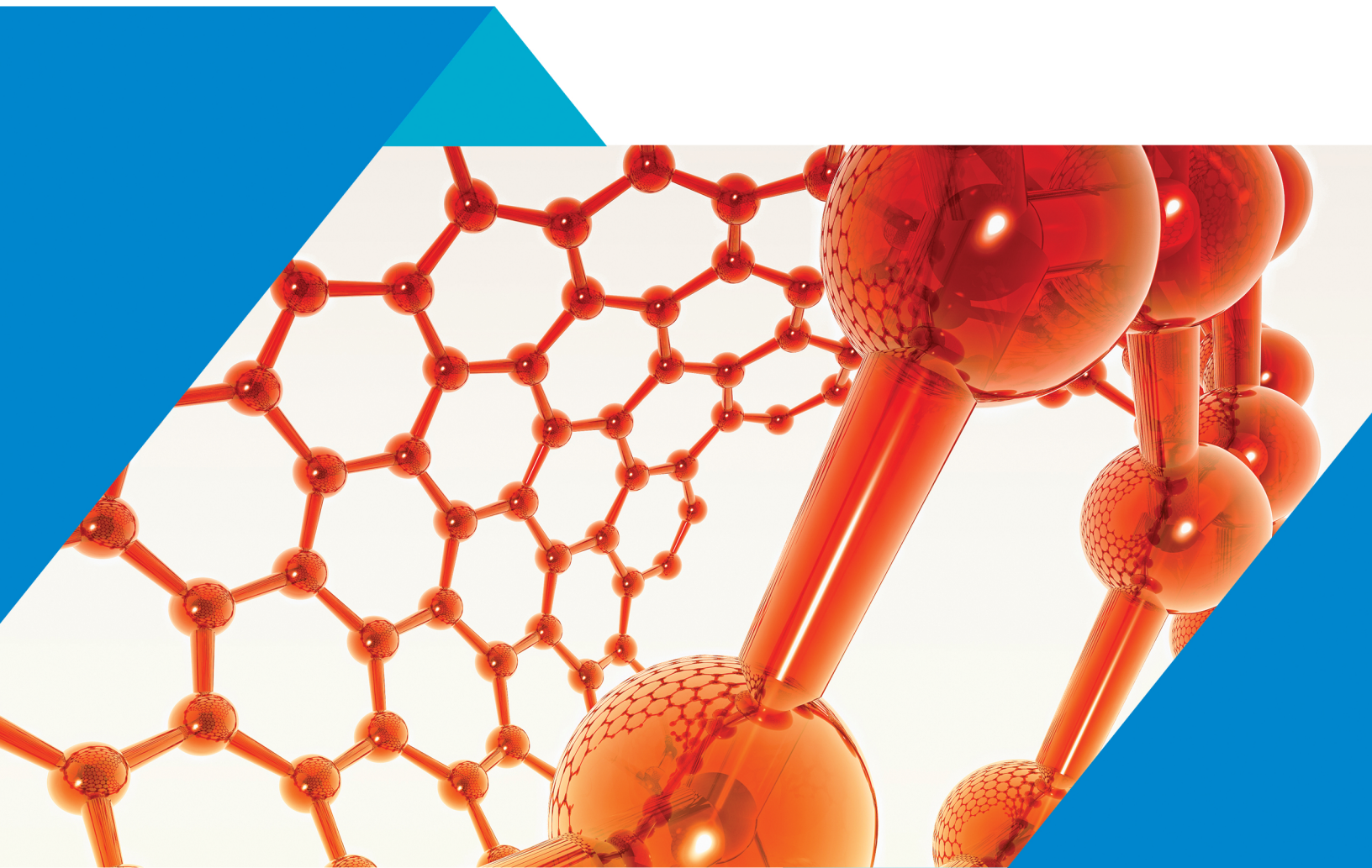


ADVANCED MATERIALS AND NANO SYSTEMS:

THEORY AND EXPERIMENT - PART-3



Editors:

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Advanced Materials and Nano Systems: Theory and Experiment

(Part 3)

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CONTENTS

FOREWORD	i
PREFACE	iii
LIST OF CONTRIBUTORS	viii
CHAPTER 1 ROLE OF PLASMONIC METAL-SEMICONDUCTOR HETERO-STRUCTURE IN PHOTO CATALYTIC HYDROLYSIS AND DEGRADATION OF TOXIC DYES	1
<i>Shomaila Khanam and Sanjeeb Kumar Rout</i>	
INTRODUCTION	1
PLASMONIC DYNAMICS	3
SYNTHESIS PROCESS OF METAL-SEMICONDUCTOR PLASMONIC PHOTOCATALYST	6
FACTORS AFFECTING PLASMONIC NANOSTRUCTURE	9
Geometrical Shape	9
Size of the Plasmonic Nanocrystal	10
Material Composition	11
Ratio of Noble Metal to the Semiconductor	12
PLASMONIC METAL-SEMICONDUCTOR HETEROSTRUCTURE FOR PHOTOCATALYTIC HYDROLYSIS OF AMMONIUM BORANE	12
PLASMONIC METAL-SEMICONDUCTOR HETEROSTRUCTURE FOR DYE WATER TREATMENT	14
PROPOSED MECHANISM	16
Schottky Barrier	17
Direct Electron Transfer	18
Enhanced Local Electric Field	19
Plasmon Resonant Energy Transfer	20
PROSPECTS AND FUTURE	21
Plasmonic as Energy Inputs	21
Quantum Dots and Quantum Dots	22
Communication with Plasmonic	23
Plasmonic Nanoparticles in the Treatment of Cancer	24
Plasmonic in Desalination of Water	24
Plasmonic Invisible Photodetector	26
Electrochromic Smart Window	26
Plasmonic Sensing	27
Antimicrobial Coating	27
LIMITATIONS AND CHALLENGES	28
CONCLUSION	29
ACKNOWLEDGMENTS	29
REFERENCES	29
CHAPTER 2 BAZRO₃-BASED CERAMICS AND CERAMIC COMPOSITES AS SMART MATERIALS FOR ADVANCED APPLICATIONS	38
<i>D. Vignesh and Ela Rout</i>	
INTRODUCTION	39
SYNTHESIS STRATEGY OF CERAMICS	41
CERAMICS AND CERAMIC COMPOSITES IN PC-SOFC TECHNOLOGY	42
Grotthuss Mechanism in Proton Conductors	47
BaZrO ₃ Based Proton Conductors (PCs) for Fuel Cells	48
BaZrO ₃ -based Thin Film Composites for Fuel Cell Technology	54

ADVANCED CERAMIC COMPOSITES IN DEFENCE	56
Mechanism of Course-Changing Bullets	57
BaZrO ₃ Based Ceramic Composites in Defence	58
CERAMIC COMPOSITES AS PHOTOCATALYSTS FOR HYDROGEN PRODUCTION	60
Photocatalytic Mechanism for Hydrogen Production	61
BaZrO ₃ Based Ceramic Composites for Hydrogen Production	63
CERAMIC PHOSPHORS FOR MEDICAL APPLICATIONS	66
Optical Activity of Ceramic Phosphors	68
BaZrO ₃ -based Ceramic Phosphor for Radiation Shielding	70
CERAMIC MATERIALS FOR MICROWAVE DIELECTRIC RESONATORS	74
Functioning of Microwave Dielectric Resonator	75
BaZrO ₃ -Based Ceramic Materials as Microwave Dielectric Resonators	76
Critical Shortcomings and Future Scope	79
CONCLUSION	80
ACKNOWLEDGMENT	81
REFERENCES	81
CHAPTER 3 A HIGH-CAPACITY ANODE MATERIAL FOR LITHIUM-ION BATTERIES IS SILI-GRAPHENE TYPE SiC₃	95
<i>M. Houmad, M. Khuli, A. El Kenz and A. Benyoussef</i>	
INTRODUCTION	95
COMPUTATIONAL DETAILS	97
RESULTS AND DISCUSSION	97
Electronic Properties of Li Adsorption on the Siligraphene	97
Li Adsorption and Diffusion on the Siligraphene	100
Li Diffusion Process	101
Voltage Profiles as a Function of Capacity for Siligraphene Li _x SiC ₃	101
CONCLUSION	104
REFERENCES	104
CHAPTER 4 AN INTRODUCTION TO THE FABRICATION OF WHITE LIGHT-EMITTING DIODES	109
<i>Naorem Premjit Singh and Yengkhom Rangeela Devi</i>	
INTRODUCTION	109
TYPES OF LEDS AND THEIR APPLICATIONS	111
CHARACTERISTICS OF A LIGHTING SOURCE	112
Color Rendering Index (CRI)	112
CIE Color Co-ordinates	113
Color Co-related Temperature (CCT)	115
Luminous Efficacy (K)	115
FABRICATIONS OF WHITE LIGHT-EMITTING DIODE	116
Mixing of Multiple LEDs Emitting Different Monochromatic Color	116
Advantages and Disadvantages	118
Mixing of an LED Chip with a Phosphor	118
<i>Luminescence</i>	119
<i>Phosphor</i>	120
DIFFERENT SYNTHETIC METHODS OF PHOSPHOR	120
Co-Precipitation Method	120
Hydrothermal/Solvothermal Method	121
Sol-gel Method	121
Combustion Method	121
Sonochemical Route	122

Microwave-assisted Synthesis	122
Solid State Method	122
Energy Transfer	123
Quenching of Luminescence	123
Thermal Quenching	124
COMBINATION OF BLUE EMITTING LED WITH A PHOSPHOR EMITTING YELLOW LIGHT	125
Advantages and Disadvantages	126
COMBINATION OF UV/NUV EMITTING LED WITH MULTIPLE PHOSPHORS EMITTING RED, GREEN AND BLUE COLOR	127
Advantages and Disadvantages	128
COMBINATION OF UV/NUV EMITTING LED WITH A SINGLE PHOSPHOR EMITTING BLUE AND YELLOW LIGHTS OR BLUE, GREEN AND RED LIGHTS	129
Doping of a Single Activator Ion into the Host Material	130
Doping of Multiple Activator Ions into the Host Material	134
CONTROLLING THE CONCENTRATIONS OF DEFECT AND REACTION CONDITIONS OF THE DEFECT-RELATED LUMINESCENT MATERIAL	135
ADVANTAGES AND DISADVANTAGES	135
CURRENT LIMITATIONS AND CHALLENGING	136
CONCLUSION	136
REFERENCES	137
CHAPTER 5 ELECTRONIC AND PIEZOELECTRIC PROPERTIES OF NON-METAL DOPED II-VI MONOLAYER COMPOUNDS	143
<i>Lalmuan Chhana, Zodinmawia, Ramesh Chandra Tiwari, Shivraj Gurung and Lalhriat Zuala</i>	
INTRODUCTION	143
COMPUTATIONAL METHODS	144
RESULTS AND DISCUSSION	146
Pristine Properties	147
Non-metal Doping	149
CONCLUSION	155
ACKNOWLEDGEMENTS	155
REFERENCES	156
CHAPTER 6 A THEORETICAL INVESTIGATION ON THE NEW QUATERNARY MAX- PHASE COMPOUNDS (Zr_{1-x}Ti_x)₃ALC₂ (WHERE X= 0-1)	159
<i>Habib Rached and Ismail Ouadha</i>	
INTRODUCTION	159
GENERALITIES ON THE MAX-PHASES	161
Chemical Elements	162
Crystal Structure	163
MAX Phases Properties	164
<i>Mechanical Properties</i>	165
<i>Electrical Properties</i>	166
<i>Thermal Properties</i>	166
Synthesis of MAX Phases	168
<i>Synthesis of Massive Samples</i>	168
<i>Synthesis of Thin Film</i>	169
Applications	169
RESULTS AND DISCUSSION OF THE FIRST-PRINCIPLE INVESTIGATIONS OF (Zr_{1-x}Ti_x)₃ALC₂) MAX-PHASE COMPOUNDS (X=0-1)	170

Details of the Employed First-principle Method	170
Structural Properties	171
Mechanical Behavior	177
Electronic Properties	182
Thermodynamic Properties	185
CONCLUSION	195
REFERENCES	195
CHAPTER 7 SURFACE SEGREGATION IN PT₃NB AND PT₃TI USING DENSITY FUNCTIONAL THEORY-BASED METHODS	202
<i>Kingsley O. Obodo, Lalrin Kima, Adedapo S. Adeyinka and Dibya Prakash Rai</i>	
INTRODUCTION	203
COMPUTATIONAL METHOD	206
RESULTS AND DISCUSSION	206
Surface Segregation in Pt ₃ X (111) Surface	206
Direct Exchange and Antisite Migration	207
Oxygen Adsorption on Pristine Pt (111) Surface	210
Oxygen Adsorption Energy on Pt ₃ X (111) Surface	211
CONCLUSION	214
ACKNOWLEDGEMENT	215
REFERENCES	215
CHAPTER 8 NANOPARTICLES AND ENVIRONMENTAL HEALTH	220
<i>Aparna Roy, Kumaresh Mandal, Shishir Tamang, Soni Subba, Saptaparni De, Divya Rai, Biswajit Roy and Rakesh Tamang</i>	
INTRODUCTION	221
NATURAL NPs	221
ENGINEERED NPs	222
THE FATE OF NPs IN THE ENVIRONMENT	223
Physiochemical Transformation	224
Biological Transformation of NPs	225
NPs IN SOIL	225
Source of Soil NPs	226
Effect on Soil	226
Soil Remediation with NPs	233
NPs IN THE AQUATIC ENVIRONMENT	234
Source	234
Effect of NPs in Water	235
Remediation of Contaminants in Water	236
NPs IN AIR	237
Source	237
Effect of NPs in the Air	239
Remediation of Pollutants in the Air by NPs	240
LIMITATIONS AND FUTURE PERSPECTIVES	240
CONCLUSION	241
ACKNOWLEDGMENTS	242
REFERENCES	242
CHAPTER 9 INVESTIGATION FOR OPTIMUM SITE FOR ADSORPTION AND POPULATION EFFECT OF LITHIUM ON SILICENE MONOLAYER	249
<i>Lalhumhima, Lalmuanchhana, Shivraj Gurung, Lalrinthara Pachuau, Lalmuanpuia Vanchhawng, Zodinmawia and Lalhriat Zuala</i>	

INTRODUCTION	249
COMPUTATIONAL DETAILS	251
RESULTS AND DISCUSSIONS	252
CONCLUSION	256
REFERENCES	256
CHAPTER 10 STRATEGIES FOR SYNTHESIZING METAL OXIDE NANOPARTICLES AND THE CHALLENGES	260
<i>Harish Bishwakarma, Mukul Anand and Alok Kumar Das</i>	
INTRODUCTION	260
NANOSCIENCE AND NANOTECHNOLOGY	261
NANOTECHNOLOGY IN THE 20TH CENTURY	262
NANOMATERIALS CLASSIFICATION	262
DIFFERENT METHODS OF GENERATION OF NPs	263
BOTTOM-UP APPROACHES	264
Sol-gel Method	264
<i>Advantage</i>	265
<i>Disadvantage</i>	265
Hydrothermal Method	266
<i>Advantages</i>	267
<i>Disadvantage</i>	267
Chemical Vapour Deposition Method	267
<i>Advantages</i>	269
<i>Disadvantages</i>	269
TOP-DOWN APPROACHES TO THE SYNTHESIS OF NPs	269
Ball Milling Method	269
<i>Advantage</i>	270
<i>Disadvantage</i>	270
Laser Ablation Method	271
<i>Advantages</i>	272
<i>Disadvantages</i>	272
Electrochemical Discharge Methods	273
<i>Influencing Process Parameter of ECDP for NPs Synthesis</i>	275
<i>Advantage</i>	276
<i>Disadvantage</i>	276
CONCLUSION	276
ACKNOWLEDGMENTS	277
REFERENCES	277
CHAPTER 11 HETEROGENEOUS SEMICONDUCTOR PHOTOCATALYSIS FOR WATER PURIFICATION: BASIC MECHANISM AND ADVANCED STRATEGIES	283
<i>Naorem Premjit Singh and Yengkhom Rangeela Devi</i>	
INTRODUCTION	283
PHOTOCATALYSIS AND ITS BASIC MECHANISM	284
STRATEGIES TO IMPROVE THE CATALYTIC EFFICIENCY AND LIGHT ABSORPTION	288
DOPING OF METAL OR NON-METAL	288
Metal Ion Doping	288
Non-metal Doping	290
SURFACE PLASMON RESONANCE	291
CONSTRUCTION OF SEMICONDUCTOR HETEROSTRUCTURE	292
Z-SCHEME HETEROSTRUCTURE FORMATION	294

FACTORS AFFECTING THE CATALYTIC EFFICIENCY	298
Effects of Particle Size, Morphology and Crystal Structure	298
Effect of pH	299
Effect of Catalyst Concentration	299
Effect of Pollutant Concentration	300
Effect of Light Intensity	300
Effect of Temperature	301
Effect of O ₂ Concentration	301
CONCLUSION	302
REFERENCES	302
SUBJECT INDEX	534

FOREWORD

First of all, I would like to congratulate Dr. Dibya Prakash Rai for successfully publishing a series of two books, Part 1 & 2, entitled “Advanced Materials and Nano Systems: Theory and Experiment”. Following the success of the previous two books, the editor is motivated for the third edition. I believe this third edition of the book will receive grand success with the support of two dynamic researchers Dr. Kingsley O. Obodo and Dr. Jitendra Pal Singh. The subjects covered in this book range from bulk to nanoscale materials at all applied levels, including some of the most significant and current issues in materials science and nanosystems. It includes introductory chapters, discussions of fundamentals, and problems with in-depth solutions. It covers practically all of the subject matter in the concerned discipline. This book walks readers through using the most basic features or utilities of a program or method. I have had the pleasure of reading several extremely fascinating chapters on the creation of nanoparticles. These chapters concentrate on the potential for reducing environmental pollution and the application of nanosystems for energy harvesting. This book also addresses the existing constraints and difficulties in the development of nanotechnology. It offers a perspective on its potential future development and application in overcoming the current energy crisis, in medicine, and the evolution of digital technology, *etc.* Over the past 20 years, there has been a tremendous increase in nanotechnology research, which focuses on the science, technology and engineering of nanoscale materials. Nanotechnology has seen a rise in global investment from all sectors, including the public, businesses, governments, institutes, *etc.* Developed nations, including the United States, Germany, the United Kingdom, France, and others, are working to advance research and development in this crucial sector and creating the scientific understanding required to address queries and worries about the potential effects of this nanotechnology on the environment, health, and safety. In both clinical care and biological research, nanotechnology is gaining importance and prominence. Nanotechnology is anticipated to have a bright future in many facets of medicine, much like other sciences. Nanoparticles can deliver medications into cells to reach illness areas because of their tiny size, which raises local drug concentrations and lowers systemic toxicities. The diversity and promise of nanotechnology products thrill me. Still, I am also conscious of the challenging research required to provide solid answers to important queries regarding their potential effects on human health and the environment. To consider the possible influence on human health that this new and promising kind of material science represents, many of the established assumptions of safety and health must be re-examined, if not modified. Technological advancements have made it possible for humans to view atoms, manipulate them individually, alter their positions one at a time, and utilize them to generate new codes. The challenge was and continues to be, how to handle the system at an atomic scale. This is a challenging undertaking, but it is still feasible. Electronics experts who work with integrated circuits participated in the race for shrinking as well as moving circuitry from micro to submicron levels and reaching ever-closer to the nanoscale. The concept of electronics will need to be completely rethought if researchers ultimately get to the point where a single electron serves as the foundation for electronics (nano-transistor). Since other scientific disciplines like mechanics, optics, chemistry, and biology have also begun to create their nanoworlds, which we now refer to as nanosystems, this evolution is not simply affecting electronics. The silicon airbag's accelerometer in automobiles refers to the example of a mass-produced nanosystem. As far as I am concerned, the application of nanosystems as nanomotors, nanorobots or nano-transistor has not been realized yet. This is because development from lab-scale to commercial-scale will take some time. In actuality, the energy situation is what is most concerning. Rapid energy use eventually threatens the viability of life and may even bring about the end of the contemporary planet one day. As a result, one should seek renewable energy sources or locations where energy may be produced without

ii

harming the environment. We may find various promising energy harvesting technologies in the field of materials science, such as thermoelectricity, piezoelectricity, solid-state batteries, *etc.* Since revolutions and technological advancement do not come naturally to people or communities, it is to be expected that certain worries will accompany these developments. We must be cognizant of the current difficulties and the issues at hand. I want to invite the readers to continue reading this book. Let's explore this new universe in all the forms of materials science while maintaining the realism of an engineer and the creative progress.

Victor Sunday Aigbodion

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PREFACE

The first two volumes of the book “Advanced Materials and Nano Systems: Theory and Experiment Parts 1 and 2” were a great success. I received numerous overwhelming responses and best wishes from both the readers and well-wishers. This has motivated me a lot and encouraged me to work on the third volume of “Advanced Materials and Nano Systems: Theory and Experiment”. Furthermore, I am supported by two dynamic and experienced scientists who are working in the field of nanoscience and nanotechnology, Dr. Kingsley O. Obodo from South Africa and Dr. Jitendra Pal Singh from India. They helped me in the selection and scrutiny of the best 11 chapters. The best 11 selected chapters contain very popular topics related to novel nanomaterials for drug delivery, environmental safety, industrial biocatalysts, energy harvest, electronics, *etc.* As usual with previous volumes of the book, this upcoming edition will be very exciting and will include interesting chapters in the said field from very expert authors and researchers from all over the world. The title of the book, “Advanced Materials and Nano Systems: Theory and Experiment”, is fascinating and truly subject-specific on an international level, which easily captures the attention of readers who are working in the field of nanoscience and nanotechnology. This book also covers a wide range of scientific topics, ranging from bulk materials to nanomaterials and their applications. Advances in materials science *via* nanotechnology have resulted in significant advancements in a variety of disciplines, such as biomedicine, biomaterials, biosensors, nanoelectronics, energy production, construction, packaging, food, health care, automotive, and defense, among others. Knowing the rapid popularity of nanotechnology and its benefits, we have decided to compile this third edited book; hence, we have invited numerous chapters from active researchers who are working in the thrust areas of nanomaterials.

The opening of Chapter 1 by Shomaila Khanam and Sanjeeb Kumar Rout contributes to the role of plasmonic metal-semiconductor heterostructure in photocatalytic hydrolysis and degradation of toxic dyes. In this experimental work, they have reported the efficiency of plasmonic metal-semiconductor heterostructure as a superior material for photocatalytic water splitting activity for clean and cheap energy generation *via* the localized surface plasmon resonance (LSPR) method. The LSPR generation by these kinds of materials has proved to be very efficient in the photocatalytic hydrolysis of the hydrogen-rich compound, photocatalytic water splitting, and photocatalytic degradation of organic dyes.

Chapter 2 gives details on BaZrO₃-based ceramics and composites as smart materials for advanced applications. This chapter's introductory section provides a brief history of ceramic materials and their schematic development. Ceramic materials have been used in everything from pottery to pellets, ammunition to antennas, and electrolytes to electronics. This chapter focuses on the barium zirconate (BaZrO₃)-based ceramic composite as smart materials for advanced applications targeting the energy sector, photocatalyst for hydrogen production, a smart bullet in defense, and microwave dielectric resonators for wireless communication systems, respectively.

In Chapter 3, Houmad *et al.* used density functional theory (DFT) to investigate the 2D graphene-like nanomaterial Sili-graphene as a high-capacity anode material for lithium-ion batteries. Herein, they predict silicon-doped graphene (Siligraphene) as an efficient anode material for potential Li-ion batteries (LIBs). They reported the most stable lithium adsorption at different sites in the hexagonal structure of the silica sheet. Also, they have calculated a very important parameter, the Li-ion migration efficiency in siligraphene, for the LIBs. The reported diffusivity was found to be about 0.095 eV for Li on top of silicon atoms and about

0.223 eV for oxygen, indicating rapid charging and discharging processes. They also report a minute variation in the voltage essential for its potential applications in LIBs.

In Chapter 4, Singh and Devi present an introduction to the fabrication of white light-emitting diodes. They have highlighted the fascinating and eco-friendly sources of white light-emitting diodes due to their high energy savings in various fields, including lighting, architecture, medicine, *etc.* In this study, they focus on the development and fabrication of cheap and eco-friendly light sources (white light emitting diodes), as the lighting sector is one of the most important and attractive fields because it consumes a large amount of electricity, about 15–20% of total electricity production in the world. They emphasize the two fabrication methods for white light-emitting diodes. The luminous efficiency and rendering index of a lamp are influenced by the type of fabrication. In this chapter, the different fabrication methods for white light-emitting diodes are discussed. The chapter is divided into three parts. The first part is devoted to the general introduction of the light-emitting diode (LED), its working principle, and its applications. In the second part, the characteristics of light, including CIE, colour temperature, and rendering index, are briefly discussed. In the last part, the different methods of fabrication and their advantages and disadvantages are discussed.

Chhana *et al.* investigated the electronic and piezoelectric properties of non-metal doped II-VI monolayer compounds in Chapter 5. In this study, they have used spin-polarized density functional theory (DFT) to calculate the electronic and piezoelectric properties of the dynamically stable II–VI monolayers: ZnO, ZnS, CdO, and CdS. They also doped the monolayer system with boron and carbon to analyze the variation of these properties for their integration into potential technological applications. They report the half-metallicity of the above-stated monolayers when doped with B and C atoms. The presence of half-metallicity in doped monolayers is promising for spintronic applications. The B-doped ZnO and ZnS monolayer results in negative structural stiffness and negative piezoelectric tensors, while C-doping provides stable and enhanced elastic as well as piezoelectric properties of the monolayer.

Habib Rached and Ismail Ouadha contributed to Chapter 6. They reported a theoretical calculation on the new quaternary MAX-phase compounds $(\text{Zr}_{1-x}\text{Ti}_x)_3\text{AlC}_2$ (where $x = 0-1$). They mainly studied the structural, electronic, mechanical, and thermodynamic properties of the MAX phases $(\text{Zr}_{1-x}\text{Ti}_x)_3\text{AlC}_2$ compounds by using the full-potential plane-wave FP-LAPW method as implemented in the Wien2k code. They have reported the importance of exchange-correlation functionally, in which they have adopted the most commonly adopted exchange-correlation (XC) energy of all electrons within the Perdew-Burke-Ernzerhof parametrization. They reported an agreement between their theoretical findings with the experimental results. They studied the formation energy to check the ground-state stability of the system. The negative value of formation energy confirms the stability of their compounds. The calculation of the electronic structure in the MAX phase found it to be metallic with prominent *p-d* hybridization. They have also studied the elastic properties by calculating the elastic constants using the Hex-elastic package. They report the mechanical stability of the MAX-phase compound. This chapter also includes a study of the temperature and pressure effects on bulk modulus, Debye temperature, and heat capacity at constant volume (CV) and constant pressure (CP), respectively.

Chapter 7 highlights the work of Obodo *et al.* Here, they studied the surface segregation in Pt_3Nb and Pt_3Ti using density-functional-based methods. In their DFT-based studies, they reported the surface segregation of the stoichiometrically ordered Pt_3X system because, due to the endothermic process of direct exchange in Pt_3Ti , the exchange of surface atoms is forbidden in the ground state. Direct exchange in Pt_3Nb was also reported as exothermic

surface segregation. They describe an intriguing phenomenon in which an overlayer forms on the Pt_3X system as a result of PtX migration into an antisite defect in an off-stoichiometric configuration. Doped surfaces, rather than pristine structures, have the optimal oxygen adsorption energy for Pt(111). The instability was found in the Pt_3X system with the X-skin surface configuration. While the Pt-skin configuration improved the adsorption energy, the inclusion of the antisite configuration improved ORR activity for both Pt_3X systems. Finally, they found that Pt_3Nb had better catalytic performance than Pt_3Ti .

Chapter 8: This chapter is contributed by Roy and his group, and their work is a review of the nanoparticles and their manipulation for capturing the toxic elements from the air to keep the environment healthy. The high surface area to volume ratio of extremely small particles (nanoparticle size between 1-100 nm) accounts for their distinct behavior. They report the importance of artificially synthesized and manipulated nanoparticles as per the specific needs. Alarming impact on the environment as a result of the massive use of nanoparticle-based industrial products degrades environmental health. Environmental health is determined by the quality of the air, water, and soil, which is reflected in a healthy ecosystem and its biodiversity. The effects of nanoparticles released into the environment vary depending on their type, surface coating, and degree of environmental transformation. Some nanoparticles are harmful to the environment, and some are beneficial. Some of the nanoparticles in the environment get bioaccumulated in plants and animals, disturbing their growth and productivity. Recognizing the potential of nanotechnology in manipulating nanoparticles, remediation has proven to be an effective technique for removing some toxic elements and compounds from the environment, thereby providing a way to reduce pollution efficiently. In this review, they have presented an overview of the sources, fate, and effects of nanoparticles available in air, water, and soil. They also promise the long-term assessment of nanoparticles and the formulation of strict guidelines for their usage by the concerned industries for better environmental health and, in turn, a healthy ecosystem.

Chapter 9 includes the research work of Lalthumhima *et al.*, who reported the optimal site for the adsorption and population effect of lithium on a silicene monolayer. This is a purely theoretical work based on density functional theory's first principles. They report the most stable site for adsorbing the lithium ions in the silicene monolayer. They discovered the active site by calculating the minimum adsorption energy required to place the lithium atom in various possible locations. They reported that the center of the hexagonal structure in silicene was the most favorable site. Using transition state search (TSS), the optimized stable state and a low diffusion energy barrier (DEB) of 0.348 eV were indicated. The metallic property of pristine silicene is maintained throughout Li atom adsorption.

Chapter 10 details the methods for synthesizing the metal oxide nanoparticles as well as the difficulties. They have emphasized the significance of nanoscience and nanotechnology in raising the standard of living. The advancement of nanotechnology is facilitated by the new class of materials known as nanoparticles (NPs). The NPs should have at least one particle dimension between 1 and 100 nm. The synthesis methods can change the size and structure of NPs, which are important in molecular biology, physics, organic and inorganic chemistry, biology, medicine, and materials research. Synthesis techniques can produce NPs with high surface areas, increasing their value and supplying necessary features like surface reactivity. They discussed the various methods for creating nanoparticles. They concentrate on the two parts, top-down and bottom-up, which are categorized according to the raw materials used to create the NPs in this study. An overview of synthesis techniques and their uses in nanotechnology and nanoscience was given in this review. The electrochemical discharge procedure, a revolutionary method for creating NPs, is covered in detail. Tables are used to discuss the synthesized materials, including ZnO, carbon, graphene, and other metal oxides,

as well as their composites. Finally, the difficulties, benefits, drawbacks, conclusions, and synthesis of NPs are examined.

The final chapter, 11 by Singh and Devi, discusses the Heterogeneous semiconductor photocatalysis for water purification: Basic mechanism and advanced strategies. In this chapter, they have discussed the different techniques based on the semiconductor photocatalysis for water purification. They specially emphasize the contribution of water pollution *via* anthropogenic activities, human waste, utilization of toxic chemicals in agricultural activities *etc.*, and the solution of purification of water to make it drinkable with the help of nanotechnology. Heterogeneous semiconductor photocatalysis is the most effective green method in this regard because it enables it to degrade into nonhazardous products like CO₂ and H₂O without releasing any harmful residue. Therefore, understanding the knowledge of photocatalysis mechanism is very significant to enable further improvement. Hence, this chapter presents the basic mechanism of photocatalysis, its drawbacks and the advanced strategies to improve the catalytic efficiency. Finally, some of the important factors that influence catalytic activity have also been discussed.

In the current book, various computational and experimental techniques of recent advances in materials science are presented, with a primary emphasis on the synthesis, characterization, and analysis of functional properties of novel nanomaterials to address a variety of problems encountered on a daily basis. This book's timely release should be of interest to scholars, professors, and students in the field of nanotechnology. Given the increasing demand for nanomaterials in various human activities, it is anticipated that the topic of advanced materials and nanosystems from theory and experimental perspectives will continue to be at the forefront of cutting-edge research in science and technology for the foreseeable future. With a focus on the synthesis, characterization, and analysis of functional properties of innovative nanomaterials to solve a variety of problems encountered on a daily basis, the current book presents numerous computational and experimental approaches to recent breakthroughs in materials science.

The timely publication of this book (Part 3) should be of great interest to professionals, educators, researchers and students in the field of materials science and nanotechnology. It is projected that the subject of nanomaterials and nanotechnology will remain at the forefront of cutting-edge research in science and technology for the foreseeable future, given the growing integration of nanomaterials in numerous human activities. I also want to express my gratitude to the editorial team of the Bentham Books for their prompt release of Parts 1 and 2 of “Advanced Materials and Nano Systems: Theory and Experiment”, which gave me the confidence I needed to quickly collect the chapters compile them and finish Part 3.

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CHAPTER 1**Role of Plasmonic Metal-semiconductor Heterostructure in Photo Catalytic Hydrolysis and Degradation of Toxic Dyes****Shomaila Khanam¹ and Sanjeeb Kumar Rout^{1,*}**¹ *Department of Physics, Birla Institute of Technology, Mesra, Ranchi, Jharkhand, India*

Abstract: Plasmonic metal-semiconductor heterostructure has become the most prominent content for water splitting by photocatalytic means. It is thought to be an effective, clean, and affordable energy source. Hydrolysis, water splitting, and destruction of organic dyes have all demonstrated the high efficiency of LSPR formation by these materials. A noble metal combined with a low bandgap semiconductor makes for the perfect photocatalyst. In this case, both semiconductors and noble metals can absorb visible light. They are prone to producing positive and negative pairs and inhibit their recombination, causing the resulting electron-hole pairs to interact with the chemicals in the immediate environment, thereby increasing photocatalytic activity. The strong SPR's combined effect with the efficient separation of photogenerated electrons and holes supported by noble metal particles can be credited with the increased photocatalytic activity. It has become a useful method for overcoming the limitations of conventional photocatalysts and promoting photocatalytic mechanisms.

This book chapter has three main goals: briefly describing plasmonic dynamics, explaining the preparation techniques, analyzing the key characteristics of the plasmonic metal nanostructure that influence photocatalysis, summarizing the reported literature, and offering an in-depth explanation of the four fundamental plasmonic energy transfer process.

Keywords: Ammonia borane, Localized surface, Plasmon resonance effect, Photocatalytic degradation, Plasmonic, Photocatalytic hydrolysis.

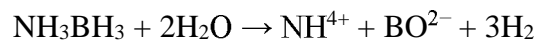
INTRODUCTION

Hydrogen is recognized as a green fuel on a worldwide scale because of its high energy density, ability to emit no harmful waste products, and status as an alternative to petroleum distillates. In recent years, hydrogen has emerged as a

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crucial fuel, satisfying society's need for fuel with minimal environmental impact. Sadly, there is still a roadblock in the way hydrogen becomes a practical source of energy due to its safe and affordable storage. In addition, applications for hydrogen outside of transportation are as important to take into account; these include its use in fertilizer production, metal treatment, food processing, petroleum refining, and food processing. Hydrogen has high gravimetric and volumetric density, and can be stored in a variety of solid-state hydrogen storage materials, including ammonia borane (NH_3BH_3 , AB), sodium borohydride, ammonium borohydride, decaborane diammoniate of diborane, and others. Ammonia borane is regarded as a standout candidate for hydrogen applications [1 - 3] because of its many benefits, like its sufficient hydrogen content (19.6% wt), lower molecular weight (30.7 g mol⁻¹), stability in solution, solubility in water, and tendency to undergo hydrolysis reaction. In order to generate three equivalents of hydrogen from one mole of AB by photocatalysis, several homogeneous catalysts have been produced. For instance, Goldberg *et al.* observed that an iridium catalyst from AB released hydrogen quickly within 20 minutes of being at ambient temperature [2, 4]. By using photocatalytic hydrolysis of AB, Baker and colleagues experimented with the acid-induced hydrolysis of AB [5] and the effectiveness of a nickel-based catalyst in the release of 94% hydrogen after 3 hours. Numerous academic papers by Xu and Chandra [6], Manners [7], and Jagirdar [8] proved the heterogeneous photocatalysis of ammonia borane for hydrogen release through combined noble metals and nanoceramics composites is very effective. Plasmonic photocatalyst is the name given to the heterogeneous catalyst consisting of noble metals and semiconductors. When the light wave of plasmonic resonance strikes them, they begin to oscillate, which eventually results in LSPR (a bound electromagnetic field). The best examples of these materials with negative real permittivity are silver and gold. Plasmonic nanoceramics have demonstrated their use for everything from organ imaging to sensors. Plasmonic materials have a special ability to create an increased electric field at the metal-semiconductor interface, which makes them ideal photocatalysts. Its ability to generate photoacoustic waves and heat is beneficial in the medical sector, in which it is employed to treat cancer and image organs. The usage of metal-semiconductor composite as a photocatalyst is very common. When exposed to light, photocatalysts can accelerate photochemical processes and start the reduction and oxidation process. It may remove a variety of toxic colours from water while also serving as a disinfectant. By starting the dehydrogenation reaction and releasing hydrogen from the hydrogen-stored compounds, it aids in the creation of hydrogen by splitting water. It can provide us with sustainable water and air purification as well as green and clean energy.

Three processes—hydrolysis, pyrolysis, and solvolysis—can liberate hydrogen from ammonium borane [2, 7, 9, 10]. Hydrolysis is the most effective technique for removing hydrogen from AB out of the three. It has low energy consumption and needs a sufficient catalyst at room temperature [7]. In contrast, pyrolysis exhausts energy and results in byproducts that are difficult to get rid of [9]. Moreover, solvolysis calls for organic solvent, which is incompatible with the need for green hydrogen [10]. In the presence of a catalyst, 1 mol of AB can produce 3 mol of hydrogen through hydrolysis. The hydrolysis equation is:



We will learn more about the function of noble metals and nanoceramics hybrid in the effective release of hydrogen from AB in this book chapter. The combination of noble metals and semiconductor catalysts has the capacity to control the rate of the reaction, release hydrogen from ammonia borane and degrade toxic dyes. By hydrolyzing ammonia borane, noble metals like Pt, Ag, and Au and their nanocomposites produce a large amount of hydrogen. The Pt-based photocatalysts can also complete the process in under a minute. However, taking into account cost-effectiveness, the less expensive metals, such as Ag and Pd, along with semiconductors, may be useful in releasing hydrogen from AB.

PLASMONIC DYNAMICS

Hot electrons can pass from metal to semiconductor and vice versa, thanks to the plasmonic structures' LSPR effect at their Schottky junction [2, 11, 12]. Due to its dependence on their structure and size, it has a confined effect [13]. In an electromagnetic wave moving in the direction of plasmonic nanocrystals, there are two types of light waves that can be observed: TE (transverse electric) modes and TM (transverse magnetic) modes. The electric field component of the transverse electric mode is parallel to the wave propagation vector. The electric field in the transverse magnetic mode runs parallel to the direction in which light travels. The surface plasmonic wave travels down the x-axis before dissipating in the z-axis.

The electric field and magnetic field equation for TE wave is written as:

$$Z > 0, \quad \vec{E} = E_1 \vec{y} e^{i(k_x x - \omega t)} e^{-a_1 z} \quad (1)$$

$$Z < 0, \quad \vec{E} = E_2 \vec{y} e^{i(k_x x - \omega t)} e^{a_2 z} \quad (2)$$

We have from Maxwell's equation,

BaZrO₃-Based Ceramics and Ceramic Composites as Smart Materials for Advanced Applications

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Abstract: Ancient human history invites significant learning with unknowing facts and fascinations. Significant development and transitions in the human lifestyle are visualized from the capitalized materials. “Ceramics”, as antique as it sounds, is frequently used for innumerable applications. From pottery to pellets, ammunition to antennas, electrolytes to electronics, all exist under the radar of ceramic materials. The dominant trait of ceramic materials for advanced applications is constantly replenished to extract peerless products for future utilization. Ionic or covalent bonding in ceramic microstructures administers their suitable mechanical, electrical and chemical characteristics. Pristine ceramics display low conductivity and chemical stability, while doped ceramics *via* implanted impurities empower their characteristics. The nature of dopants and defect substitution differs on the target application. The vastly introspected energy sector is permeated with acceptor-doped perovskite ceramics, while the defense sector inquests over piezoelectric ceramics and ceramic composites. The trivial facet amongst all is the use of Barium Zirconate (BaZrO₃) based ceramic compositions. It has been substantially contemplated to visualize the role played by BaZrO₃ in multiple domains. Either as a parent material or as an additive, BaZrO₃ attracts research groups from diverse sectors. Compiled with innumerable advantages, it accompanies a few limitations. The vital thing is the high sintering temperature along with the trade-off between proton conductivity and chemical stability. However, BaZrO₃-based ceramics are keenly monitored and tailored in an attempt to subsidize the maximum possible drawback with a simultaneous improvement in their properties. In the following chapter, we emphasize BaZrO₃-based ceramic and ceramic composites as smart materials for advanced applications. The extended applications in the energy sector, photocatalysts for hydrogen production, smart bullet systems in defense and microwave dielectric resonators for wireless communications are elaborately introspected with key insights.

Keywords: BaZrO₃, Dielectric resonator, Hydrogen production, Photocatalyst, Proton conductor, Smart bullets.

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INTRODUCTION

Material Science, as it is much heard of, is concerned with the study of contemporary materials for diverse applications which pave as an eye-opener for future technologies. Of the frontline nature of materials known to date, ceramics are undoubtedly influential and demanding. It wouldn't be erroneous to affirm us all besieged by ceramics. The root for ceramics arrives from the Greek word 'keramikos' for clay products. Ceramics are non-metallic, inorganic and often crystalline materials, with clay being traditionally recognized. Ceramic artifacts date long back to ancient human history as a source of evolution and survival [1, 2]. Archaeologists and multiple research groups consider 'ceramography' as an effective strategy to examine and unveil numerous unanswered questions about human history and development. While fundamental ceramics remain as handy products, ceramic matrix composites, on the other hand include advanced domestic and industrial products over monolithic ceramics [3, 4]. The spectrum of material architecture using ceramic materials has flourished with a subsequent revelation of multiple domains. The physical and chemical properties of ceramics inevitably rely upon their crystalline nature. The underlying study of solid-state chemistry reveals an interrelation between the properties and microstructure of ceramics. The elementary idea of material assessment for future advancement lies in an appropriate choice with requisite characteristics. Analysis and characterizations of ceramic microstructure occur at similar microscopic scales that vary from a few Angstroms (Å) to micrometers (μm). This invites ceramics and their composite counterparts for utilization in optics.

From the material's perspective, Barium Zirconate (BaZrO₃) and their allied compositions establish suitable bulk, mechanical, optical and dielectric properties due to supportive microstructures [5 - 7]. BaZrO₃ is used in distinct sectors either as a host material or as an additional reagent. This illustrates our former claims of their growing demand in the energy sector [8, 9]. Population growth and rapid decline in the intermittent and usable form of eco-friendly energy sources impels researchers and practitioners to introspect efficient energy storage technology. Solid oxide fuel cells (SOFC) and proton-conducting solid oxide fuel cells (PC-SOFC) showcase promising results as a spark for future technological advancements [10]. The study of Bi, Lei *et al.* [11] gauges the proton conductivity and power density of 20%Yttrium (Y) doped BaZrO₃. the outcome reveals considerable proton conductivity of $0.53 \times 10^{-3} \text{ S-cm}^{-1}$ under ambient conditions. The following observation attributes to the large grain size that enables unimpeded proton mobility. In support of the former literature, the works of Satapathy [12], showcase a rise in proton conductivity in Yb-doped BaZrO₃ under the N₂ atmosphere from 10^{-5} to 10^{-3} between $x = 0.05 - 0.20$, respectively. The conductivity, however decreased after that with a subsequent increase in dopant

concentration due to the proton trapping. In compliance with former discussions, Draber *et al.* [13] certified the proton trapping effect *via* a comparative difference in the activation energy for proton conduction between pure and doped BaZrO₃ compositions. While the activation energy in pure BaZrO₃ varies between 0 - 0.27 eV, the activation energy in the latter case with high doping concentrations ($x > 0.25$) elevates close to ~ 0.5 eV. This affirms the inability of long-range proton diffusion due to dopant-proton interaction. Recent studies by Vignesh [14, 15] as a continuum, highlights the optimal acceptor substitutions to desirable outcomes and eliminate the trapping effect. The material characteristics is preserved at lower doping concentrations ($x < 0.25$) while the predominant and early instance of proton trapping effect emerges at elevated acceptor substitutions ($x > 0.25$). While intermediate doping concentrations showcases multiphase co-existence and refrains adequate proton conductivity due to compositional induced structural phase transitions. This provides an optimal doping range between $x = 0.125 - 0.25$ which varies among different acceptor substituents.

Following the applications of BaZrO₃-based ceramics in different domains, the works of Fu *et al.*, Zuo *et al.* and Wang *et al.* [16 - 18] depict the use of BaZrO₃ and Sb⁵⁺ as additives too $(_{0.97-x})(K_{0.48}Na_{0.52})Nb_{0.965}Sb_{0.035}$ (Sb-KNN) which leads to the dispersion and broadening of dielectric peaks and enables relaxor like ferroelectric characteristics with low hysteresis. This grants their implication as multilayer capacitors, dielectric resonators and also in advanced defense technologies. Probing an eco-friendly and alternate source of energy, hydrogen fuel is preferably indicated as the best possible option among all available sources [19, 20]. Production of hydrogen through electrolysis of water depicts slow chemical kinetics. A recent study conducted by Tao *et al.* [21] in 2021 concerns hydrogen production using photocatalytic activity *via* perovskite-based ceramics. The machine learning models were proposed to predict the accurate bandgap (E_g) of the resultant ceramic. The predicted outcomes suggest an active hydrogen production rate (R_H) and extend the scope of ceramics as a potential photocatalyst with trivial modulations. Kolodiaznyi *et al.* [22] on the other hand investigated the plausibility of BaZrO₃-based ceramics as a microwave dielectric resonator. Established studies over resonators demand and operate materials with high dielectric constant, quality factor and high absorption coefficient with large bandwidth. The following requirements allow the material to serve as an accomplished sensor and actuator. Pure BaZrO₃ manifests high dielectric loss at room temperature to serve as a microwave dielectric resonator [22, 23]. The product of quality factor (Q) and resonator frequency (f) at $f = 10$ GHz is evaluated to lie in the range of 5 – 20 THz, which goes in agreement with the works of Stetson *et al.*, Yamaguchi *et al.* and Sivasubramanian *et al.* [24 - 26] respectively. To overcome the high dielectric loss, BaZrO₃ is used as an alloy with a host ceramic material to obtain an overall ceramic composite

A High-capacity Anode Material for Lithium-ion Batteries is Sili-graphene Type SiC_3

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Abstract: In this study, we have proposed an anode material based on Silicon doped graphene (Sili-graphene) for developing the Li-ion batteries (LIBs). We have predicted that Sili-graphene can be an anode material for lithium batteries. In particular, we have found that the Sili-graphene sheet can adsorb lithium atoms in different sites in a hexagonal structure. Also, we have found that Lithium atoms can be diffused along the plane of sili-graphene. The energy of diffusion of sili-graphene (SiC_3) is about 0.095eV, and for Li on top of silicon atoms is about 0.223eV, indicating rapid charging/discharging processes. During charging and discharging, the electrode Li_xSiC_3 exhibits small variations in voltage, making them a potential candidate for Li-ion batteries.

Keywords: Capacity, Charging/discharging processes, Diffusion barrier, DFT, Lithium batteries, Voltage.

INTRODUCTION

A key challenge for rechargeable Li batteries is to propose an appropriate theory to realize the experimental results for a novel application as an anode material with high efficiency and good performance [1 - 3]. The research in this area is devoted to developing a new rechargeable Libattery to overcome the energy crisis and provide sustainable energy resources [4, 5]. The anode of Li-battery was developed in 1979 by Yazami *et al.* [6] and successfully launched in the market during the early 1990s by Sony Corporation [7]. After that, great efforts have been made to improve the stability and efficiency [8, 9]. Also, it has paved the way in a

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great deal for the development and investigation of new materials that can possibly be integrated into Li batteries. Intensive studies were done after the discovery due to the following reasons; their good life [10], higher reversible capacity [11, 12], and higher energy density [13, 14]. Graphite is used in commercial batteries; the Li-ion has a storage capacity between two layers of graphite because it has a charge capacity of ~ 372 mA h/g with acceptable reversibility as well [15, 16]. In addition, the demand for its application is increasing in different areas, such as portable electronic devices and electric vehicles [17, 18]. The growing demand for market valuation and rigorous research conducted in parallel may improve the capacity of lithium-ion batteries [19].

The recent development for fabricating the Li-battery used 2D materials, such as the transition metal dichalcogenides (TMDs) [20, 21], which are used thanks to their high charge capacity, dimensionality, and structural flexibility [22]. Graphene battery is similar to traditional lead-batteries in that it is composed of an electrolyte solution between the two electrodes to facilitate the transfer of ions in solution between the electrodes. Graphene-based batteries are quickly becoming more favorable than their graphite predecessors. A variety of graphene-based batteries has been developing in their nanocomposites, such as Li-ion batteries [23 - 26], Na-ion batteries [27 - 29], Zn-batteries [30, 31], K-ion battery [32] and Li-S battery [33 - 35]. The batteries are composed of three parts: the anodes, cathodes, and interface, to improve the performance of batteries. It is necessary to improve all three parts for better performance. The mechanical instability and the structural phase transition due to Li insertion in 2D materials have outclassed the performance of all batteries. Moreover, the improvement of life durability and reversible capacity is still a focal point of core research.

The presence of remarkable chemical and physical properties makes this material a promising component in different technological devices such as conversion systems and advanced energy storage [36]. The graphene anodes have already been used for Lithium batteries, and several research groups are involved in the development of their storage capacity [37, 38]. These successes in the application of graphene have encouraged the scientific community to invent a new class of graphene-like 2D materials [39 - 41]. At the same time, the discovery of graphene has brought a great change in the field of electronics. For example, the construction of the novel nano-transistors is based on graphene [42, 43]. However, graphene is a gapless material, and many efforts are made to open the band gap. Avetisyan *et al.* and Mak *et al.* apply the electric field to open the band gap of a graphene [44]. Denis *et al.* and Dai *et al.* studied the variation of physical properties of heteroatom-doped graphene material [45, 46]. Houmad *et al.* have doped silicon on graphene to tune the electronic properties [47] by opening the band gaps from zero to 2.51 eV as a function of silicon concentration. Similar

facts have already been confirmed by Z. Shi *et al.* [48, 49]. Wu *et al.* experimentally verified the results of the opening of band gap (0.13-0.25eV) on silicon doped with a concentration level of 2.7-4.7% by using electrical measurements of field effect transistor. The presence of a band gap in the range of ultraviolet has been confirmed by the photoelectron spectroscopy measurement. This result gives a new hope for its possible application in solar cell devices. In addition, it is possible to control the band gap with silicon doping graphene. Also, they found that silicon has increased the optical conductivity in the visible light region. Denis *et al.* have successfully demonstrated the opening of the band gap in graphene (monolayer or bilayer) by doping with aluminum, silicon, phosphorus or sulfur [50]. Other groups used the chemical functionalization [51].

Here, we have proposed sili-graphene as a novel anode material for Li-ion batteries (LIBs). Based on the first principles calculation, we will study the diffusion of Li-ion on the siligraphene as an anode material. The energy of diffusion of siligraphene (SiC_3) is rapid in charging/discharging processes. Also, the electrode of the siligraphene has a small variation of voltage in Li_xSiC_3 siligraphene during charging and discharging. This best advantage makes this 2D-material modified (g-SiC_3) a good candidate for Li-ion batteries.

COMPUTATIONAL DETAILS

The structural and electronic properties are investigate using the plane-wave projector-augmented wave method as implemented in the QUANTUM-ESPRESSO package [52]. Electron-ion interactions are described using ultrasoft pseudo potentials with a kinetic energy cut-off of 38 Ry, and the convergence criteria for energy are assumed to be 10^{-8} Ry. We perform Brillouin-zone integrations using Monkhorst-Pack grids of special points with $10 \times 10 \times 2$ meshes for the calculations of structural and electronic properties. For structural relaxation, lattice constants and atomic coordinates were optimized based on the PBE Perdew Burke Ernzerhof [53, 54]. The band structures obtained from the first principles are key factors in determining all the carrier transport properties.

RESULTS AND DISCUSSION

Electronic Properties of Li Adsorption on the Siligraphene

After relaxing the structure of Li adsorption on the Siligraphene we have got the following information: the first observation on the surface of siligraphene has become a buckled structure. The buckling distance between the carbon and silicon atoms along a Z-axis is given by $\Delta l = +0.36\text{\AA}$, and the distance between Lithium atoms and the surface of siligraphene is $\Delta l = +1.75\text{\AA}$ (Fig. 1).

An Introduction to the Fabrication of White Light-emitting Diodes

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Abstract: Light-emitting diodes, especially white light-emitting diodes are very attractive and fascinating lighting sources at this present time because they have the potential for high energy saving and environmental friendliness as compared to conventional lighting sources such as incandescent and fluorescent lamps and also have wide applications in a variety of fields including in lighting, architectural and medical *etc.* Among the various applications, the lighting sector is one of the most important fields because it consumes a large amount of electricity. About 15-22% of total electricity production in the world is consumed in the lighting sector. Therefore, understanding how to fabricate a white light-emitting diode is very necessary in order to improve its practical application further. Basically, there are two methods of fabrication for white light emitting diode, mixing of multiple LEDs and phosphor converted white light emitting diode (pc-WLED). The luminous efficiency and rendering index is influenced by the type of fabrication. In this chapter, the general introduction of light emitting diode (LED), its working principle, characteristics of light including CIE, color temperature and rendering index, the different modes of fabrication for white light-emitting diodes, and their advantages and disadvantages have been discussed.

Keywords: LED, Fabrication methods, pc-WLED.

INTRODUCTION

Electrical energy is one of the very essential parts of modern life, which is required in every household for various applications. The lighting sector is one of the fields in which a substantial quantity of electricity is being consumed. Around (15-22) % of the total electricity production is being used in the lighting sector [1 - 3]. At this point, light emitting diode (LED), especially white light emitting diode (WLED), is highly fascinating because they have the potential for low

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energy consumption, high efficiency, long lifetime, no heat production, compactness and environmental friendliness [4]. Therefore LED, LED-based lighting sources are considered as next-generation lighting sources and nowadays, conventional lighting sources such as incandescent light and halogen lamps have been replaced gradually by WLED in many sectors, including street lamps.

LED is a semiconductor-based lighting source. The light emission in LED is due to the recombination of electrons and holes inside the diode. LED consists of at least two semiconductors, n-type and p-type and a diode junction is formed between them. When electric current is passed in forward biased condition, the negative terminal of the battery is joined to the n-type and the positive terminal is joined to the p-type semiconductor. The electron from the n-type combines with the hole of the p-type; which results generation of light in different electromagnetic waves depending on the energy gap between the electron and the hole to be combined [5]. The working of an LED is diagrammatically shown in Fig. (1).

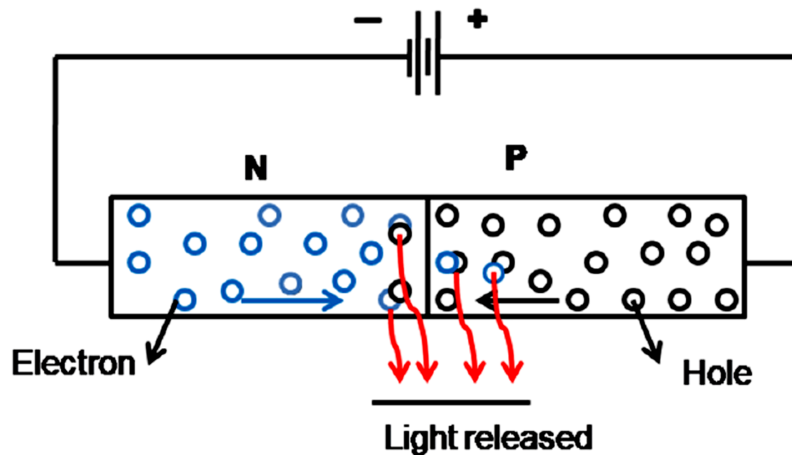


Fig. (1). The schematic diagram of an LED showing how it generates light.

The amount of energy released from an LED material can be calculated by using the formula given below:

$$\Delta E = h\nu = \frac{hc}{\lambda} \quad (1)$$

Here, ΔE represents the emission energy, h is Planck's constant, c is the velocity of light, which is equal to the velocity of emitted electromagnetic light, and λ is the wavelength of the emitted light.

TYPES OF LEDS AND THEIR APPLICATIONS

Based on the amount of energy released, LEDs can be classified into different types such as UV- LEDs ($\lambda_{\text{Emi}} < 400 \text{ nm}$), Visible-LEDs ($\lambda_{\text{Emi}} = 400\text{-}800 \text{ nm}$) and Infra-Red-LEDs ($\lambda_{\text{Emi}} > 800 \text{ nm}$). They have applications in different fields. For instance, Infrared-LEDs are used in remote control circuits such as in Televisions, DVD players and other domestic appliances *etc.*, UV-LEDs are used in industries for curing and hardening such as printing and manufacturing, and as disinfectants or sterilizers in the purification of air and water *etc.* [5]. whereas visible light emitting LEDs are found applications in several fields. Some of the applications of visible light-emitting LEDs are shown in Fig. (2).

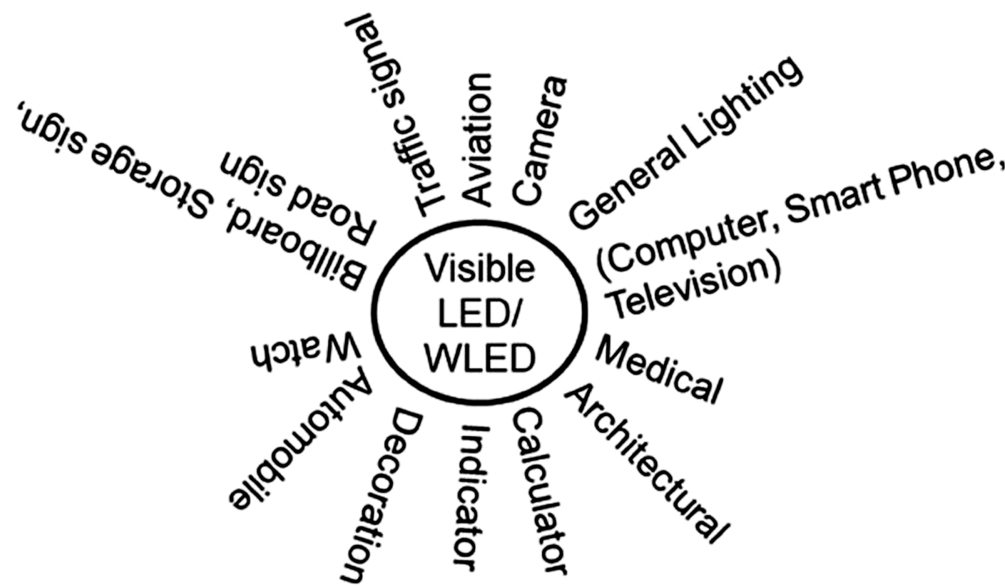


Fig. (2). Various applications of visible LED.

It is known that the visible light electromagnetic spectrum is extended in the wavelength (λ) range between 400 to 800 nm. The color of emitted light from a visible LED depends on the magnitude of the energy gap between the electron and hole to be combined. In Table 1, the variation of color with wavelength of visible light is shown [6].

Among the various applications, the lighting sector is one of the most interesting and attractive fields. The first practical visible light-emitting LED (red) was invented by Nick Holonyak Jr. in 1962 while he was working at General Electric

CHAPTER 5

Electronic and Piezoelectric Properties of Non-metal Doped II-VI Monolayer Compounds

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Abstract: The enhancement of nano-system properties, particularly low dimensional structures, is of great importance for future devices. Using spin-polarized Density Functional Theory (DFT), electronic and piezoelectric properties of II-VI monolayer (ZnO, ZnS, CdO and CdS) are studied. Variations of these properties are further studied under substitutional doping of non-metal atoms (boron and carbon). Doping with a B/C atom transforms all the monolayers into half-metallic ferromagnet, with changes arising mainly from *p*-orbitals of the dopant (B/C) atom. Reduction of band gap energy from its pristine structure is observed in all the doped cases. Observations predicted that the B-doped ZnO and ZnS monolayer showed negative structural stiffness and negative piezoelectric tensors, while C-doping remains stable with enhanced elastic as well as piezoelectric properties of the monolayer.

Keywords: Dynamic stability, Non-metal doping, Piezoelectric property, II-VI monolayer.

INTRODUCTION

The existence of two-dimensional material piezoelectricity, which is absent in its bulk form, has already been the focus of several theoretical predictions [1] and experimental reports [2]. In monolayer piezoelectric materials, crystal structure plays a crucial role in piezoelectricity and can lead to flexo-electricity [3]. Since the majority of the atoms in monolayer materials are surface-based, the impact of the surface on its physical properties cannot be disregarded. Thus, surface changes resulting in surface piezoelectricity and ferroelectricity can significantly modify the piezoelectric characteristics of monolayer materials [4 - 6]. For designing

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piezoelectricity, such universal surface characteristics of the monolayer materials are intriguing. In fact, some monolayer materials that are fundamentally non-piezoelectric due to the preservation of their inversion symmetry, even in their monolayer counterpart, can nonetheless be converted to this property through surface or structural changes. As a result, there are a lot more piezoelectric materials in two dimensions, and it is theoretically possible to develop materials with better piezoelectric capabilities.

Among the low dimensional materials, group II-VI monolayer compounds with wide band gaps are widely studied due to their versatility as a result of their tunable band gap nature. After the stabilities and possible realization of monolayers were verified experimentally [7], theoretical investigations of ZnO, ZnS, CdO, and CdS monolayers and their properties attracted huge attention among the II-VI monolayer compounds [8 - 15]. Later experimental reports of two monolayer thick ZnO films, in which the hexagonal ZnO sheets possess smaller buckling, confirmed the prediction of DFT calculations [16, 17]. Following the experimental confirmation of ZnO monolayer, a single layer of ZnS was also successfully grown on Ag (111) substrate [18]. Successful prediction of *ab initio* DFT calculation inspires further theoretical investigation on various properties of wide band gap II-VI semiconducting compounds. Reported calculations on CdO and CdS have also shown that these materials possess low formation energy in their two-dimensional structure with sp^2 hybridized orbitals [19, 20]. These studies motivate deeper insight into these monolayers and their properties and to find a way to enhance them by introducing dopant atoms.

The additional benefits of monolayer materials can also be vital for the design of piezoelectric monolayer devices in addition to these specific benefits, which include the availability of other piezoelectric materials and piezoelectricity manufacturing. Besides, monolayer materials are fundamentally flexible and strong. Furthermore, a limited number of atoms in these monolayers significantly enables atomistic-level simulations for a practical approach. Moreover, free charges in semi-conductive monolayer materials can be electrostatically controlled by gates without gates and interconnects. In this study, variation of piezoelectric properties of the proposed monolayers will be studied via induction of structural defects as a result of non-metal doping.

COMPUTATIONAL METHODS

For the study, a 4x4x1 supercell of each monolayer is taken for the pristine structure. A vacuum of 15 Å is inserted along the *z*-direction to avoid periodic interaction between monolayers. For each of the doped structures, one of the oxygen/sulfur atoms in a supercell is substituted with a non-metal (B/C) dopant

atom. Structural optimization is performed until the forces on each atom become less than 0.01 eV/Å with energy convergence criteria of 10^{-5} eV.

All the computations are performed with spin-polarized plane-wave density functional theory (DFT) as implemented in the Vienna ab initio simulation package (VASP) [21]. The ionic potentials are represented by Projector Augmented Wave Potentials (PAW) [22] with its electron exchange-correlation treated by Generalized Gradient Approximation (GGA) in the form of Perdew, Burke and Ernzerhof (PBE) for solids [23]. An energy cut-off of 400 eV is used for the plane-wave expansion of the electronic wave function. Brillouin zone integration is performed using $8 \times 8 \times 1$ k-point mesh within the Monkhorst-Pack scheme [24], with the properties calculation sampled by denser $16 \times 16 \times 1$ k-point mesh.

Elastic and piezoelectric calculations for zero external electric field can be expressed as:

$$\begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_6 \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & 0 \\ C_{12} & C_{11} & 0 \\ 0 & 0 & \frac{C_{11}-C_{12}}{2} \end{bmatrix} \begin{bmatrix} S_1 \\ S_2 \\ S_6 \end{bmatrix} \quad (1)$$

and

$$\begin{bmatrix} P_1 \\ P_2 - P_2^0 \end{bmatrix} = \begin{bmatrix} 0 & 0 & -d_1 \\ -d_1 & d_1 & 0 \end{bmatrix} \begin{bmatrix} S_1 \\ S_2 \\ S_6 \end{bmatrix} \quad (2)$$

respectively. In the above expressions, σ_1 and σ_2 are the normal stresses along x and y directions, respectively. S_1 and S_2 are the normal strains along the x and y directions, respectively. σ_6 and S_6 are the in-plane shear stress and shear strain, respectively. P_2^0 is the spontaneous polarization in the y -direction. P_1 and P_2 are polarizations along x and y directions, respectively. C_{11} and C_{12} are two independent elastic constants, while d_i is an independent piezoelectric constant.

Piezoelectric coefficients for monolayer system are related by the equation:

$$e_1 = d_1(C_{11} - C_{12}) \quad (3)$$

To analyze the relative stability of doped monolayer, formation energy is calculated using,

CHAPTER 6

A Theoretical Investigation on the New Quaternary MAX-phase Compounds $(\text{Zr}_{1-x}\text{Ti}_x)_3\text{AlC}_2$ (where $x=0-1$)

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Abstract: The physical properties of the $(\text{Zr}_{1-x}\text{Ti}_x)_3\text{AlC}_2$ MAX-phase compounds have been studied using the first-principle plane-wave method in the framework of the DFT theory. The Perdew-Burke-Ernzerhof parametrization was chosen for the exchange correlation (XC) energy. The equilibrium ground-state properties of the named compounds were calculated and compared with the reported experimental and theoretical data. The stability of our compounds has been analyzed. The electronic structures were predicted, indicating all our compounds exhibit a metallic behavior. The mechanical stability and elastic moduli were evaluated from the elastic constants. The effect of temperature and pressure on Bulk modulus, Debye temperature and heat capacity have been investigated and discussed in detail.

Keywords: Electronic structures, First-principles calculations, Quaternary MAX-phases, Thermo-mechanical properties.

INTRODUCTION

The growing interest in materials science has led to a true technological revolution of our time. The need to develop new materials that can meet the rapidly changing and renewable needs of society is one of the major challenges in the field of engineering and new technologies. Materials science is concerned with the elaboration and characterization of materials of whatever types, and constantly searching for new materials that meet the increasing demands of technological applications. In fact, before choosing a material to be used in a particular technological application, the possibilities of its use must be first stud-

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ied by determining its physical and chemical properties (structural, electronic, mechanical ... *etc.*) through both experimental and theoretical methods. For example, improving aircraft engines must include an increase in operating temperature, so the materials used should be lighter and more resistant to high temperatures. In recent decades, researchers have shown that even the strongest metal alloys become soft at temperatures above 1000°C. Scientists have developed a new class of materials known as ceramics, but unfortunately, it is characterized by fragility that limits its use despite undeniable progress in this field. Generally, brittleness, hardness and low usability are closely related to good resistance to high temperatures.

During the 1990s, the team Barsoum *et al.* [1] from Drexel University in Philadelphia discovered interesting properties of Ti_3SiC_2 . In addition to being inexpensive, this material is distinguished by its hardness, lightness, useable, resistance to oxidation and thermal shock and ability to remain solid at temperatures above 1300°C in air. About fifty compounds with similar properties were synthesized and classified into a new family known as MAX phases, referring to their formulations.

MAX phases are ternary ceramic materials based on carbides or nitrides, which constitute a new class of nano lamellar materials combining the properties of metals and ceramics, which give them exceptional properties such as high elastic stiffness, high melting temperature, high thermal shock resistance and high electrical conductivity [2, 3]. Due to the exceptional and desirable properties of MAX phase materials is well-recognized that they are used in various new industrial applications such as in aerospace, defense, nuclear reactors, automotive, and medical [4 - 7].

Recently, in 2016, a successful experimental study of the new compound Zr_3AlC_2 of the MAX-phase family was reported [8]. After that, Zapata-Solvas *et al.*, have also synthesized experimentally solid solutions of MAX-phases $(Zr_{1-x}Ti_x)_3AlC_2$ for different x concentrations [4, 9, 10].

In addition to experimental work, there are many theoretical studies related to the properties of MAX phases, for example, elastic properties and electronic-structure calculations. Moreover, a theoretical study has significance in stimulating experimental research on the synthesis and application of the new MAX-phase compounds with better characteristics, reaching some results that are difficult to reach experimentally.

According to the theory of quantum mechanics, the electronic structures of materials can be theoretically determined by solving the Schrödinger equation, where defining the electronic structures of materials is fundamental to

understanding and explaining experimental results obtained on their properties or even predicting their properties even if they have not yet been experimentally determined.

In order to expand and compare the previous works on Zr_3AlC_2 and Ti_3AlC_2 compounds, we have studied the structural, mechanical, electronic and thermodynamic properties of the uninvestigated MAX-phases $(Zr_{1-x}Ti_x)_3AlC_2$ using the first-principle full potential linearized augmented plane wave (FP-LAPW) method [13], in the framework of density functional theory (DFT) [11, 12] and simulated in the WIEN2k code [14].

GENERALITIES ON THE MAX-PHASES

The $M_{n+1}AX_n$ compounds are recognized as MAX-phase materials where M is an early transition metal, A is an A-group element, and X is C and/or N. During the last two decades, the MAX-phase materials have attracted intensive interest from scientists due to their combined best properties of metals and ceramics. The first study of this type of compound was done in the 1960s on the Ti_3SiC_2 powder to determine its specific properties [15]. However, interest in these phases remained limited for many years. Significantly renewed interest in the MAX phases since the mid-1990s after the intrinsic properties of the compounds became known, where Barsoum and El-Raghy reported on the synthesis and characterization of bulk and pure samples of Ti_3SiC_2 [1, 16, 17]. A major research effort has been carried out to synthesize pure MAX-phase compounds in the form of bulk or thin film [18, 19].

Several MAX-phases have been synthesized and many have been investigated for their interesting properties. Characterization and understanding of their physical, mechanical and chemical properties have fundamental and development goals for potential applications. Many recent articles focus on compounds such as Ti_3SiC_2 [20] and Ti_3AlC_2 [21], especially on their elastic and mechanical properties.

T. Laupauw *et al.* were the first team who experimentally synthesized a new 312-MAX-phase compound Zr_3AlC_2 [8]. Barsoum *et al.*, have also successfully synthesized the 413-MAX-phase compound Ti_4AlN_3 [22]. The MAX-phases have now been shown to include over 90 different compounds. The majority consists of 211 compounds, most of which were discovered by Nowotny [23]. There is a lot of work being done regarding the theoretical prediction of the stability of these types of compounds and there is still definitely an undiscovered chemical group [24]. Finally, it is interesting to note that it is possible to make a large number of solid solutions at sites M, A, and X, of which only a few have been synthesized thus far, so this will be particularly important to modify and

Surface Segregation in Pt₃Nb and Pt₃Ti using Density Functional Theory-based Methods

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Abstract: First-principles DFT calculations were used to investigate surface segregation processes in ordered Pt₃X (where X=Nb, Ti) alloys. Using pristine Pt (111) surface as a reference, the effect of surface segregation on the adsorption energy of O₂ atoms in Pt₃X alloys was evaluated. Our results showed that surface segregation due to direct exchange is only feasible for the Pt₃Nb alloy ($E_{\text{segr}} = -0.3833$ eV) but not for its Ti analogue ($E_{\text{segr}} = 0.516$ eV). In contrast, for both Pt₃X alloys, surface segregation due to antisite migration and leading to the formation of a Pt-skin or overlayer, favouring oxygen atom adsorption, an essential step in ORR, is possible. Interestingly, reverse migration of X atoms from the bulk to replace Pt atoms on the surface is an endothermic process and is thus very unlikely. Analysis of the surface segregation energy for configurations involving a direct exchange of Pt atoms located beyond the third layer in the slab model with Nb atoms at the surface indicates the formation of pristine bulk like Pt (111) surface from Pt₃Nb surface is unlikely. The energy of adsorption for the O-atom on pristine Pt (111) surface shows that the presence of minute quantities of dopant Nb atoms in the sub-surface layer could enhance its suitability for ORR. Comparison of O-atom adsorption energy on the various surface segregation models of Pt₃X alloys to that of pristine Pt (111) surface shows that the formations of a Pt-skin or overlayer on the Pt₃Nb surface due to surface segregation change the O-atom adsorption energy on this surface to 0.34 eV which is just 0.14 eV higher than the optimal value of 0.20 eV. Our results also show that the binding of an oxygen atom to the fcc Pt site in Pt₃Ti is lower in energy compared to its binding on a pristine Pt (111) surface. In comparison, the binding of an oxygen atom to the fcc Pt site in Pt₃Ti is of the same magnitude as that of the pristine Pt (111) surface.

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Keywords: Density functional theory, Platinum, Surface segregation, ORR.

INTRODUCTION

Developing improved polymer electrolyte membrane fuel cells (PEMFC) is an active area of research within the industry and academia. In industry, manufacturing long-lasting and durable PEMFC at a meager cost (reduction of platinum usage) is one of the key drivers of research in this area [1 - 3]. The PEMFC could provide a viable means of on-board energy for different applications such as transportation, stationary generators, etc. This industrial development is only possible if specific academic questions are tackled. Some interesting questions currently addressed within the academic domain are the improvement of the fuel cell catalyst, segregation issues in alloyed materials, reaction kinetics, nanoparticle optimization, *etc.* [1 - 4].

One key reaction carried out by the fuel cell membrane is the oxygen reduction reaction (ORR), which involves the reduction of water to produce oxygen and energy. The ORR reaction proceeds slowly, even in the presence of platinum, the archetypal catalyst for this process. Several Pt alloys have been investigated as catalysts for this reaction, and some of them have displayed enhanced catalytic activity. However, their long-term durability and stability are still in question due to the possibility of surface segregation in the alloys. Hence, this work investigates the segregation of Pt₃Nb and Pt₃Ti-based alloy catalysts in ORR. Surface segregation involves the movement of atoms from the bulk or vice versa due to the prevailing chemical environment, which might result in a difference between the chemical composition of the surface region and the bulk region. Surface segregation could significantly affect the overall properties of materials overall properties encompassing crucial aspects such as wetting, electrical contact, adsorption, oxidation, crystal growth, corrosion, friction and wear, and catalysis. This effect could occur in both ordered and disordered alloys [5 - 8].

Various Pt alloys, including late transition metals such as Ni, Co, Cr, and Fe, as well as partially dealloyed core-shell catalysts derived from Pt-Cu nanoparticles, have undergone extensive investigation [1 - 11]. This chapter introduces a novel collection of Pt alloys and intermetallic compounds that exhibit promising properties for the oxygen reduction reaction (ORR). The ORR is a challenging reaction to catalyze because the catalyst material must possess both stability under highly corrosive conditions at a fuel cell cathode and chemical activity to activate O₂, while also being capable of releasing oxygen from the surface in the form of H₂O. O₂ activation typically involves proton and electron transfers to form adsorbed OOH before breaking the O-O bond [12]. Therefore, the catalyst must moderately stabilize OOH. After dissociation, the catalyst surface forms adsorbed

O and OH, and these species should not bind too strongly to facilitate rapid H₂O desorption. Our focus lies on metallic ORR catalysts comprised of alloys or intermetallic compounds, hereafter referred to as alloys. Specifically, systems that form Pt overlayers or “skins” on the surface are explored. These two metallic elements are the only ones stable under the high potentials and acidic conditions of a PEMFC while also exhibiting surface chemical properties that closely align with the optimum requirements for the ORR. The ultimate objective is to discover Pt₃X alloy meeting the following criteria: (1) they should form Pt or Pd overlayers with greater ORR activity than Pt, and (2) they should demonstrate maximum stability [9 - 15].

The approach involves employing density functional theory (DFT) calculations initially to identify intriguing candidates, followed by experimental testing. While the primary goal of this approach is computational electrocatalyst discovery, it also serves as a valuable exploration of the current understanding of the ORR. In the realm of catalysis, nothing attests to the robustness and accuracy of a theoretical framework more convincingly than its ability to identify new active materials.

Surface segregation can manifest in ordered and disordered alloys, driven by three primary physical mechanisms in solid solutions or disordered binary alloys. Firstly, for alloys with heat of solution negative, the majority component enriches the surface towards maximizing the bulk component mixing. Next, when there is a significant difference in atomic sizes between the components, the smaller component segregates to the surface to reduce strain energy. The component with lower surface energy, in its pure elemental form, segregates to the alloy surface. Lastly, surface segregation in ordered alloys can occur due to the generation and movement of antisite defects caused by the off-stoichiometric effect. Surface segregation in disordered alloys is always exothermic and results in a decrease in the system's configurational entropy. In contrast, surface segregation in ordered binary alloys would increase the system configurational entropy, and it can be exothermic or endothermic. The prediction of surface segregation in binary alloys is long been a subject of research [13 - 19] utilizing theoretical models such as tight-binding theory (TBT), embedded atom method (EAM), density functional theory (DFT), and statistical mechanics methods to evaluate energy and sample different configurations [18 - 22].

Previous studies have primarily focused on surface segregation in disordered alloy configurations. In this work, we employ a similar computational approach to predict the feasibility of surface segregation in ordered Pt₃Nb and Pt₃Ti alloys. The surface structure and composition of bimetallic alloys greatly influence their catalytic activities. Therefore, surface segregation models can be used to design

Nanoparticles and Environmental Health

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Abstract: The size range of nanoparticles between 1-100nm is unique because of their extremely small structure with a very high surface area to volume ratio. Besides naturally produced nanoparticles, there is a huge worldwide demand for synthetic nanoparticles. These synthetic nanoparticles are modified to some extent according to the specific need. These manipulations at the nano-scale paved the way for a popular branch of science called nanotechnology. However, with the massive use of nanoparticle-based industrial products in our day-to-day lives, we knowingly or unknowingly ignore their impact on the environment. The air, water, and soil quality determines environmental health, which is reflected by a healthy ecosystem and its biodiversity. The existing intricate interaction between humans and their surrounding environment is important for maintaining a fine balance in the ecosystem. Any change in this interaction may lead to adverse consequences. The nanoparticles released in the environment cause a varying degree of effects on the ecosystem based on the type, surface coating, and degree of its environmental transformation. Some nanoparticles are harmful to the environment and some are beneficial. Some of the nanoparticles in the environment get bioaccumulated in plants and animals, disturbing their growth and productivity. Remediation by nanoparticles has been effective in removing some toxic compounds from the environment, thereby providing a way to minimize pollution efficiently. Thus, in this review, we have tried to present an overview of the sources, fate, and effects of nanoparticles available in air, water, and soil. We strongly advocate for the long-term assessment of nanoparticles, and the formulation of strict guidelines for their usage by the concerned industries for better environmental health, and in turn a healthy ecosystem.

Keywords: Environment, Nanoparticle, Nanotechnology, Pollutant, Remediation.

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INTRODUCTION

The definition of nanoparticles (NPs) or nanomaterials put forward by the European Commission says the nanoparticles are natural, incidental, or manufactured material containing particles in the unbound or aggregated form where 50% or more of the particles are in the size range of 1nm-100nm in at least one dimension [1]. Since the discovery of nanotechnology in 1959 by physicist Richard Feynman, its application in different industries like electronics, healthcare, energy storage and production, construction, cosmetics and personal care, pest control, agriculture, water treatment, *etc.* has increased tremendously. The NPs are found in all environmental compartments: soil, water, and air, with the ocean holding the largest amount of NPs on earth [2]. The largest market for nanomaterials is North America, and its fastest-growing market is in the Asia Pacific. In the Asia Pacific region, the leading countries in terms of nanomaterial production are China, India, Japan, and South Korea [3]. Mainly, the surge in demand for nanomaterials is noted in the fields of energy storage and conversion, treatment of diseases, agricultural productivity, personal care products, water treatment, and remediation. This increased use of nanoparticle-based products has resulted in growing concern over its effect on environmental health. This may be due to the scattered research on its risk assessment and unaccounted disposal in the environment. Thus, this review intends to summarize the available research articles in nanoparticles pertaining to environmental health, and put forward the future perspective on its sustainable use.

NATURAL NPs

The NPs can be produced naturally as well as synthetically. Natural NPs are either organic or inorganic. Organic natural NPs are produced by various natural processes, like photochemical reactions, weathering of rocks and minerals, wind erosions, occasional forest fires, volcanic eruptions, organismal activities, and extra-terrestrial processes. Examples of natural organic NPs are Oceanic spray, volcanic ash, mineral NPs, naturally produced carbon-based NPs, aerosols, forest fire smoke, *etc.* Some typical representatives of naturally occurring inorganic are FeS_2 , Ag, Au, SiO_2 , Fe_2O_3 , Al_2O_3 , and MnO_2 [4]. Natural NPs play an important role in the biogeochemical processes on Earth. The natural nano-sized geomaterials perform key roles in the distribution of different minerals on Earth by complex physiochemical interactions with biotic and abiotic factors, different transformation procedures, and weathering [2]. Due to their high surface area to volume ratio and high reactivity, NPs contain a significantly higher amount of minerals than bulk soil mass, which ultimately leads to increased mineral availability to plants, microorganisms, and higher taxa [5]. The nano-sized mineral dust, particulate matter generated by forest fires, and volcanic ashes can

cause serious environmental and human health issues [6]. Moreover naturally formed metal NPs are highly stable, and thus can be transported to large distances without transformation to any other forms. The coating of organic matter and ROS on these metal NPs significantly affect their toxicity [4].

ENGINEERED NPs

Nanoparticles that are developed with synthetically definite chemical composition, size, and surface coatings, either simple or conjugated with other bioactive molecules to enhance some specific properties are called Engineered nanoparticles (ENPs) [7]. Designed for specificity, controlled reactivity, increased sensitivity, and cost-effectiveness, The ENPs have become an integral part of several industries worldwide, such as electronics, medical diagnosis, personal care, textile, food packaging, construction, *etc.* The different types of ENPs are produced using metal, metal oxide, carbon, nano-clay, quantum dots, *etc.* The ENPs get released into the environment during their production, use, and disposal. Currently, its fate in the environment is mostly unaccountable or unmanaged. Thus, it is essential to study the fate of ENPs in the environment and their mechanisms of interactions with aquatic and terrestrial ecosystems. There is a high possibility of ENP entry into the environment during production. Therefore, production volumes are a good indicator of ENPs released in the environment. Of the total ENPs produced, 0.1-2% are released into the environment. Of these released ENPs, 20-80% go directly into the environment, from which 10-40% go to the air and 10-40% to the water bodies. The direct release of ENPs during product use is dependent on the type of product produced. A significant amount is released if the product is in liquid, gas, or powder form [8]. The indirect emission of ENPs in the environment occurs *via* effluents of wastewater treatment plants and the disposition of untreated biosolids produced as by-products of NPs into soil landfills. During the whole life cycle from production to disposal, the global estimation of ENPs released into the environment is almost 63-91% into the landfills, 8-28% in soil, 7% in the aquatic environment, and 1.5% in the air [9].

Among engineered NPs, Quantum Dots (QDs) are also used frequently. QDs are nanocrystalline structures having semi-conductivity and unique fluorescent properties. The characteristic fluorescent property described as “quantum yield” of QDs is based on the ability of QDs to emit light (quantum) after absorption, and it is directly proportional to the QDs efficacy in different fields like imaging, display industry (liquid crystal display, light emitting diodes), medical imaging, solar cells. QDs can be engineered to be made of only one element, like carbon or silicone, or they can be combined with other compounds based on the properties of the desired material. The release of QDs in the environment most likely occurs during the synthesis step and end-product formation step. After release in the

CHAPTER 9

Investigation for Optimum Site for Adsorption and Population Effect of Lithium on Silicene Monolayer

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Abstract: This investigation holds the search for optimum sites for Lithium on Silicene Monolayer, by studying the adsorption energy on putting the Lithium atom on different possible sites. The center of the hexagonal structure in silicene was found to be the most favourable site. Using transition state search (TSS) the optimized stable state is confirmed. A low Diffusion Energy Barrier (DEB) of 0.348 eV indicates that the adsorption of Li over silicene can occur easily. Multiple adsorptions are considered, up to 4 Li atoms upon silicene substrate. The metallic property of pristine silicene is maintained throughout Li atom adsorption. Large adsorption energy in each of the adsorption suggests that silicene may be promising for Li-based battery material.

Keywords: Diffusion energy barrier, Lithium, Lithium-ion battery, Silicene monolayer.

INTRODUCTION

Over the years, electronics have been growing, and the search for newer technology comes with various challenges to make various components compact which involves an even more compact power source. Since the discovery of Lithium-ion Battery (LIB), its application has been widely explored for many electronics and automobiles [1 - 3], and it has been used conventionally in almost all electronics. For a long time, graphite has been used as an anode (the negative terminal of the battery); however, due to various limitations such as thickness, low capacity and safety concerns, newer materials such as SiO₂, alloy anodes, and conversion-type transition-metal compounds have been proposed by various researchers [4 - 6].

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2D materials have found a wide area of applicability due to their large surface-to-volume ratio. Among them, silicene is one of the most considered materials. Silicene is a low-dimensional buckled monolayer of silicon. Lately, experimentally-fabricated materials with buckling structures have been developed. In fact, in recent experimental works, silicene monolayers have been synthesized by various methods such as Molecular-beam-epitaxy (MBE), by condensation of Silicon atoms on silver crystals in a vacuum chamber, Wet-chemical exfoliation method, and various methods of synthesis have also been presented by Balendhran. S. *et al.*, [7 - 10].

In general, the so-called silicene, a silicon (Si) equivalent of graphene, also receives a great deal of scientific attention. Similar to graphene, silicene is composed of hexagonal rings. However, they are not planar due to symmetric buckling caused by a pseudo-Jahn Teller effect forbidding them from being flattened; the instability of the high buckled and the planar silicene has also been proven by Roome. N.J. *et al.*, [11]. Interestingly, due to its buckled honeycomb structure compared to graphene, silicene demonstrates a substantially higher level of chemical reactivity, as well as significantly stronger adsorption of atoms and molecules [12 - 18] than graphene with promising new silicene-based electronic device applications [19, 20], Li-ion storage batteries [14, 21 - 23], hydrogen storage [24 - 26], catalysts [18, 27], thin-film solar cell absorbers [28, 29], and hydrogen separation membranes [30, 31], gas sensor and detection [32 - 34]. While sp^2 hybridization is favoured for 2D graphene, Si strongly favours sp^3 [35]. Li-ion secondary batteries are a prospective form of energy storage that can be used in both mobile and grid applications [36, 37]. Their energy density is significantly influenced by the individual charge capacities of the constituent electrodes [38]. Silicene has long been proposed as a substitute for conventional graphite electrodes in LIB. Low specific capacity is one of the few drawbacks of a graphite electrode (372 mAh g^{-1}) [39]. It is worth noting that the clustering of lithium atoms reduces the chargeability of the LIB and is also the primary cause of deterioration of battery health. A high theoretical capacity of silicon (4200 mAh g^{-1}) and a suitable operating voltage make it one of the most promising anode materials for a LIB [40]. The interaction between silicene and Li is stronger than that of graphene [41]. These characteristics have indicated the promising capabilities of silicene as an anode in lithium-ion batteries.

Specific optimum site adsorption of fully occupied lithium on silicene monolayers has not been observed in our literature survey. In this work, we have studied the adsorption for a single lithium atom to find the most optimum site considering four different sites. A transition state search is performed, taking energy footprints along the transition. We have interpreted its electronic properties and determined its character for an anode in Li-ion battery by implementing the optimum site for

specific site adsorption and checking the effects of lithium population on silicene. Although this is not a large scale, this study provides a rough description of how a lithium atom reacts with a silicene monolayer monolayer (Fig. 1).

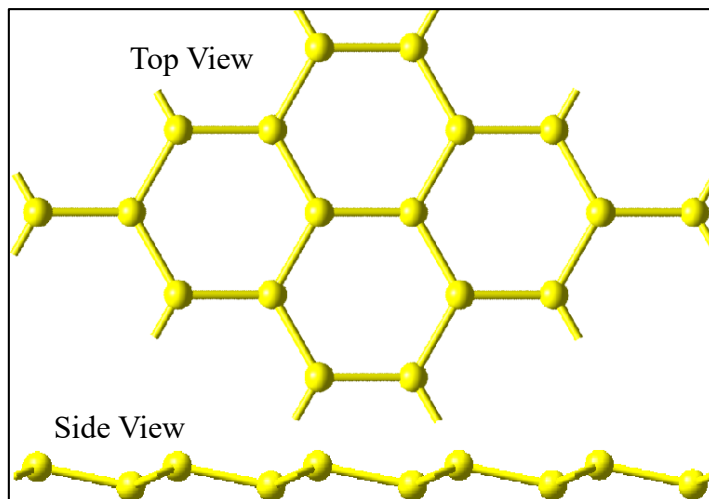


Fig. (1). Top view and side view of silicene.

COMPUTATIONAL DETAILS

In this work, all the calculations were based on density functional theory and the Generalized Gradient Approximation made simple by Perdew, Burke and Ernzerhof [42] exchange-correlation function was incorporated to describe the interactions which are integrated with VASP (Vienna Ab-initio Simulation Package). Van der Waals interactions are taken into consideration using DFT-D3 dispersion correction. Spin-polarized magnetic calculations were carried out (in case the compound is magnetic) using 'normal' precision and a plane-wave cutoff energy of 400 eV. Electronic iterations convergence of 10^{-5} eV is employed using the Fast (Davidson and RMM-DIIS) algorithm and reciprocal space projection operators. A k-mesh of $4 \times 4 \times 1$ was employed, and Tetrahedron with Bloechl corrections [43] was chosen for the smearing method.

The study of adsorption energy helps in finding the most favourable site for adsorption. For this, we considered 8 Si (P1) $2 \times 2 \times 1$ lattice. Geometric optimization is carried out, from which VASP energy is considered for the energy of the systems. Equation 1 (given below) is incorporated for determining adsorption energy (E_{ads}).

$$E_{ads} = \frac{(E_{sil} + N_{Li}E_{Li} - E_{Total})}{N_{Li}} \quad (1)$$

Strategies for Synthesizing Metal Oxide Nanoparticles and the Challenges

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Abstract: The development of nanoscience and nanotechnology has improved our quality of life. The new class of materials known as nanoparticles (NPs) contributes to the development of nanotechnology. For the NPs, at least one dimension of particles should be 1 to 100 nm. The synthesis approaches can modify NPs structure and size, which is crucial in molecular biology, physics, chemistry, medicine, and material science. The high surface area of NPs can be achieved *via* synthesis approaches, providing increased value and imperative parameters like surface reactivity. Several approaches to synthesizing NPs can be used, mainly categorized into two parts: bottom-up and top-down. These two categories are classified based on the starting materials used to synthesize the NPs. This review discussed the brief of synthesis approaches and their utilization in the field of nanotechnology and nanoscience. The novel approach to the synthesis of NPs *i.e.*, the electrochemical discharge process, is discussed in detail. The materials synthesis like ZnO, carbon, graphene, and other metal oxide and their composite are discussed in tabular form. Finally, the challenges, advantages, disadvantages, conclusions and NPs synthesis are discussed.

Keywords: Bottom-up, Nanoscience, Nanotechnology, Nanoparticle, Top-down.

INTRODUCTION

The NPs are a class of materials that have high demand in molecular biology, physics, chemistry, medicine, and material science [1]. The study, structure, formation, synthesis, manipulation, and utilization of materials, devices, and functional systems through nanoscale control are all included in nanoscience and nanotechnology (NST). This also consists of exploiting phenomena and properties of the material at the nanoscale. The word “nano” comes from the Greek word “nanos” or the Latin word “nanus,” both of which mean “dwarf” or “extremely little” and represent one-millionth of a meter (10^{-9} nm) [5]. The dimension of nano can also be understood through the best example, the arrangement of five silicon

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atoms in a line, or the arrangement of ten hydrogen atoms in a line is considered as one nano-meter [6]. The daily life object, which we can see from an open eye or not in size scale (atom to meter), is shown in Fig. (1).

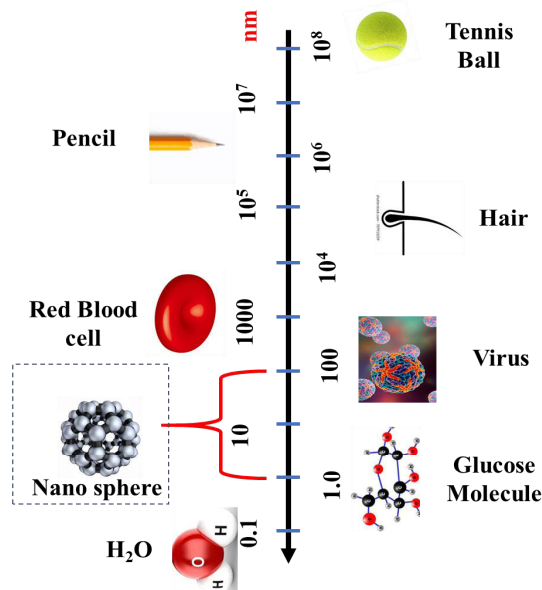


Fig. (1). Size distribution of NPs with different element.

NANOSCIENCE AND NANOTECHNOLOGY

At the time of Democritus and the Greeks in the fifth century B.C., scientists debated whether the matter is continuous and thus infinitely divisible into smaller pieces or whether it is made up of tiny, indivisible, and unbreakable particles or atoms. This debate is the result of people starting to think about nanoscience. It can observe, measure, assemble, control and manufacture the materials at the nanoscale. Nanotechnology can be stated as the development, synthesis, characterization and application of materials and devices at the nanoscale. The nanoscience and nanotechnology are co-related, under which knowledge of physics, materials science, chemistry, solid-state physics, and quantum mechanics is required. As a result, profound knowledge in one field will not be sufficient; a combination of physics, chemistry, material science, solid state, and biosciences is required. The nanoscience provides knowledge of atom arrangements and their fundamental properties at the nanoscale. Nanotechnology controls matter at the atomic level to create novel nanomaterials with various properties [6]. Nanotechnology has engulfed almost the entire engineering field. However, most people are unaware of its applications despite the fact that it covers almost every branch of science. Even after progress over time, there is still space for

improvement in the era of nanotechnology and nanoscience for developing new materials and their application for humanity.

NANOTECHNOLOGY IN THE 20TH CENTURY

The term nano was first introduced by scientist Richard P. Feynman (1959-1960) in his lecture that. “Feynman posed the question, “Why can't we write the entirety of the 24 volumes of the Encyclopedia Britannica on the head of a pin?” in this lecture. “and presented a vision of building everything from larger machines down to molecules using machines”. They introduce materials that can be broken into minor portions, *i.e.* nano and movement can be done from atom to atom to form nano-size [7]. Further future discovered the scanning electron microscope by Binning and Rhorer in 1983. Recent progress has made it possible for scientists to create unique nanomaterials and miniature technologies.

NANOMATERIALS CLASSIFICATION

NPs are the building block of nanotechnology, which is one billion meters. All the physics laws applied in our daily life use materials, but in the case of nano, it differs. It is observed that physics law is not applicable in NPs as the gold colour is nice yellowish, but 100 atoms of gold in the cube are red. It has a high surface-to-volume ratio, making it different physicochemical properties than bulk. Unexpectedly, the shape and size of the nanomaterials are altered at the nanoscale level, giving them a distinct personality with new powers. NPs can be synthesized in different forms, including rods, sheets, and flowers; each shape has unique features due to its dimensionality. Nanorods and nanotubes fall within the one-dimensional category of nanostructures, while films and layers-type particles are two-dimensional nanomaterials. Their individual functions typically classify them. The attractiveness of nanomaterials lies in the fact that their physical properties can be changed by combining them with other NPs. The following categories can be applied to materials based on their dimensions (< 100nm) [8].

1. Zero-dimension particles (0-D) – Nanomaterials with all three dimensions are at the nanoscale referred to be zero-dimensional NPs. The graphene quantum dot is the best example of a zero-dimensional nanoparticle because all three dimensions are on the nanoscale.
2. One-dimensional nanoparticle (1-D)- In this category, nanomaterials having one of the dimensions need to be nanoscale; the other two can be any size. Materials in this category comprise nanotubes, nanowires, and nanorods.

Heterogeneous Semiconductor Photocatalysis for Water Purification: Basic Mechanism and Advanced Strategies

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Abstract: Water is essential for all living things, whether it is human beings, animals or plants. Around 70% of the total earth's surface is covered by water, however only a small fraction of it (2.5%) is found as fresh water. On the other hand, due to anthropogenic activities like industrialization, a huge increase in population, utilization of toxic chemicals in agricultural activities *etc.*, the available freshwater bodies have been contaminated by various kinds of pollutants, including toxic chemicals released mainly from industries like textile, which causes hazardous to both human being and aquatic life. Therefore removal of these toxic chemicals before entering into fresh water bodies is of great importance. Heterogeneous semiconductor photocatalysis is the most effective green method in this regard because it enables to degrade the pollutants into non hazardous products like CO₂ and H₂O without releasing any harmful residue. Therefore, understanding the knowledge of photocatalysis mechanism is very significant to enable further improvement. Hence, this chapter presents the basic mechanism of photocatalysis, its drawbacks and the advanced strategies to improve the catalytic efficiency. Finally some of the important factors that provide strong influences on the catalytic activity also have been discussed.

Keywords: Basic mechanism, Heterostructure formation, Metal and non-metal doping, Photocatalysis, Surface Plasmon resonance.

INTRODUCTION

Water is one of the basic necessities for all forms of life. Around 70% of our total earth's surface is covered with water. However, only about 2.5% is found as fresh water in the form of river, glaciers, groundwater and water vapours in the atmosphere [1]. Furthermore, due to anthropogenic activities like industrialization, huge increase in population, use of different hazardous

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chemicals in agriculture and domestic waste *etc.*, the available freshwater bodies are contaminated by different kinds of pollutants, including various toxic chemicals that lead hazardous to both aquatic and surface lives of our planet. Hence, water pollution is one of the major concerns all over the world at the present time. According to a literature report, approximately 3.2 million people die per year in the world due to the use of unsafe water, poor sanitation and inadequate hygiene [2]. The very important toxic chemicals include various coloring organic dyes released mainly from industries like textile, chlorinated and non-chlorinated organic aliphatic and aromatic compounds, inorganic compounds like heavy metals, insecticides, herbicides and byproducts of fertilizers from agricultural activities and antibiotics from agriculture and hospitals [3 - 5]. These toxic chemicals are non-biodegradable and stable in the natural cycle and cause both acute and chronic pollution to our environment [5, 6]. Hence, removal or degradation of these toxic chemicals before entering into freshwater bodies is highly essential. During the past few decades, several traditional treatment methods like adsorption, chlorination, chemical co-precipitation, reverse osmosis and electrochemical methods have been applied in order to solve the above problem. However, all these efforts resulted in some sorts of limitations like high cost of operation, generation of toxic byproducts and transfer of the pollutants from one dumping site to another site *etc.* [7 - 9]. Therefore, they are restricted from practical application. Nevertheless, fortunately, semiconductor heterogeneous photocatalysis is found to degrade these toxic chemicals into non-hazardous products like CO₂ and H₂O effectively without releasing any harmful residues [5]. So, it is considered as the promising green method for solving environmental problems, especially for the degradation of toxic chemicals in wastewater. In addition, applications of semiconductor photocatalysis were also found in other fields, such as the generation of hydrogen and oxygen from water, storage of sunlight energy in chemical bonds and anti-fogging and self-cleaning of windows and lenses [10]. Therefore, understanding the knowledge of photocatalysis mechanism is highly significant in order to enable further improvement. Hence, the present chapter presents the basic mechanism of heterogeneous semiconductor photocatalysis, its limitations and the advanced strategies that enable to improvement of the catalytic activity for the purification of waste water. Some of the important factors that have strong influences on catalytic activity have also been discussed.

PHOTOCATALYSIS AND ITS BASIC MECHANISM

Catalysis can be defined as a branch of science that deals with the acceleration of the rate of reaction by using a substance called a catalyst, and photocatalysis is a type of catalysis involving the utilization of light (photon) energy as a driving force for catalyzing the reaction and the catalyst substance is called photocatalyst.

Since then, the first semiconductor photocatalysis was reported by Fujishima and Honda in 1972 for water splitting into H_2 and O_2 by using semiconductor TiO_2 as anode and Pt as cathode [11, 12], extensive research on semiconductor photocatalysis has been conducted, and so far many semiconductor materials that enable light absorption in UV and visible regions have been developed for various applications including degradation of toxic organic pollutants in wastewater.

In the basic mechanism of semiconductor photocatalysis, the photocatalyst material absorbs light (UV, Visible or IR) energy greater than the width of the band gap energy of the semiconductor, which induces the excitation of electrons from the valence band to the conduction band and leaves holes behind in the valence band of semiconductor. These photo-induced electrons (Conduction band) and holes (Valence band) move to the surface of the catalyst and then promote redox reactions by reacting directly with the adsorbed toxic organic contaminants present in wastewater or by producing some other highly oxidizing and reducing species such as OH^\cdot and O_2^\cdot via reacting with water as well as hydroxyl ion and adsorbed oxygen molecules [4, 9, 12, 13]. However, the direct participation of the photo-induced electrons and holes rarely occurs as the amount of water molecules present is very large compared to the contaminants [4, 13]. When the photo-excited electron reacts with the adsorbed dissolved oxygen on the surface of the catalyst, it reduces the dissolved oxygen and gives rise to a superoxide radical anion ($O_2^{\cdot-}$). Furthermore, this superoxide radical can get protonation and form hydroperoxyl radical (HOO^\cdot). On the other hand, the hole reacts with water as well as hydroxyl anion (HO^-) and forms hydroxyl radical (HO^\cdot) [14, 15]. These radical species can mineralize the organic pollutants. However, the generation of these radical species is allowed only if the potential of the corresponding reaction falls within the potential gap of the valence band and conduction band of the photocatalyst. For instance, TiO_2 has three crystalline phases: anatase, brookite and rutile. The anatase phase has a conduction band potential of $E_{CB} = -0.51V$ at $pH = 7$ and the valence band potential of $E_{VB} = +2.69V$ at $pH = 7$ [15]. So, both the reduction of adsorbed oxygen ($E_{O_2/O_2^{\cdot-}}^0 = -0.33V$, $E_{O_2/HOO^\cdot}^0 = -0.45V$) and oxidation of water and hydroxyl ion ($E_{H_2O/HO^\cdot}^0 = +0.82V$, $E_{HO^-/HO^\cdot}^0 = +2.29V$) [15] can take place since their potential falls within the gap of conduction and valence band potentials of the catalyst. However, in the case of the rutile phase, it has the conduction band potential of $E_{CB} = -0.31V$ [15], which is less negative than the potential for reduction of dissolved oxygen, so the reduction reaction cannot take place. In addition, a scavenging reaction such as the recombination of the photo-induced electron-hole pair can also take place, which occurs at a very short time and retards the rate of redox reaction. So, for an efficient photocatalyst material, the photo-induced electron-hole pair would have a low recombination rate, high separation and high diffusion rate to the surface of the catalyst. Fig. (1) shows the

SUBJECT INDEX

A

Acid 121, 234
 citric 121
 humic 234
 Activity 228, 232
 antifungal 228
 phosphatase 232
 Acute respiratory syndromes 239
 Adsorption energy 202, 206, 210, 212, 215,
 249, 251, 252, 253, 254, 255, 256
 integrated oxygen 210
 Air 2, 111, 240
 pollutant remediation 240
 purification 2, 111
 Alcoholysis 264
 Alloying of nanomaterials 270
 Alloys, bimetallic 204
 Aluminium membrane, porous 25
 Anisotropy 167, 177, 179
 elastic 179
 Anthropogenic 60, 237
 productions 60
 sources 237
 Anti-fungal agent 227
 Anti-microbial agents 226
 Antibacterial agents 227
 Antimicrobial 27, 227
 agents 27
 Coating 27
 Antisite migration 207, 214
 configurations 207
 effects 214
 Atomic-simulation environment (ASE) 206
 Autoclave conditions 266, 270
 Autonomic nervous system 239

B

Ball milling 269, 270, 271, 276
 mechanical 269
 method 269

process 271
 Behavior 26, 99, 104, 153, 159, 166, 171, 177,
 182, 195
 macroscopic mechanical 195
 metallic 99, 104, 153, 159, 182, 195
 Bioelectrocatalysis 19
 Biotransformation 225
 Boltzmann's constant 186

C

Calculated elastic constants 148
 Calculations, electronic-structure 160
 Capillary liquid electrode 273
 discharge (CLED) 273
 microplasma 273
 Carbon-based nanoparticles 228, 237
 Catalyst 2, 3, 12, 13, 15, 203, 205, 284, 285,
 287, 288, 289, 298, 299, 300, 302
 fuel cell 203
 nickel-based 2
 photosensitized 12
 Ceramic(s) 39, 80, 229
 dental 80
 industry 229
 monolithic 39
 Charge 14, 289, 292
 carriers, photo-induced 289
 separation property 14
 transfer mechanism 292
 Chemical 44, 103, 121, 203, 223, 250, 264,
 266, 267
 composition 121, 203, 223
 reactivity 44, 250
 stoichiometry 103
 vapour deposition method 264, 267
 waste 266
 Color rendering index (CRI) 112, 117, 127,
 128, 129, 135, 137
 Colossal dielectric constant (CDC) 78
 Combustion 45, 121
 method 121

Subject Index

reaction 45
Composites 8, 26, 39, 42, 62, 68, 70, 71, 73, 75, 77, 80
ceramic-based polymer 73
ceramic matrix 39
ceramics and ceramic 42, 62, 71, 75, 80
Compounds, toxic organic 292, 302
Concentration quenching effect 123
Conditions, thermodynamic 61
Contaminants, adsorbed toxic organic 285
Conversion 22, 42, 120, 128, 221
electrochemical energy 42
thermoelectric energy 22
Copper, polycrystalline 268
Corrosion 68, 182, 169, 203, 228
protection 228
resistance 182
Crystal lattice 71, 133, 187
atomic 187
distorted 71
Crystallized microphases 44

D

Debye temperature and heat capacity 159, 195
Degradation, pollutant 240
Density functional theory (DFT) 65, 143, 145, 155, 161, 170, 195, 203, 204, 206, 214
Dental implants 41
Deposition, chemical vapor 7, 169, 276
DFT theory 159
Dielectric 4, 39, 76, 77, 78, 81, 273
fluctuations 77, 81
properties 4, 39, 76, 77, 78
temporary 273
Diffuse reflectance spectroscopy 64
Diffusion of Lithium ions 101, 104
Direct exchange energy 208
Discovery, computational electrocatalyst 204
Disorder 42, 72
stoichiometric 42
Dispersion, global radiation 70
Dissolved 225, 285
organic matter (DOM) 225
oxygen 225, 285
DNA damage response 239
Dopant 49, 63
host compatibility 49
non-metallic 63

Advanced Materials and Nano Systems Part 3 313

Doping 51, 52, 53, 59, 60, 64, 130, 131, 133, 143, 149, 151, 154, 155, 288, 289, 290
concentration 51, 52, 53, 59, 60, 64
metal ion 288, 289, 290
Down-conversion 71, 119
luminescence 119
mechanisms 71
Drug delivery gene therapy 228
Duration 44, 47, 67, 168, 270
milling 270
Dyes Irradiation Light Synthetic Method 287

E

ECDP technology 273
ECM-Electrolysis 273
Economic facets 42, 71
Economical facet 55
Effect 14, 15, 72, 226, 227, 233
eco-toxicological 233
photocatalytic 14, 15, 226, 227
photoelectric 72
Elastic coefficients 148
Electrical 77, 109
conductivity 77
energy 109
Electrochemical 43, 47, 48, 49, 260, 273, 275
activity 48
discharge methods 273
discharge process (EDP) 260, 273, 275
impedance spectroscopy 49
kinetics 43, 47
process 273
Electrochromic smart window 26
Electrolyte 18, 38, 43, 79, 273, 274, 276
material 43
polymer 79
Electromagnetic field 27
Electron 19, 289, 290
hole recombination 289, 290
transfer processes 19
Electronic 70, 96, 97, 126, 127, 130, 131, 132, 133, 134, 154, 155, 182, 228, 229, 230, 250, 252, 254, 256
behaviour 254
devices 70, 228, 229, 230
properties 96, 97, 154, 155, 182, 250, 252, 254, 256
transition 126, 127, 130, 131, 132, 133, 134

Electrons 1, 5, 6, 10, 12, 13, 17, 18, 19, 20, 22, 61, 63, 110, 133, 288, 289, 298
 photogenerated 1, 10, 61
 transferring 12
Embedded atom method (EAM) 204
Emission, blue 130
Endothermic segregation energy 214
Energy 14, 18, 22, 72, 95, 250, 284
 crisis 14, 95
 density 250
 electromagnetic 22
 photon 18, 72
 sunlight 284
Energy sources 21, 60, 62
 pollutant-free 60
 radiation-induced 21
 solar 62
Energy transfer 16, 20, 21, 69, 119, 123, 124, 129, 130, 131, 132, 133, 134
 plasmon resonant 16, 20, 21
Environment 27, 206, 220, 221, 222, 223, 224, 226, 227, 228, 229, 230, 231, 233, 240, 241
 atomic-simulation 206
Exothermic 43, 121
 electrochemistry 43
 reaction heats 121

F

Factors 9, 60, 61, 75, 78, 118, 130, 135, 181, 221, 271, 272, 298
 abiotic 221
 shear anisotropic 181
Fermi energy 148, 150, 152
Ferroelectricity 143
Field 97, 292
 effect transistor 97
 electromagnetic mechanism 292
Food packaging 222
Free energy variations 43
Freshwater 25, 223, 226, 234, 235
 aquatic systems 223
 ecosystems 234, 235
Fuel 1, 239
 fossil 239
 green 1
Fuel cell(s) 39, 42, 43, 47, 48, 54, 56, 62, 79, 80, 203
 application 42

 membrane 203
 technology 48, 54, 56, 79
 proton exchange membrane 43
 solid oxide 39, 47

G

Gas 230, 250, 267
 phase processes 267
 sensors 230, 250
Glasses 71, 121, 268
 fluorine-doped tin oxide 268
Gold 10
 nanoshells 10
 nanosphere 10
Green nanoparticle synthesis 276
Groundwater regulation 234

H

Harmful organochlorine pesticide 227
Heat 26, 270, 271
 absorption 26
 energy 270, 271
Heating 22, 25, 27, 121, 123, 237
 artificial 27
Hematopoiesis 235
High processing time 266
Hydrolysis reaction 2
Hydrothermal 8, 266, 267, 294
 method 266, 267, 294
 process 8, 266
 synthesis technique 8
 technique 266

I

Imaging 222, 231
 biomedical 231
 medical 222
Immune system 235
Implanted mechanical flexibility 80
Industrial products 39, 220, 237
 nanoparticle-based 220
Ionic 42, 48, 50, 51, 181
 bonding 181
 conductivity 48, 50, 51
 mobility 42

Subject Index

K

Kinetic energy 56, 206, 270

L

Laser hypothesis 271

Lattice 55, 71, 79

 damage 79

 disorder 55, 71

Legitimate use 61

Light 110, 117, 118, 120, 128, 131, 135

 efficiency 117

 emission 110, 118, 120, 128, 131, 135

Liquid cathode glow discharge (LCGD) 273

Localized surface plasmon resonance (LSPR)

 2, 6, 10, 12, 14, 18, 19, 291, 292

Low energy electron diffraction (LEED) 205

Lowest unoccupied molecular orbital (LUMO) 12

Luminescence response 69

Luminous efficacy 115, 116

M

Mass 65, 72, 73, 80

 absorption coefficient (MAC) 72, 73, 80

 storage property 65

Material 6, 11, 42, 76, 118

 composition 6, 11

 processing techniques 76

 polycrystalline 42

 polymer 118

Materialistic architecture 58

Maxwell's equation 3

Mechanical 55, 63, 148, 159, 161, 163, 165,

 168, 177, 179, 195

 properties 148, 161, 163, 165, 168

 stability 55, 63, 159, 177, 179, 195

Medical diagnostics 10

Mesoporous silica 8

Metabolic activity 228, 233

Metal-semiconductor plasmonic photocatalyst

 6

Metallic properties 169

Metallurgical industries and chemical

 industries 237

Methods, non-toxic 241

Microbial cells 27

Advanced Materials and Nano Systems Part 3 315

Mineralizing agent 46

Molecularly-imprinted polymers (MIPs) 241

Monkorst-Pack method 170

Monolayers 97, 143, 144, 146, 148, 149, 150,

 152, 153, 154, 155, 205

 carbon-doped 153, 154

N

Nanoparticle(s) 55, 73, 74, 220, 221, 222, 226,

 232, 234, 237, 238, 239, 241, 260, 275

 inorganic 226

 production 275

 toxic 237

Nanoscale devices 27

Nature 38, 43, 44, 45, 46, 47, 51, 68, 69, 72,

 224, 229

 anti-corrosive 229

Neutrophils 235

Nuclear reactors 67, 160, 169

Nutrient 225, 234

 cycling 225

 recycling 234

O

Organic 44, 285

 -inorganic hybrid polymer 44

 pollutants, toxic 285

ORR reaction 203, 214

Oxidation, photocatalytic 66

Oxidative stress 230, 231, 233

Oxygen 48, 51, 62, 72, 77, 78, 79, 202, 203,

 204, 205, 206, 210, 211, 212, 213, 214,

 215, 239, 273, 285, 289

 adsorbed 211, 285

 adsorption 206

 reduction reaction (ORR) 202, 203, 204,

 205, 206, 212, 215

 releasing 203

 supply 239

 vacancies 48, 72, 77, 78, 79, 289

P

Photo 7, 8, 225

 deposition 7, 8

 transformation 225

Photocatalysts, plasmonic semiconductor 291

- Photocatalytic 1, 2, 12, 13, 14, 15, 16, 61, 62, 63, 64, 66, 229, 230, 239, 289, 290, 291, 292, 295, 298, 299, 301
activity 12, 13, 61, 62, 63, 64, 66, 230, 289, 290, 291, 292, 295, 298, 301
degradation 1, 14, 15, 16, 229, 239, 299
destruction 15
hydrolysis 1, 2, 13, 14, 16
mechanism 1
Photochemical processes 2
Photodegradation 230, 237, 301
Photoelectric mechanism 21
Photoelectron spectroscopy measurement 97
Photosynthesis 228, 233, 294
Photovoltaic cells 229
Physical vapor deposition (PVD) 169
Physiochemical transformation 223, 224, 233
Plants 222, 227, 232
tobacco 227, 232
tomato 232
wastewater treatment 222
wheat 232
Plasmon 6, 19, 21, 25, 27, 291
dynamics 19
energy 21
enhanced fluorescence 27
enhanced solar desalination system 25
resonance 6, 291
Plasmonic 8, 12, 21, 24, 27, 29
activity 8
mechanism 21
metal 12
metal-semiconductor nanoparticles 29
sensing 27
solar desalination method 24
Pollutants 61, 237, 240, 241, 276
chemical 276
remediation, organic 237
removing environmental 241
toxic 61, 240
Pollution, environmental 14, 230
Polymerization technique 241
Pressure 44, 121, 123, 159, 168, 171, 172, 175, 185, 188, 192, 273
atmospheric 273
PRET process 20
Process 60, 63, 202, 209, 221, 294
biogeochemical 221
endothermic 202, 209
natural 221
photocatalytic 63, 294
thermochemical 60
Projector-augmented wave method 97
Properties 18, 26, 38, 39, 49, 59, 74, 120, 121, 143, 144, 150, 160, 161, 162, 166, 168, 169, 203, 222, 223, 230, 235, 237, 240, 241, 249, 260
biochemical 230
catalytic 18
ceramic 169
electrical 59, 166
electrophysical 49
half-metallic 150
heat-blocking 26
metallic 249
photo-oxidative 240
photocatalytic 237
physiochemical 235, 237
thermal 166, 168
Proton 39, 43, 45, 46, 47, 48, 50, 51, 203, 204, 232, 233
conducting solid oxide fuel cells (PCSOFC) 39, 47
conductors (PCs) 43, 45, 46, 47, 48, 50, 51, 232, 233
exchange membrane fuel cells (PEMFC) 43, 203, 204
- Q**
- Quenching, thermal 119, 124
- R**
- Radiation, electromagnetic 66, 271
Reactive oxygen species (ROS) 27, 222, 231
Redox reactions 47, 61
electrochemical 47
photo-induced 61
Reduced graphene oxide (RGO) 295
Reduction, electrospinning 11
Removal 227, 235, 241, 236, 283, 284
pollutant 241
- S**
- Salt flux dissolution (SFD) 77, 78
Scanning electron microscope 262
Segregation energy 206, 208, 210

Subject Index

Semiconductor 283, 284, 291, 299
 photocatalyst 299
 photocatalytic activity 291
 photocatalysis, heterogeneous 283, 284
SERS sensitivity 10
SFD technique 77
Sink, photo-induced electron's electron 17
Soil 220, 221, 222, 225, 226, 232, 233, 239
 agricultural 232
 biosolid-laden 226
 heavy metal-contaminated 233
 community 226
 microbiota 225
Sol-gel 7, 121, 264, 265
 methods 7, 121, 264, 265
 process 264
Solar 21, 25, 60, 62, 63
 energy 21, 25, 60, 62
 radiations 62, 63
Solid oxide 39, 44, 46, 47
 electrolytes 44
 fuel cells (SOFC) 39, 46, 47
Solid state reaction (SSR) 43, 58, 78
Solution anode glow discharge (SAGD) 273
Solvothermal process 8
Spatial separation 294, 295
Stability, thermodynamic 176, 195
Stiffness, high elastic 160
Stoichiometric deviations 79, 81
Storage 21, 60
 magnetic memory 21
 technology 60
Surface 4, 6, 14, 19, 21, 23, 24, 27, 283, 288,
 291, 292, 295, 302
 plasmon resonance (SPR) 4, 6, 14, 19, 21,
 27, 283, 288, 291, 292, 295, 302
 propagation plasmons (SPP) 6, 23, 24

T

Techniques, flash pyrolysis 51
Thermal 10, 79, 166, 167, 168, 169, 187
 ablation therapy 10
 conductivity 79, 166, 167, 169, 187
 shock resistance 168, 169
Thermo-mechanical properties 159
Thermodynamics 185
Thermoset polymers 74
Tight-binding theory (TBT) 204
Transformation 220, 224, 225, 226, 239

Advanced Materials and Nano Systems Part 3 317

 chemical 224, 225, 239
 environmental 220
 physicochemical 226
Transition metal dichalcogenides (TMDs) 96
Transmission electron microscope 164

U

UV light irradiation 301, 302

V

Vacuumed environment 276

W

Waste 228, 229, 284
 domestic 284
 toxic 229
Wet 7, 73, 250, 264, 266
 chemical exfoliation method 250
 chemical methods 73, 264, 266
 impregnation method 7
Wetness impregnation method 8
Wireless 38, 74, 81
 communications 38, 74
 data transmission 81



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