

## Preface

Nanoscience has been defined as the manipulation of matter at the nanoscale, as well as the discovery of new nanomaterials with fascinating properties (mechanical, electrical, optical, thermal, catalytic, etc.) and performances due to the quantum size effect, whereas Nanotechnology deals with the manufacturing of nanodevices. Nanotechnology offers a broad range of technological applications and industries including semiconductors, auto and aerospace, pharmaceutical and biomedical, cosmetics, biotechnology, energy and environment, food, forensic, military, etc. Known as the 5<sup>th</sup> industrial revolution, it has and continues to attract a large number of scientists worldwide. It is reported that by 2015, Nanotechnology may spawn a \$ 1 trillion market and the job projection is around two million with additional 5 million jobs in support industries. Additionally, the emergence of Nanotechnology has created a new dynamism in our scientific and academic world: (1) drastic increase of the research funds towards nanotechnology and national nanotechnology initiatives were developed by many countries; (2) the number of conferences and publications (papers, books, proceedings) has increased drastically due to the extensive research work carried out by the researchers; (3) new established academic programs at all levels; (4) new courses and disciplines emerged including nano-chemistry, nano-physics, nano-biotechnology, nano-medicine, nano-engineering, nano-ethics, etc; (5) commercialization of new products and the establishment of new technologies and industries based on nanotechnology leading to the creation of new and important number of jobs, which will have great effects on the future of global economy; (6) new journals and books which attract a wide and large audience; etc.

The handbook consists of 2 volumes with a total number of 19 chapters covering a wide range of topics from point of view experimental, fundamental, and applications view, written by experts and eminent scientists in each field.

This handbook will present experimental and fundamental approaches and in depth understanding of the chemical/physical/mechanical/electrical/biological/etc. properties of nanostructured/advanced materials followed by some potential applications in biomedical field, renewable energy, semiconductors industry, etc. In addition, it will promote the emerging field of nanotechnology in various science and engineering disciplines.

This handbook contains various hot topics related to energy conversion and storage, biomedical field, semiconductors, construction, telecommunication, etc., and thus will target a large audience such as academics, scientists, post-graduates students, engineers, etc.

The first chapter “Self-Healing Materials Systems as a Way for Damage Mitigation in Composites Structures Caused by Orbital Space Debris,” consists of a review on materials self-healing when subjected to any chemical or/and mechanical or/and thermal, etc. It contains some important concepts (such as quantification of healing efficiency which can be assessed by various tests such as Fatigue, Tear, etc.)

and presents some self-healing systems including thermoplastic and thermosetting materials then coating systems for metallic structures, etc. The new concept/property of self-healing being considered in engineering applications is incorporated as during the design and manufacturing of materials, thus adding new functionality of self-repair for counteracting service degradation. Additionally, it was reported that self-healing results in increasing material lifetime, reducing replacement costs, and improving product safety. In terms of self-healing systems, a variety of polymers and metallic material can be used.

Chapter 2 is devoted to the study of functionalisation of carbon (fullerene, carbon nanotubes, graphene)-based nanocomposites by ruthenium (Ru-bipyridine and Ru-terpyridine)-based complexes. This type of material shows some particular catalytic, electrochemical, or magnetic properties, and offers some potential applications in energy storage, biochemical sensors, photo-induced mechanical actuation, etc. The chapter focuses the synthesis methods of Bipyridine/Terpyridine ligands followed by Complexation with a metal center then Polymerization. After that, it presents the design of organic terpyridine Ligand spacer and polymerization complex for Nanohybrid; then it gives a detailed overview on the functionalization (non-covalent and covalent) of some carbon nanostructures such as fullerene, carbon nanotubes, and graphene, with Ru bipyridine and terpyridine complexes and finally self-assembly of Ru-terpyridine metal-connected diblock metallopolymers on graphene nanoribbons.

Chapter 3, “Nano Indentation Response of Various Thin Films Used for Tribological Applications,” addresses one of the most powerful techniques to investigate the mechanical properties of nanostructured materials. The author focused particularly on three materials, where a detailed study is presented: (1) ZrN films showing better corrosion resistance, improved mechanical properties, and warm golden color, thus very suitable for tribology applications; (2) amorphous carbon (a-C) known as Diamond-Like Carbon (DLC) and hydrogenated a-C:H films show the combination of some useful properties such as high nanohardness, good thermal conductivity, low friction coefficient, excellent wear resistance, ultra-smoothness, and chemical inertness (applications as magnetic hard disc, MEMS, biocompatible coating, etc.); and (3) W-S-C films with a nanocomposite structure and showing reasonable nanohardness and low friction coefficient, offering some potential applications such as space-related technologies, in vacuum or in aggressive environment. It was found that  $H/E$  and  $H^3/E^2$  ratios are considered as important parameters for coatings (H: nanohardness; E: elastic modulus).

Chapter 4, “Synthesis and Characterization of Iron Oxide Nanoparticles,” covers various aspects of Fe oxides including: (1) crystal structure and properties; (2) synthesis of different morphologies (nanospheres, nanowhiskers, nanocubes, nanoplates, nanoflowers, etc) using various methods; (3) dispersion and functionalisation of NPs using chemical processes such as ligand exchange, lipid encapsulation, polymer encapsulation, etc.; and (4) characterizations. Finally, some potential applications are presented.

Chapter 5, “Si-NWs: Major Advances in Synthesis and Applications,” is devoted to Si nanowires due to their potential and broad applications including the fabrication of integrated circuit, DNA sensors, array-based electrical and electrochemical systems, vertical surround-gate field effect transistor, high resolution Atomic Force Microscope, etc. The authors discussed some synthesis aspects of Si-NWs (lithography, physical, or chemical vapor deposition PVD or CVD methods, etc.) where a particular emphasis on catalyst role during Vapor-Liquid-Solid (VLS) growth mechanism. After that, Nanoscale Chemical Templating (NCT) using oxygen reactive materials was presented in detail followed by some potential applications of Si-NWs such as high-resolution AFM tips, photovoltaic cells, thermoelectric devices, and sensors to end up giving directions for future research on Si-NWs.

Chapter 6, “Principles of Raman Scattering in Carbon Nanotubes,” presents background and in-depth theoretical study of carbon nanostructures (nanotubes-CNTs, nanofibers-CNFs, graphene-G) properties

then focusing mainly on CNTs. It presents crystal structure and Brillouin zone, electronic band structure, and electronic Density Of States (DOS), which represent the backbone to access vibrational properties through Raman spectroscopy technique.

Chapter 7, “Pharmacokinetics of Polymeric Nanoparticles at Whole Body, Organ, Cell, and Molecule Levels,” deals with an important and crucial aspect of using Nanoparticles (NPs) for the biomedical field in terms of interaction at different levels. It starts by discussing the fate of NPs in the human body including efficiency and toxicity (which are strongly dependent on NPs shape, size, surface charge modifications, chemical composition, etc.), through ADME (Absorption, Distribution, Metabolism, and Excretion). Both experimental and modeling of pharmacokinetic of polymeric NPs have been presented. Then, pharmacokinetics at different levels of interaction inside the body was discussed from point of view of: (1) organ and sub-organ (lung, physiological, and biological barriers, tumor); (2) at cellular and sub-cellular level (cell surface binding, cellular uptake [endocytosis] kinetics, intracellular traffic and biotransformation kinetics, exocytosis kinetics); (3) at molecular level (protein binding, ligand-targeting).

Chapter 8, “Applications of Nanomaterials in Construction Industry,” presents a short overview of the potential and challenging applications of Nanotechnology in some areas of construction industry. In recent years, some studies devoted to the construction industry report on some interesting results such as: (1) nanoparticles (Zn, SiO<sub>2</sub>, Fe<sub>2</sub>O<sub>3</sub>, and halloysite clay) were embedded into a commercial epoxy resin for the enhancement of mechanical and chemical properties; (2) nano-SiO<sub>2</sub> was investigated as additive to cementation system, as well as nano-Fe<sub>2</sub>O<sub>3</sub> and nano-Al<sub>2</sub>O<sub>3</sub>; (3) nano-TiO<sub>2</sub> has been reported to produce “self-cleaning” and “depolluting” concrete as well as on roadway for pollution reduction; and (4) Carbon Nanotubes/Nanofibres (CNTs/CNFs) as potential candidates for use as nano-reinforcements in cement-based materials. Then the author discusses the challenges related to the use of nanomaterials as well as strategies for using them for the next ten years with some concluding remarks.

Chapter 9, “Silicon Nanostructures-Graphene Nanocomposites: Efficient Materials for Energy Conversion and Storage,” starts by highlighting energy resources/demand and that renewable energies represent only 16% (mainly solar), as well as some background about some fundamental concepts of solar cells energy efficiency and graphene as a potential material for energy conversion/storage. Then a particular focus on the potential use of Si-graphene for energy conversion and storage, Si-NWs/graphene heterojunction device for photoelectrochemical water splitting, Si-nanostructures/graphene as anode for Li-ion batteries showing high reversible discharge capacity, and supercapacitors. Finally, the authors present various methods for the preparation of various Si (NPs, NWs)/Graphene nanocomposites.

Due to the importance of graphene, Chapter 10, “Metal Oxide-Graphene Nanocomposites: Synthesis to Applications,” was dedicated to metal oxides / graphene composites due to their potential application. Several oxides / methods were presented: in-situ techniques such as precipitation (Fe<sub>3</sub>O<sub>4</sub>, CuO); sol-gel (TiO<sub>2</sub>); hydrothermal/solvothermal (ZnO); photo-assisted reduction (TiO<sub>2</sub>); microwave-assisted synthesis (Fe<sub>3</sub>O<sub>4</sub> and Co<sub>3</sub>O<sub>4</sub>); atomic layer deposition (TiO<sub>2</sub>); followed by ex-situ methods such as layer-by-layer self-assembly (TiO); etc. Then, the authors presented some potential applications of MO/graphene nanocomposites including Li-ion battery, supercapacitors, water purification, photovoltaic cells, biomedicine, and end by giving some future research directions.

Chapter 11, “In<sub>2</sub>X<sub>3</sub> (X=S, Se, Te) Semiconductor Thin Films: Fabrication, Properties, and Applications,” presents a review on the recent progress on Indium chalcogenide thin film semiconductor compounds as potential candidates as window/buffer-layer for photovoltaic devices. The authors discuss in more detail the evolution of structure and microstructure as well as optical/electrical properties modifications due to the deposition method (metal-organic chemical vapor deposition, atomic layer chemical vapor deposi-

tion, chemical bath deposition, spray pyrolysis, molecular beam epitaxy, etc.); the effect of deposition parameters (temperature, time, pH of the solution, type of substrate, etc.); and post-deposition treatment. Then a particular interest is devoted to the synthesis, characterizations and properties of some selected compounds including  $\text{In}_2\text{Se}_3$ ,  $\text{In}_2\text{Te}_3$ ,  $\text{In}_2\text{S}_3$  then ternary compounds such as  $\text{In}_2\text{Se}_{3-x}\text{Te}_x$ .

Chapter 12, “Carbon Nanotubes for Photovoltaics,” reports an in-depth review about the use of CNTs for PV. After introducing the outstanding physical properties of CNTs, the authors present some potential applications of CNTs in various PV/DSSS/OPV: CNT-Si hetero-junction solar cells based on aligned CNTs and Si-NWs, as well as some PV simulations based on molecular dynamics; Dye Sensitized Solar Cell (DSSC) where CNTs replace Pt as CNT as counter electrode; incorporating CNT networks in the cell’s conducting electrode to promote charge transport in the  $\text{TiO}_2$  layer, CNT as Transparent Conducting Oxide (TCO) layer which is usually Indium Tin Oxide (ITO) in DSSC; and CNTs in Organic PV devices (OPV). After that, the authors discuss a very important aspect of PV, trends to improve the efficiency, followed by a discussion and some recommendations and concluding remarks.

Chapter 13, “Overview on Hydrogen Absorbing Materials: Structure, Microstructure, and Physical Properties,” presents some important aspect of hydrogen storage in materials. The authors start by giving some fundamental background on hydrogen storage, thermodynamics, and kinetics, properties, and mechanisms. Then a particular focus is devoted to some potential materials including: binary hydrides; intermetallics ( $\text{LaNi}_5$ ,  $\text{FeTi}$ , Laves phases  $\text{AB}_2$ ); Mg-based materials; amorphous alloys; quasicrystals; carbon nanostuctures (nanofibers); light complex hydrides based on alkali-metals (Li, Na, Al, B); rare-earth based hydrides thin films with optical switchable properties; and zeolites.

Chapter 14, “Conductive Probe Microscopy Investigation of Electrical and Charge Transport in Advanced Carbon Nanotubes and Nanofibers-Polymer Nanocomposites,” is devoted to the fundamental and some experimental aspects to access some properties of CNTs-Polymer nanocomposites by using some advanced probe microscopies such as Atomic Force Microscopy (AFM); Electrostatic Force Microscopy (EFM); Current-Sensing Atomic Force Microscopy (CS-AFM). After that, a particular focus is dedicated to DC(AC)-EFM imaging of embedded CNT-polymer nanocomposites films, followed by a CS-AFM investigation of bulk and surface percolation as well as electrical conductivity measurements.

Chapter 15, “Nanostructured Materials for the Realization of Electrochemical Energy Storage and Conversion Devices: Status and Prospects,” presents an interesting overview on some nanomaterials as potential candidates for energy conversion and storage. After a good introduction related to fundamental aspects of electrochemical energy storage, the authors discuss each application separately: (1) nanocatalysts (Pt, Pt-M core-shell,  $\text{Pt}_3\text{M}$ , graphite- $\text{C}_3\text{N}_4$ , etc.) for fuel cells; (2) photoelectrochemical water splitting (such as nanocrystalline  $\alpha\text{-Fe}_2\text{O}_3$  and nano- $\text{CdSe}$ ); (3) dye-sensitized solar cells DSSCs (oxide semiconductors like  $\text{TiO}_2/\text{ZnO}/\text{SnO}$ , nanoporous film coated with oxides  $\text{Al}_2\text{O}_3/\text{SnO}_2/\text{ZrO}_2/\text{SrTiO}_3/\text{ZnO}$ , etc.); cathode for Li-ion batteries (such as  $\text{LiMO}_2$  and spinel-type  $\text{LiM}_2\text{O}_4$  where  $\text{M}=\text{Co}$ ,  $\text{Mn}$ , etc.); and anode for Li-ion batteries (graphite,  $\text{Li}_2\text{Si}_5$ ).

Chapter 16, “Nucleic Acids Based Nanotechnology: Engineering Principals and Applications,” focuses on the engineering of functional systems at the molecular level offering potential applications such as molecular sensors, actuators, drug delivery devices, etc. After a good introduction on some very important aspects such as nanobiotechnology, nanomedicine, etc., the author presents in more detail some applications such as: (1) passive nanostructures based on DNA using self-assembly; (2) engineering active nanostructures based on allosteric ribozymes; (3) RNA-based nanocircuits; (4) integrated RNA-based nanodevices with a complex logic function as a tool for molecular diagnostics; (5) allosteric ribozymes as

designer cis-acting gene control elements; and (6) gene silencing techniques via trans-acting ribozymes to end up with some future research work in this field.

Chapter 17, “Theoretical Assessment of the Mechanical, Electronic, and Vibrational Properties of the Paramagnetic Insulating Cerium Dioxide and Investigation of Intrinsic Defects,” presents a very detailed study of some properties (ground-state properties, elastic stiffness constants, and electronic structure with the inclusion of on-site Coulomb interaction, dielectric properties, lattice dynamic, and thermodynamic properties) of  $\text{CeO}_2$  by *ab-initio* calculations (calculations based on Density Functional Theory [DFT] as implemented in WIEN2K and CASTEP packages). A particular focus is dedicated to investigate the presence of intrinsic defects (oxygen or cerium vacancies) in un-doped  $\text{CeO}_2$  (cubic structure of  $\text{CaF}_2$ , space group Fm-3m) to create ferromagnetic behavior.

Chapter 18, “Implementation of Nanoparticles in Cancer Therapy,” is devoted to the application of nanotechnology in the biomedical field. The authors start by stating conventional method used for cancer therapy (surgery, radiotherapy, chemotherapy, etc.) then present how Nanoparticles (NPs) present a potential alternative. Then some general fundamental/experimental aspects related to some selected NPs that are used in drug delivery and targeting in cancer therapy are presented, including Polymeric NPs, Liposomal NPs, Dendrimer NPs, Protein NPs, Polymersome NPs, Inorganic NPs, etc. Additionally, the authors discuss NP toxicity and safety, followed by some major cancer targets for NPs systems (including cell marker targeting *via* antibodies, targeting signaling pathways, niche targeting, angiogenesis-associated targeting) as well as targeting schemes (including passive, active, and triggered targeting), and end with nanoparticle-mediated gene therapy with future research perspectives.

Chapter 19, “Understanding the Numerical Resolution of Perturbed Soliton Propagation in Single Mode Optical Fiber,” deals with an important matter related to optical fibers used for telecommunications such as terrestrial broadcasting by a fundamental approach: how to reduce the noise to acceptable levels by acting on device parameters such as the structure of the fiber device. Then, the authors present a detailed theoretical background to study soliton propagation in a mono-modal optical fiber followed by frequency domain filter system, which allow one to create a model followed by simulations using numerical models that allow one to understand the behavior of solitons.

This handbook presents the recent advances and future prospects of several nanotechnology applications. In addition, it highlights various technological applications in biomedical, renewable energy, electronics, etc., which will improve future life by offering solutions in health, energy, etc. It contains chapters dealing with various topics starting from experimental approaches, simulation, and modeling, and ending with applications and future perspectives.

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