SYNTHESIS AND CHARACTERIZATION OF NANOMATERIALS: STUDY OF THEIR PROPERTIES AND POSSIBLE APPLICATIONS

ABSTRACT

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ABSTRACT
Polymers materials are of profound interest to society and are replacing metals in diverse fields of life, they seem to provide a solution to almost every deed in life, from preparing daily commodities to the highly sophisticated artificial heart valve. Since desirable properties can be conveniently attained by tailoring the polymer structure and also by incorporating additives. Scientists have been enthusiastic to explore the possibility of transforming insulating polymers into materials envisaging such special characteristics like low density, low cost, ease of fabrication, flexibility of design, low energy and labour requirements for fabrication and processing, which make them a class of versatile materials capable of meeting even the most stringent specifications of modern technology. Due to the excellent properties synergistically derived from polymer and inorganic materials, polymer nanocomposite materials are used in many fields. In the recent years, these nanocomposite materials replaced the pristine polymers due to their strength and stiffness and possess evolutionary means of achieving properties that cannot be realized with single materials.
The work embodied in Ph.D. thesis entitled “Synthesis and Characterization of Nanomaterials: Study of their Properties and Possible Applications” is divided into six chapters.

Chapter. 1.
Introduction
Nanoscience and nanotechnology are extending actively in almost every field of technology, science and engineering as it is possible to develop super functional properties of material at nano scale. In view of the fact that the nanoscale properties of the material are different from macroscopic properties thus become the basis of development of nanotechnology. In nanotechnology materials are designed, characterized and applied by controlling their size to form materials, devices and systems with new properties and functions. The surface area effect becomes exceptionally important as soon as materials are considered at nano scale. Nanoscience is the study of phenomena and application of materials at atomic, molecular and macromolecular range where properties differ considerably from those at larger scale. Therefore, the field of nanocomposites and nanomaterials become the basis for further researches to investigate their structural features and applications.
Chapter 2.

Review of literature and characterization techniques.

The chapter 2. of the Ph.D thesis describes the review of literature in the relevant field of nanocomposites and nanomaterials, the aim and objectives of the research work done and the basic principles and theories, techniques involved in characterization of various nanomaterials such as FT-IR, SEM, TEM, TGA, DTA, Electrical Conductivity, etc.

Chapter 3.

Electrical conductivity, isothermal stability and ammonia sensing performance of newly synthesized and characterized organic-inorganic polycarbazole-titanium dioxide nanocomposite.

Electrically conductive polycarbazole-titanium dioxide nanocomposite (PCz/TiO₂) have been synthesized for the first time by in-situ chemical oxidative polymerization of carbazole (Cz) in the presence of titanium dioxide (TiO₂) nanoparticles. FTIR, SEM, TEM, XRD, TGA and DTA were used to characterize PCz/TiO₂ nanocomposites. The characterization results confirmed that there is a strong interaction between PCz and TiO₂ nanoparticles and the nanocomposites showed higher thermal stability than pure PCz. The composite showed electrical conductivity and isothermal stability in terms of DC electrical conductivity retention under ambient condition below 100⁰C. A nanocomposite based sensor was fabricated for the detection of aqueous ammonia, it was found that the resistivity of the nanocomposites increases on exposure to ammonia at room temperature (25⁰C) and there showed a linear relationship between the responses and the concentration of ammonia. The comparative antimicrobial activities of PCz, its PCz/TiO₂-7 nanocomposite and ciprofloxacin drug with different bacteria have also been studied.

Chapter 4.

Interaction mode of polycarbazole-titanium dioxide nanocomposite with DNA: molecular docking simulation and in-vitro antimicrobial study.

Polycarbazole-titanium dioxide (PCz/TiO₂-8) nanocomposite was synthesized for the first time by in-situ oxidative polymerization with APS as an oxidizing agent in the presence of TiO₂ nanoparticles and characterized by SEM, TEM, FTIR, DTA and TGA techniques. The results of analysis confirmed that the incorporation of TiO₂ in
PCz indicating the formation of nanocomposite due to strong interaction between TiO₂ and PCz matrix responsible for enhancing the properties as compared to pristine PCz. The PCz/TiO₂-8 nanocomposite was tested for antimicrobial activity and was found to exhibit activity against gram negative and gram positive strains at micromolar concentrations. SEM and TEM results show that PCz has polymerized on the surface of the TiO₂. The four types of 3D molecular field descriptors or field points as extrema of electrostatic, steric, and hydrophobic fields are explained. These field points are used to define the properties necessary for a molecule to bind in a characteristic way into a specified active site. A molecular docking simulation was used to predict the modes of interactions of the drugs (PCz and PCz/TiO₂-8) with DNA. The molecular docking conclusion indicated that the modes of interactions between two (PCz and PCz/TiO₂-8) and DNA helix can be regarded as groove binding.

This chapter deals with the synthesis of polymers, PCz and its nanocomposite, PCz/TiO₂-8 have been exploited as new DNA binding materials strived vociferously for the first time to the best of the knowledge for molecular simulation applying field description parameter and created pharmacophore models for investigating the possible binding sites. These studies revealed that compounds (PCz and PCz/TiO₂-8) with wide chemical diversity can enhance our understanding of ligand-receptor interactions. Moreover, computer-aided molecular simulation studies were performed to visualize the binding modes of PCz and its PCz–TiO₂-8 nanocomposite with DNA bases.

Chapter 5.
Photocatalytic and biological studies on electrically conductive and isothermally stable POT-TiO₂ nanocomposites.

The Poly(o-toluidine)-titanium dioxide (POT-TiO₂) doped with organic sulfonic acids (dodecylbenzene sulfonic acid, camphor sulfonic acid, and p-toluene sulfonic acid) were synthesized by in-situ polymerization of o-toluidine (OT) with the TiO₂ nanoparticles. The thermogravimetric analysis (TGA) and differential thermal analysis (DTA), Fourier transform infrared (FTIR) spectroscopy, X-ray diffraction (XRD) analysis, transmission electron microscopy (TEM), scanning electron microscopy (SEM), were used to characterize DBSA/POT-TiO₂, PTSA/POT-TiO₂ and CSA/POT-TiO₂ nanocomposites. The characterization results demonstrated that the
nanocomposites revealed superior thermal stability than that of pure POT. The characterization results of investigation confirmed that the inclusion of the TiO$_2$ nanoparticles in pristine POT signifying the development of nanocomposites as a result of the interaction among the TiO$_2$ nanoparticles and pure POT moiety accountable for higher thermal stability than that of pure POT. The nanocomposite display isothermal stability as well as electrical conductivity in terms of DC electrical conductivity retention under ambient condition below 90°C. The anthelmintic and antimicrobial and photocatalytic activities of pristine POT and its nanocomposites have also been studied with earthworms and separate bacteria.

Chapter 6.

Synthesis and characterization of cobalt selenide nanoparticles and assessment of its photocatalytic activity.

This chapter deals with the synthesis, characterization, and photocatalytic studies of cobalt selenide (CoSe) nanoparticles (NPs). The Cobalt Selenide nanoparticles (denoted as ‘CoSe NPs’) were synthesized by simple and controlled precipitation method and were characterized using transmission electron microscopy and X-ray diffraction, which showed that the NPs are highly crystalline, circular and having particle size of 20-25 nm in diameter. Furthermore, structural, optical, thermal and photocatalytic properties of the synthesized CoSe NPs were also evaluated. The TGA/DTA results revealed that the Co and Se are strongly interacting, which is also supported by the selective area EDAX analysis. The application of synthesized CoSe NPs for an efficient photocatalysis of Rhodamine B (RhB) dye under UV light irradiation, resulted in the productions of reactive oxygen species (ROS) by the CoSe NPs. It may be concluded that the synthesized CoSe NPs have great environmental significance based on the results obtained. Moreover, the energy band gap as calculated by the Tauc relation was found to be in the range of Eg=1.8 eV.
LIST OF PUBLICATIONS:

1. Electrical conductivity, isothermal stability and ammonia sensing performance of newly synthesized and characterized organic-inorganic polycarbazole-titanium dioxide nanocomposite.

2. Interaction mode of polycarbazole-titanium dioxide nanocomposite with DNA: Molecular docking simulation and in-vitro antimicrobial study.
   Farha Firdaus, Noor-e-Iram and Mohd Shoeb Khan [Communicated]

3. Photo catalytic and biological studies on electrically conductive and isothermally stable POT-TiO$_2$ nanocomposites
   Farha Firdaus, Noor-e-Iram and Mohd Shoeb Khan [Communicated]

4. Synthesis and characterization of cobalt selenide nanoparticles and assessment of its photocatalytic activity
   Farha Firdaus, Noor-e-Iram and Mohd Shoeb Khan [Communicated]