

## Abstract

The aim of thesis is to prepare polythiophene, multiferroic BiFeO<sub>3</sub> and their graphene based nanohybrid for photocatalytic and solar cell applications. The work describes synthesis, characterization, device fabrication and future prospective of polythiophene, BiFeO<sub>3</sub> nanoparticles and BiFeO<sub>3</sub>-graphene nanohybrid. Nucleation and growth process of electrodeposited polymer determines its morphology, thus its function and applicability. Here, we show how minute changes in the polymerization condition, like current density and electrolyte concentration, alter nucleation pattern of polythiophene. Polythiophene was electrochemically synthesized on indium tin oxide (ITO) coated glass slides using boron trifluoride diethyl etherate (BF<sub>3</sub>.Et<sub>2</sub>O) electrolyte. Two distinct morphologies of the polythiophene *i.e.*, dendritic and compact uniform films have been obtained. Due to the higher surface roughness in the dendritic structured samples electrical properties seem to decrease. However, dendritic structures can efficiently guide light and proved to be a good candidate for the photonic and energy application. On the other hand, compact uniform films of polythiophene shows enhanced redox capacity and high electrical conductivity. It also shows substantial photovoltaic performance when used as a Hole-Transporting Layer (HTL) in the photovoltaic device. This shows that electrochemically synthesized polythiophene with/without dendrites has potential application in the field of optical waveguide and photovoltaics.

BiFeO<sub>3</sub> nanoparticles were prepared by simple green route as well as conventional synthetic route. An extract of *Calotropis gigantea* flower was used as a reaction medium in the green route. In each case so formed BiFeO<sub>3</sub> nanoparticles are of comparable quality. These pure phase BiFeO<sub>3</sub> nanoparticles were first time surface modified effectively using two silanes viz., tetraethyl orthosilicate and (3-Aminopropyl)triethoxysilane. Modified BiFeO<sub>3</sub> comprise superior dispersion characteristics, improved ferroelectric properties and favorable magneto-dielectric properties than unmodified BiFeO<sub>3</sub>. The BiFeO<sub>3</sub> nanoparticles grafted on graphene nanosheets (BiFeO<sub>3</sub>-g-GNS), and their morphology, photocatalytic activity, structural and magnetic properties were investigated. Well decorated graphene sheets with spherical perovskite type BiFeO<sub>3</sub> nanoparticles of size 50–80 nm are obtained as confirmed by FESEM and HRTEM analysis. Enhanced interactions between BiFeO<sub>3</sub> and graphene are observable from XPS and Raman spectra. BiFeO<sub>3</sub>-g-GNS exhibits enhanced photovoltaic performance and photocatalytic activity over pristine BiFeO<sub>3</sub>. These improvements are attributed to increase in absorption intensity in the visible region (above 550 nm), reduced band gap, and limited recombination of charge carriers by the incorporation of graphene. Overall, electrodeposited polythiophene, BiFeO<sub>3</sub> and their graphene based nanohybrid have potential application in the field of photovoltaics and photocatalysis.

**Keywords:** Structured Polythiophene, Electrochemical Synthesis, Solar cell, Multiferroics, Bismuth Ferrite, Graphene, Photocatalysis, Waveguide, Nanophotonics.