SUMMARY OF THE THESIS

The work incorporated in the thesis is based on the synthesis, characterization and application of modified TiO$_2$ nanoparticles as photocatalysts and antimicrobial agents. The thesis is divided into five chapters. First chapter gives a brief introduction with reference to Photocatalysis and photocatalysts, the second chapter describes the experimental methodology used for preparing TiO$_2$ samples and details of the characterization techniques employed in this present work. The third, fourth and fifth chapters account for the results and discussions related to synthesis and applications of TiO$_2$, and Nd doped and Ag coated TiO$_2$ and TiO$_2$-Fe$_3$O$_4$ nanocomposites respectively. The data is supported with well reviewed list of references and outcome of the work in the form of list of publications is given at the end of thesis.

First chapter begins with the overview of challenges of 21$^{st}$ century and the discussions about the application of photocatalysis as a principle key to overcome these challenges. The use of TiO$_2$ is justified appropriately. Various methods used for synthesizing TiO$_2$ have been briefed along with their advantages and disadvantages. Further, the drawbacks of the TiO$_2$ as a photocatalyst are also mentioned together with the ways of modifying it so as to improve its photocatalytic efficiency with the help of well reviewed survey of literature. The chapter concludes with the scope of the present work.

Second chapter accounts for the detailed experimental methodology and characterization techniques adopted for the synthesis and characterization of TiO$_2$. Various methods such as sol-gel, sol-hydrothermal and ultrasound assisted sol-gel and sol-hydrothermal were used for the synthesis of modified TiO$_2$. The details about the photodeposition and sonochemical deposition of noble metals on TiO$_2$ are given therein.

The characterization techniques used for analyzing the samples have been briefly discussed together with the basic principles involved. The different techniques include Fourier transform infrared (FTIR), Diffuse Reflectance UV-Visible (DRUV) and Photoluminescence (PL) spectroscopy, X-ray Diffraction (XRD) analysis, N$_2$-Brunauer–Emmett–Teller (BET) surface area analysis, Scanning electron microscopy
(SEM) and Transmission electron microscopy (TEM) and Vibrating sample magnetometry (VSM). The protocols used for the photocatalytic and antimicrobial investigations of the synthesized materials are also illustrated in this chapter.

The third chapter presents the results on TiO$_2$ nanoparticles synthesized by various methods such as sol-gel, sol-hydrothermal and ultrasound assisted sol gel and sol hydrothermal methods. Small amount of brookite phase (less photoactive) observed in ultrasonically treated samples could be completely eliminated by addition of mineralizers during the sonication treatment. Among all the mineralizers (Hexamine, Glycine, Urea and NaOH), glycine is found to be the best yielding particles with smallest size of 2-3 nm which has been confirmed from the TEM analysis of the samples. Additionally, to achieve enhanced charge separation, some of the catalysts were coated with silver ions by sonochemical and photochemical method of deposition. Amongst the two, sonochemical method of deposition yields product with better optical and morphological properties.

The fourth chapter is divided into two sections. Fourth chapter section 1 includes the results of Ag (1%) coated Nd (0-5%) doped TiO$_2$ nanoparticles based on various characterization techniques. XRD analysis confirms the formation of anatase phase of TiO$_2$. Nd doping and Ag coating could be ensured from the EDAX analysis of the samples. The improvement in the optical properties of TiO$_2$ on Nd doping and Ag coating was confirmed by Diffuse Reflectance UV–Visible (DRUV) and Photoluminescence (PL) spectroscopy. The catalysts are found to be active in both UV and solar light, however, the degradation yields are lower in solar light in comparison with UV light. 1.0% Nd doping appears to be optimum, yielding highest degree of degradation in both UV and solar light irradiation.

Section 2 of this chapter reviews the results of the antibacterial activities of TiO$_2$, 1% Nd doped TiO$_2$ and Ag coated Nd doped TiO$_2$ nanoparticles in dark and solar light irradiation using *E. coli* and *S. aureus* bacterial strains. All the samples are found to be inactive in dark except Ag coated TiO$_2$ nanoparticles. In case of solar light irradiation, the extent of activity shows the order as undoped TiO$_2$ < Nd doped TiO$_2$ < Ag coated TiO$_2$. The mechanism of bactericidal action of the nanoparticles, in presence of sunlight has been explained with the help of microscopic analyses (SEM
and TEM). The bacterial damage is observed to proceed through initial perforation of the cell, damage of cell wall and finally the bacterial death.

**Fifth chapter** deals with the results of Fe$_3$O$_4$-TiO$_2$ magnetic nanocomposites. The presence of peaks corresponding to both, Fe$_3$O$_4$ and TiO$_2$ in the XRD diffractograms indicate the formation of crystalline nanocomposites. The magnetic properties of pure Fe$_3$O$_4$ and composite samples have been evaluated by the VSM analysis. The TEM micrographs reveal the formation of nanocomposites (heterojunctions) with TiO$_2$ particles surrounding the Fe$_3$O$_4$ nanoparticles.

The heterojunctions probably increase the rate of recombination in TiO$_2$ sample thereby decreasing the photocatalytic activity of the composite samples. Further, one of the composite samples (15% Fe$_3$O$_4$ -TiO$_2$) has been coated with the Ag ions which show the highest antibacterial activity as Ag acts as electron acceptors and reduce the rate of recombination reactions. This chapter also describes the results on the antibacterial activities of the Fe$_3$O$_4$, TiO$_2$, Fe$_3$O$_4$-TiO$_2$ and Ag coated Fe$_3$O$_4$-TiO$_2$ nanocomposites. The results indicate that the pure phase TiO$_2$, Fe$_3$O$_4$ and its composites do not show any antibacterial activity in dark as well as in light. However, the Ag coated composite sample shows significant antibacterial activity with lower MIC values.