CHAPTER - VI

SUMMARY, CONCLUSIONS AND FUTURE SCOPE

This chapter presents the summary of the research work carried out and the major conclusions arrived at. In addition, future scope of research work in this section is also pointed out.

6.1 Summary and Conclusions

Nanotechnology is an emerging field that spreads out in various fields which include physics, chemistry, materials, electronics, optics, electronics, information storage, sensors, communications, energy conversion, environmental protection, aerospace and many more. Materials reduced to nanoscale can show different properties when compared to what they exhibit on macroscale. Nanomaterials of metal oxides such as ZnO, TiO$_2$, SnO$_2$ etc. possess a variety of applications in the field of Nanotechnology.

Among the metal oxides, TiO$_2$ is a popular semiconducting material on the nanoscale because of its wide range of application in the field of photocatalysis to remove organic effluents. TiO$_2$ is a large band gap, 3-3.2 eV (for rutile and anatase phases respectively) semiconducting nanoparticle.

In this present work, pure (prepared and calcinated) and metal ions (Fe$^{2+}$, Zn$^{2+}$, Ag$^+$, Ni$^{2+}$ and Cu$^{2+}$ separately each with 3 different concentrations, viz 1, 3 and 5 wt%) doped TiO$_2$ nanoparticles have been successfully prepared by Sol-Gel method.
The prepared pure and metal ions doped TiO$_2$ nanoparticles are characterized structurally by X-ray powder diffraction (PXRD) and chemically by energy dispersive spectroscopy (EDS). The crystallite sizes of the TiO$_2$ nanoparticles are found out using Scherrer formula and Williamson–Hall plot model. The size calculated by both these methods matched well and are in the range from 9-44 nm. From the PXRD pattern the phase is identified as anatase and is confirmed by the JCPDS (JCODS 21-1272). The reflection in various planes indexed is in accordance with the JCPDS. The lattice parameter values of pure and metal ions doped TiO$_2$ nanoparticles are calculated. For all the samples, it has been observed that the volume of the unit cell either increases or decreases. Thus, it is concluded that the doped metal ions deform the crystal lattice without altering the crystalline phase.

The presence of elements Ti, O and the doped metal ions is clearly understood from the EDS spectrum. The presence of doped metal ions is further confirmed by the existence of doped metal ion in the EDS spectrum of metal ions doped TiO$_2$ nanoparticles.

The morphologies of pure and doped TiO$_2$ nanoparticles are identified from scanning electron microscopy and atomic force microscopy. The increased surface roughness is identified from AFM images of doped TiO$_2$ nanoparticles. SEM images show that the pure, Fe$^{2+}$ and Zn$^{2+}$ doped TiO$_2$ nanoparticles are in the cluster form. In addition, Ag$^+$, Ni$^{2+}$ and Cu$^{2+}$ doped TiO$_2$ nanoparticles show grain morphology with uneven distribution.
FTIR spectra reveal the presence of functional groups in the pure and metal ions doped TiO₂ nanoparticles. High intense peak below 1000 cm⁻¹ is mainly attributed to the Ti-O network vibrations of TiO₂ nanoparticles.

The samples are optically characterized by UV-Visible and Photoluminescence spectra. The optical band gap value of pure and metal ions doped TiO₂ nanoparticles are calculated from Tauc plot. All the samples show indirect bandgap values and decrease from 3.31 eV. This concludes that no quantum confinement effect is observed by the influence of doping. Photoluminescence spectra conclude that the PL emission spectra are mainly due to oxygen and self-trapped excitons. PL intensity is altered by metal ions and is either increased or decreased.

Decolourisation efficiency of pure and doped TiO₂ nanoparticles is identified from photocatalytic studies. 1, 3 and 5 wt% Zn²⁺ and 1 wt % Ag²⁺ doped TiO₂ nanoparticles show higher photocatalytic activity than pure TiO₂ nanoparticles. Other samples show lower efficiency than the pure TiO₂ nanoparticles because of higher rate of recombination. Hence, it is concluded that metal ions must be added with a minimum level to get enhanced photocatalytic performance.

In effect, the results obtained in the present study manifest that the method preferred is found to be an effective and economical one for preparing TiO₂ nanoparticles with high purity, smaller size, and is highly useful in optical and photocatalytic applications.
6.2 Future Scope

There is ample scope to synthesize pure and metal ions doped TiO$_2$ nanoparticles with various synthesis processes such as Solvothermal and Hydrothermal method.

In addition, in the present work, poor photocatalytic performance at higher doping concentration could be received. Therefore, metal ions doped TiO$_2$ nanoparticles with lower percentages shall be prepared by this method and their photocatalytic performance shall be analysed.

Moreover, it is possible to perform High Resolution Transmission Electron Microscopy (HR-TEM), Electrical studies, X-ray photoelectron spectroscopy (XPS), FT- Raman spectroscopy for TiO$_2$ nanoparticles.

Similarly, there is scope to find out the sensing behavior and solar cell efficiency of these pure and metal ions doped TiO$_2$ nanoparticles by fabricating relevant devices.