# ABSTRACT

The objective of the present thesis is laid on the synthesis and characterization of various concentrations (0.05,0.10, 0.15) of rare earth metal ion ($Ce^{3+}$ and $Nd^{3+}$) doped zinc oxide nanoparticles. The mentioned nanoparticles had been synthesized by co-precipitation method. The synthesized nanoparticles were characterized through X-Ray Diffraction (XRD), X-ray Photoelectron Spectroscopy (XPS), Scanning Electron Microscope (SEM), Transmission Electron Microscopy (TEM), Energy Dispersive X-ray analysis (EDAX), PhotoLuminescence (PL) spectra, Fourier Transform Infra-Red spectroscopy (FT-IR) and Micro-Raman studies in order to study the structural, morphological, elemental compositional, optical properties , functional group and phases respectively. The present work is also extended to determine the antibacterial and anticancer properties.

The X-ray diffraction of ZnO and various concentration of Ce doped ZnO revealed wurtzite hexagonal structure without any secondary phase of $Ce^{3+}$/ $Ce^{4+}$ ions with cerium oxide between $CeO_2$ and $Ce_2O_3$. The XPS measurement of Ce doped ZnO confirmed that the oxidation state of Zn (2p) signal has been splitted into two symmetric peaks corresponding to Zn ($2P_{3/2}$) at 1022.57 eV and Zn ($2p_{1/2}$) at 1045.57 eV. O (1s) asymmetric signal has been splitted into three symmetric peaks I1 (531.36 eV), I2 (532.63 eV) & I3 (533.64 eV) and the binding energy of Ce (3d) values were observed at 882.57 eV, 888.91 eV, 898.92 eV, 902.32 eV, 909.06 eV, 917.76 eV and 922.88 eV for $Zn_{0.90}Ce_{0.10}O$ NPs.

The morphological analysis of ZnO and Ce doped ZnO NPs were found to exihibit nanoflower and spherical like structure respectively. The Ce doped ZnO NPs agglomerates with each other due to the increasing

nucleation of $Ce^{3+}$ ions and subsequent growth of ZnO NPs. The elemental analysis showed the increase in percentage of Ce as the concentration of Ce in Ce doped ZnO increases. This confirmed the incorporation of Ce in Ce doped ZnO nanoparticles.

The photoluminescence emission spectra of ZnO and Ce doped ZnO NPs exhibited UV and Visible region which depends on nature as well as concentration of $Ce^{3+}$ ions. The Photoluminescence spectra of the ZnO and Ce doped ZnO NPs were observed with excitation wavelength 325 nm. The blue emission wavelength at 440 nm, 439 nm, 439 nm and 446 nm for ZnO and Ce doped ZnO NPs, is due to the single ionized Zn vacancies. Thus the changes in emission confirmed the substitution of Ce ion into ZnO lattice.

The FT-IR spectra showed the Zn-O stretching vibrations at 418 and 416 $cm^{-1}$ for ZnO and Ce doped ZnO NPs respectively. Raman studies also confimed the wurtzite structure of ZnO and Ce doped ZnO NPs. The phonon mode intensity has decreased with increase in Ce ion concentration.

The antibacterial studies were performed against a set of bacterial strains as Gram positive bacteria (*S. aureus and S. pneumonia*) and Gram-negative *(E. coli, P. aeruginosa, P. vulgaris, K. pneumonia, and S. dysenteriae)* bacteria. From the antibacterial activity, $Zn_{0.85}Ce_{0.15}O$ NPs possessed more antibacterial effect as compared to the other ZnO, $Zn_{1-x}Ce_xO$ (x=0.05 and 0.10) NPs. The cytotoxic effect of ZnO and Ce doped ZnO were analyzed in cultured (A549) human lung cancer cell line. Among which, $Zn_{0.90}Ce_{0.10}O$ NPs possesed the highest cytotoxicity activity. With respect to cell death, as low a concentration of 68 ± 0.05 μg/ml of $Zn_{0.90}Ce_{0.10}O$ NPs was good enough to cause loss of viability of 50% of the cell as compared to ZnO and $Zn_{1-x}Ce_xO$ (x=0.05 and 0.15) NPs.

The X-ray diffraction of ZnO and various concentration of Nd doped ZnO revealed wurtzite hexagonal structure without any secondary phase of $Nd^{3+}$/ $Nd^{4+}$ ions with neodymium oxide of $Nd_2O_3$. The XPS measurement of Nd doped ZnO nanoparticles confirmed that the oxidation state of Zn (2p) signal has been splitted into two symmetric peaks corresponding to Zn ($2P_{3/2}$) at 1022.38 eV and Zn ($2p_{1/2}$) at 1045.50 eV. O (1s) asymmetric signal has been splitted into three symmetric peaks 530.99 eV, 532.60 eV & 534.30 eV respectively. Binding energy of Nd (3d) state values were observed at 978.26 eV, 983.28 eV, 997.29 eV, 1002.18 eV and 1023.37 eV for $Zn_{0.90}Nd_{0.10}O$ NPs.

The morphological analysis of ZnO NPs exhibited nanoflower like structure and Nd doped ZnO NPs as nanoflake and spherical like structure. These morphological changes are due to the substitution of $Nd^{3+}$ ions in ZnO lattice sites or on the ZnO surface. The percentage composition of elements such as Zn, O and Nd were identified using EDAX spectra. The percentage of Nd has been increased since the concentration of Nd in Nd doped ZnO increases. This confirmed the substitution of Nd in Nd doped ZnO.

The Photoluminescence spectra of the ZnO and Nd doped ZnO NPs were observed with excitation wavelength 325nm. The green emission bands are observed at 519 nm, 520 nm, 520 nm and 522 nm for ZnO and Nd doped ZnO NPs, is due to the oxygen vacancies and intrinsic defects. These emission changes confirmed the substitution of $Nd^{3+}$ ions into ZnO lattice surface.

From the FTIR spectra, the Zn-O stretching bands were observed at 423, 466, 423 and 452 $cm^{-1}$ for ZnO and Nd doped ZnO NPs respectively. In Raman spectra, ZnO and Nd doped ZnO NPs confirmed the wurtzite

hexagonal sturcture. A1 (LO) phonon modes intensity decreased with the increase in concentration of $Nd^{3+}$ ions. This is due to the incorporation of $Nd^{3+}$ ions in ZnO lattice surface.

The antibacterial studies were performed against a set of bacterial strains such as Gram positive bacteria (*S. aureus* and S. *pneumonia*) and Gram-negative (*E. coli, P. aeruginosa, P. vulgaris, K. pneumonia, and S. dysenteriae*) bacteria. From antibacterial activity, the $Zn_{0.85}Nd_{0.15}O$ NPs possessed more antibacterial effect as compared to the other ZnO and $Zn_{0.95}Nd_{0.05}O$ and $Zn_{0.90}Nd_{0.10}O$ NPs. The cytotoxic effect of pure ZnO, $Zn_{0.95}Nd_{0.05}O$, $Zn_{0.90}Nd_{0.10}O$ and $Zn_{0.85}Nd_{0.15}O$ were examined in cultured (A549) human lung cancer cell line. Among them, the $Zn_{0.95}Nd_{0.05}O$ NPs produced the highest cytotoxicity activity. With respect to cell death, as low a concentration of 118.5 ± 0.05 μg/mL $Zn_{0.95}Nd_{0.05}O$ NPs was good enough to cause loss of viability of 50% of the cell as compared to the pure ZnO, $Zn_{0.90}Nd_{0.10}O$ and $Zn_{0.85}Nd_{0.15}O$ NPs.