ABSTRACT

In this work mixed metal oxides nanoparticles were synthesized containing "Mo" and "Sr" as basic elements and lanthanides (La & Gd) were doped using sonication, sol-gel and hydrothermal methods with variation in calcination temperature and reaction time. The nanomaterials synthesized were computed theoretically and later on compared photo-catalytically.

MoO_3 nanoparticles were synthesized using sonication and sol-gel methods for 04 hours and calcined at 03 different temperatures 250, 350 and 450 °C. To conclude the best suitable method for the synthesis of MoO_3 nanoparticles were characterized using fourier transform infra-red (FTIR), thermogravimetric analysis-diffraction scanning calorimetry (TGA-DSC), scanning electron microscopy-energy dispersive X-ray (SEM-EDX) spectroscopy, high resolution transmission electron microscopy (HRTEM), dynamic laser scattering-particle size analyser (DLS-PSA), X-ray diffraction (XRD) analysis and UV-Visible spectrometer. The optical properties like band gap, extinction coefficient (K), refractive index (n), optical conductivity (ρ), dielectric functions (ε_r and ε_i) and Urbach energy (E_U) were determined. The sol-gel method were concluded the better one and later on used for the synthesis of MoO_3 nanoparticles with the reaction time of 10 and 24 hours.

$SrMoO_4$ nanocomposites were synthesized by varying the "Sr" and "Mo" concentration with change in reaction time of 04, 10 and 24 hours using the sol-gel method. The nanocomposites were characterized using FTIR, Raman analysis, SEM-EDX, HRTEM, DLS-PSA, XRD and UV-Visible spectrometer. The refinement parameters were calculated with the help of XRD-data using FULLPROFF and PROFEX software. The optical properties like band gap, extinction coefficient (K), refractive index (n), optical conductivity (ρ), dielectric functions (ε_r and ε_i) and Urbach energy (E_U) were determined.

Lanthanides (La and Gd) doped $SrMoO_4$ nanocomposites were synthesized using hydrothermal method and characterized using FTIR, Raman analysis, SEM-EDX spectroscopy, TEM, DLS-PSA, XRD analysis and UV-Visible spectrometer. The refinement parameters were calculated with the help of XRD-data using FULLPROF and PROFEX software. The optical properties like band gap, extinction coefficient (K), refractive index (n),

optical conductivity (ρ), dielectric functions (ε_r and ε_i) and Urbach energy (E_U) were determined.

All the synthesized nanomaterials were computed theoretically using SCM-ADF/BAND and VESTA software using Density Function Theory (DFT) principles with Kohn-Sham approach. Different parameters like change in basis set, Hubbard potential, XC-functional (LDA, GGA, Meta and Model) were run to obtain the results closet to the experimental one. Relationship between theoretical and experimental band gap was observed. Density of state (DOS) analysis was performed and contribution of elements "Mo", "O", "Sr", "Gd" and "La" were observed with respect to fermi energy. MOPAC software results in the geometry and frequency optimization using semi-empirical Hamiltonians calculations with PM7 code. VESTA software gives the complete 3D structural representation of synthesized nanoparticles and nanocomposites with the detailed lattice and structural parameters.

The photo-catalytic activity of all the nanoparticles and nanocomposites were done against anthropogenic organo-pollutants 2-methyl-4-nitrophenol and 2-methyl-4,6dinitrophenol. These both organo-pollutants are used in military and textile industries. The results of photo-catalysis are in relation to type of metal oxide, synthesis method, synthesis conditions, change in particle size and band gap are compared with respect to percentage degradation and k-values.