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Effect of Mg on structural, morphological and optical properties of Mg-doped V_2O_5nanostructures

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Abstract

The spray pyrolysis is the simple and most promising thin-film fabrication technique in the deposition of Vanadium pentoxide (V_2O_5) thin film. Thin films of pure $V_2O_5$and Magnesium (Mg) doped V_2O_5were fabricated by spraying precursor solution on a glass substrate by spray pyrolysis at 350°C. The doping concentrations of 1, 3, 5, & 10wt% of Mg deposited followed by the heat treatment process at 350°C. Field emission scanning microscopy (FESEM) and atomic force microscope (AFM) images have been used to study the morphology of the film showed the presence of white nanoparticles and surface roughness thereby effect of doping have been noticed. The XRD study shows the increase in the growth of film in (200) direction and enhancement in crystallite size with increase in doping. EDAX study confirms the presence of vanadium and doped Magnesium. Optical property study using UV-visible spectroscopy shows a rapid decrease in absorbance whereas transmittance increases with an increase in wavelength and also observed varying optical bandgap (Eg) from 3.55eV to 3.75eV for pure and Mg-

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Experimental ^{1}H and ^{13}C Solid-State NMR Signal Assignment of Paramagnetic Copper (II) 2-Pyrazine-Carboxylate Complex using Density Functional Theory Calculations

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Abstract. We have acquired ^{1}H and ^{13}C solid-state NMR (ssNMR) spectra of the paramagnetic Cu(II)-2-pyrazine-carboxylate (Cu-Py) complex and assigned paramagnetic $^{1}H/^{13}C$ signals using density functional theory (DFT) calculations. The unpaired electron in Cu(II) ionexacerbates the ^{1}H and ^{13}C chemical shifts in the Cu-Py complex through hyperfine interactions, making the conventional NMR signal assignment non-feasible. Further, the nuclear fast relaxation in paramagnetic metal-organic system hampers application of routine ssNMR techniques for signal acquisition. In our work we have employed simple DEPTH experiment at 50 kHz magic angle spinning (MAS) for acquiring ^{1}H and ^{13}C 1D ssNMR spectra of the paramagnetic Cu(II)-2-pyrazine-carboxylate (Cu-Py) complex. The paramagnetic augmented (diamagnetic chemical shift + paramagnetic shift) 1D ^{1}H and ^{13}C ssNMR signals (shifts) from Cu-Py complex have major contribution from Fermi contact interaction due to proximity of the organic arm to Cu^{2+} ion (Cu^{2+}-C/H atoms 0-5 Å). The unpaired electron spin density distributed over the pyrazine-carboxylate organic arm is crucial in understanding Fermi contact shifts and hence accounts for ^{1}H and ^{13}C ssNMR signal assignment. The theoretical Fermi contact shifts together with diamagnetic shifts, calculated using density functional theory (DFT) at B3LYP level with basis sets *viz.* 6-311G, 6-311G+(D) and 6-311G++(D), were compared with the experimental shifts to facilitate the process of signal assignment. Vibrational analysis of Cu-Py complex was performed at B3LYP level of theory with various basis sets in comparison with experimental IR data. This further assisted in double validation of DFT optimized Cu-Py structure used here for extracting Fermi contact shifts. Furthermore molecular orbital analysis on the DFT optimized Cu-Py structure articulates the spin density distribution mechanism, thereby stipulating the location of the unpaired electron in the Cu(II) $d_{x^2-y^2}$ orbital in Paramagnetic Cu-Py complex.

Keywords: Paramagnetic Solid-state NMR, Cu(II) 2-pyrazine-carboxylate, Density Functional Theory (DFT) calculations, Fermi-contact shifts, Metal-organic complex

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