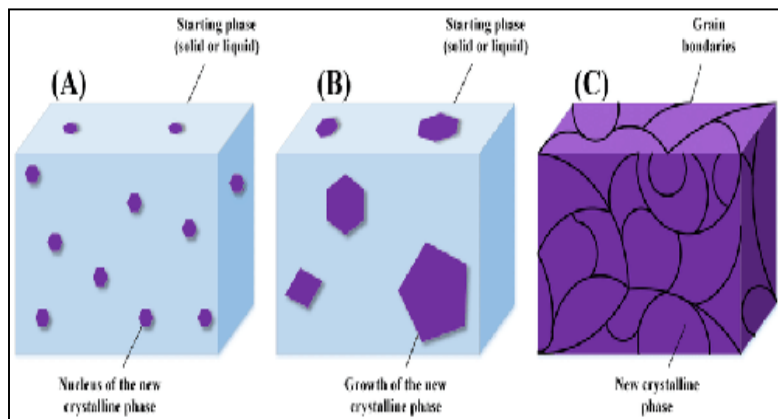




CO²⁺ DOPED CdSe NANOPOLYMER ITS INVESTIGATION ON SPECTROSCOPIC

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ABSTRACT

The Co^{2+} doped CdSe nanopolymer was prepared using polyvinyl alcohol (PVA). The prepared samples were characterized by X-ray diffraction, optical absorption, photoluminescence, EPR and FT-IR studies. The XRD pattern reveals a cubic zinc blend crystalline phase of CdSe and the average size is in nano range order. The optical absorption spectrum characterized Co^{2+} in distorted octahedral symmetry. The EPR spectrum displayed two resonance signals at $G = 4.33$ and 2.12 . Four characteristic bands are displayed in the center of 430, 459, 487 and 539 nm and the corresponding CIE chromaticity indices are calculated. The FT-IR spectrum shows the basic mode vibration of PVA in CdSe.

KEYWORDS: crystalline phase, characteristic bands.

INTRODUCTION:

The development of nano-structured polymer-semiconductor hybrid materials has evolved in the critical research areas of nanoscience and nanotechnology. These nanocomposites combine the beneficial properties of polymers with other properties of shape-tunable optical, electronic, catalytic and semiconductor nanoparticles. In general, the role of polymers is to reconcile nanoparticles and better absorb their characteristic properties. However, polymers cannot be considered as the perfect host material, as they can also be used to modify surfaces and / or to control the growth of nanoparticles. Surface correction may be important for potential use

of semiconductor nanoparticles in biomedical applications and diagnostics. Semiconductor nanocrystals with physical dimensions smaller than the Exciton Bohr radius exhibit electronic, optical, chemical, magnetic and mechanical properties, which cannot be obtained from their bulk counterparts. Among the different semiconductors, colloidal II-group metal chalcogenides, such as CdS, CdSe, and CdTe, have been studied in depth with their size-based photoimmunity properties and their quantum confinement effects, due to the latest developments in synthesis. However, CdSe has been studied extensively as a model system that monitors various applications, because their emissions can be easily controlled in the visible range by changing its shape. The spectroscopic properties of these CdS semiconductors are good with the inclusion of transition metal ions. In general, impurity concentration and coordinate geometry can be examined by optical absorption and electron paramagnetic resonance (EPR) studies. The electron configuration of the neutral cobalt atom [Co] is written as $4s^2 3d^7$. The most common oxidation states are +2, +3. Cobalt that shows cobalt +2 oxidation

state is called cobaltus, while cobalt which shows +3 oxidation state (Co³⁺) is called cobaltic. Both Co²⁺ and Co³⁺ form numerous coordinate compounds or complexes. The coordinate number of packages is usually six. In octahedral coordination, the ionic radius of Co²⁺ (0.86 Å) is smaller than that of Cd²⁺ (0.92). The presence of Co²⁺ in various hosts activates luminescence emissions in the UV and visible regions, and the surrounding environment has strong effects on spectral properties such as symmetry, covalence, coordination, and crystal field strength. The aim of the paper is to describe the synthesis and spectroscopic characteristics of Co²⁺ doped CdSe nanoparticles using XRD, optical absorption, EPR, PL and FT-IR spectroscopy.

EXPERIMENT:

Synthesis of Co²⁺ Doped:

The solution was left for 24 hours to inflate at room temperature. The solution was then heated to 65°C and stirred magnetically until a viscous transparent solution was obtained. One ml of NaHSe (50mM) was added to the solution to obtain a red transparent solution and then 0.01 mol% CoCl₂ solutions were added to the above solution with constant stirring. The solution is poured onto flat glass plate dishes. After non-solvent evaporation, a thin film containing Co²⁺ doped PVA capped CdSe nanopolymer was obtained. The film was washed several times with deionized water to remove other insoluble salts before measurements. Synthesized polymers were used for the following characteristics.

Characterization:

The optical absorption spectrum is recorded in the range of 210-1450 nm using a JASCO V-670 spectrophotometer. The photoluminescence spectrum is recorded at room temperature on the Horiba Jobin-Yvan Fluorology-3 spectrofluorometer as the excitatory source. EPR Spectrum X - The JES-FA series operating at the band microwave frequency is recorded at the temperature of the EPR spectrometer. FT-IR spectrum up to 700 - 4500 cm⁻¹ was recorded on the Shimadzu IRInfinity-1S spectrophotometer in the region.

Studies of X-Ray Diffraction:

X-ray diffraction pattern of Co²⁺ doped PVA capped CdSe nanopolymer. An acute peak is observed at an angle spread around 20.5° relative to PVA. Strong intermolecular interactions between PVA result in a crystalline form of PVA through intermolecular hydrogen bonding. Other scattered peaks of Co²⁺ doped CdSe nanoparticles have been observed at 2θ = 42.38°, 51.23° (230) and (322) are planes of zinc mixed cubic structure consistent with standard JCPDS data 78- 2963. Average crystallite size and the micro strain of Co²⁺ doped CdSe nanopolymer is measured using Scherrer's formula.

Optical Absorption Studies:

It is a powerful technique to explore the optical properties of semiconductor nanoparticles. Optical absorption spectrum of Co²⁺ doped PVA capped CdSe nanopolymer, demonstrated six characteristic absorption bands of Co²⁺ ions in the spectral site symmetry in the spectrum.

Theoretically Transitions ${}^4T_{1g}(F) \rightarrow {}^4A_{2g}(F)$: ν_2 and ${}^4T_{1g}(F) \rightarrow {}^4T_{2g}(F)$: 2.2 in 1.1 to 2.6 is. According to the present study, the ratio of ν_2 to ν_1 from the band positions is found to be around 2.36 and this value indicates the characteristic nature of the Co²⁺ ion in the symmetry of the octahedron. (D7) Different sets of energy matrix crystal fields for configuration (DQ) and inter-electronic repulsion (B and C) parameters as $Dq = 990$ and $B = 970$, $C = 3900$ cm⁻¹ solved these problems; these parameters gave well observed bands. Fit with positions. Observed and calculated band head data of Co²⁺ doped CdSe nanopolymer.

Study of Electron Paramagnetic Resonance (EPR):

Generally, the EPR spectrum of Co²⁺ is observed only at low temperatures because the spin mesh resting period is too short for the octahedral coordination of Co²⁺ ions. At higher temperatures, the spectrum will be wider due to the short rest time characteristic of the high spin phase of the Co²⁺ ion. In

precise octagonal symmetry, the D7 configuration has an orbital triplet state with the lowest spin-orbit coupling dividing the duplication of the ground state energy by $g = 4.69$. The next excited states are only a few hundred eV in energy. Distortions that reduce symmetry mix these states. Therefore, G values become anisotropic and are sensitive to changes in the crystal field. In the present investigation, the display of the CdSe nanopolymer's PL spectrum shows an echo signal at a temperature of 100 K of $G = 4.69$ and $G = 2.11$. In numerical symmetry and g the value $G = 4.69$ is given to the line $\text{Co}^{2+} = 2.01$ is due to random distribution of line distortion.

Study of Photoluminescence:

Defects such as gaps in the photoluminescence (PL) spectrum of CO²⁺ doped PVA capped CdSe nanopolymer, local mesh matching, or dangling bonds exhibited different bands in the visible region. Included Co²⁺ ions greatly affect the luminescence properties of the host material. Four characteristic bands in the center of 430, 458, 489, and 540 nm were displayed in the PL spectrum of CO²⁺ doped CdSe nanopolymer. Blue emission peaks at 430 and 458 nm are associated with trap state emissions. The trap status acts as an electron hole receiver and recombines radiatively. These trapped states thus form a series of metastable energy levels in the band gap resulting in a strong PL signal at room temperature. The strong peak above 499 nm is due to CD defects or surface defects related to the interstitial. Small peaks above 545 nm can be given for induced crystalline defects during growth.

Studies of FT-IR:

The FT-IR spectrum of CO²⁺ doped PVA capped CdSe nanopolymer exhibits various molecular vibrations of PVA in CdSe. The bands observed at approximately 3310 cm⁻¹ arrays that cause O-H stretching vibrations indicate the presence of hydroxyl groups. Asymmetric and symmetrical stretching vibrations of CH₂ are found at 2961 and 2910 cm⁻¹, respectively. The C = O stretching mode caused by the absorption of atmospheric CO²⁺ on the surface of the polymer has bands between 2308 and 1586 cm⁻¹. The bands at 1313 and 1448 cm⁻¹ are in C = O, C = C stretching mode respectively. The bending vibrations of the CO₂ groups, respectively, have an absorption band occurring at 1433 cm⁻¹. The bands in 1273 cm⁻¹ correspond to the stretching C-O of the acetyl groups present on the PVA spine. The band at 1132 cm⁻¹ has been assigned stretching vibrations. The bands seen at 1231 cm⁻¹ are assigned to C-O stretching and O-H bending vibrations. A band seen at 944 cm⁻¹ is assigned to the C-stretching vibration. The band at 828 cm⁻¹ corresponds to the stretching vibrations of the C-C group.

CONCLUSION:

In summary, Co²⁺ doped PVA capped CdSe nanoparticles were synthesized using wet chemical pathways. The effect of doped CO²⁺ ions on the structural and optical properties of PVA capped CdSe nanopolymer was investigated. The XRD pattern reveals zinc mixed cubic composition of CdSe and polycrystalline nature. The average crystallite of CO²⁺ doped CdSe nanopolymer was found to be 8 nm. The optical absorption spectrum in the octahedral site symmetry displayed the characteristic band for Co²⁺. The values of the crystal field and Racah parameters were assessed as $Dq = 990$, $B = 990$ and $C = 3900$ cm⁻¹. The EPR spectrum displayed two resonance signals at $G = 4.69$ and 2.111 . By correlating optical and EPR studies, the bonding nature of Co²⁺ ions with coordinate geometry and host lattice are distorted octahedral and moderately covalent, respectively. The PL spectrum and the corresponding CIE chromaticity diagram show the blue emission for the generated sample. The FT-IR spectrum exhibited characteristic bands of PVA in CdSe polymers and other functional groups.

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