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Luminescence Study of CdSe Quantum Dots Using Machine Learning Techniques

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Abstract

The photoluminescence study of synthesized CdSe quantum dots and comparison with literature based on machine learning (ML) techniques are studied in this paper. Quantum dot is a promising photovoltaic material for thin film solar cells and also shows power superior lasing efficiency higher than existing quantum-well devices. It is possible to create a quantum dot that can generate and absorb energy across the whole solar spectrum. Quantum dots (QDs) are special in a variety of applications due to their distinct size-dependent band gap. Since their photo luminescent properties can be considerably enhanced by optimization of the techniques by which they are synthesized, and are useful in application of optoelectronic disciplines. X-ray diffraction and photoluminescence were used to determine how CdSe quantum dots formed. Later the particle size is calculated by the Debye-Scherrer equation. Because of the quantum confinement effect and size variation, the FWHM of the CdSe samples exhibit greater values in photoluminescence than an ordinary bulk semiconductor, which is also in accordance to the literature based on ML techniques.

Keywords: *Luminescence, Quantum dots, Machine Learning.*

Introduction

Brus and Alexei Ekimov made their initial discoveries of quantum dots in colloidal liquids in the 1980s[1] and a glass matrix[1]. CdSe has a strong absorption of solar spectrum. Compared to physically created nanoparticles, chemically generated nanoparticles can be produced with more ease. The characteristics of epitaxial growth or sputtering, which are readapted to various forms and sizes, pose a challenge for conventional procedures. Nanoparticle sizes and morphologies can be controlled by the synthesis conditions and reagents[1]. By adjusting the size and shape of the nanoparticles, quantum dots that can absorb and emit light over the entire solar spectrum can also be produced. This enables us to widely vary the band gap of the nanoparticles. Quantum dots also supremely show the superior lasing efficiency higher than existing quantum-well devices[2,3]. From the ancient history, quantum dots have been among the most generally investigated nonmaterial's, both from a fundamental viewpoint and for their use for various applications[4,5]. Quantum dots are sometimes referred to as tiny patches in semiconductor materials that are the same size as an electron-hole pair's distance [6,7]. Quantum dot physics develops into a hot and productive subject. Quantum

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confinement gives quantum dots their distinctive optical, photochemical semiconductor, and catalytic capabilities.

CdSe is a semiconductor of the II-VI compound family which has a high potential application like solar cells, transistors, quantum dots, photoconductors, electro-optic devices, memory devices, Gama ray detectors, and biological applications[8,9]. Due to their strong brightness and good quantum yield, cadmium selenide (CdSe) QDs are more widely used than other QD types. Due to its exceptional incident photon to carrier efficiency and enhanced photo physical, photochemical, and electrochemical capabilities, cadmium selenide (CdSe) has been chosen as the most promising choice for nanocomposite materials[10,11].High-quality CdSe-based quantum dots are ideal fluorescent tag candidates for solar cells, single-electrode transistors, light-emitting diodes, laser materials, and biological imaging [1,12]. The distinct size dependence of quantum dots distinguishes them from all other bulk materials because of quantum confinement[13]. The direct band gap of CdSe is 1.74eV at 300K[14,15]. Solid hexagonal or cubic crystal structures are both possible for CdSe. Because of CdSe quantum dots, the power conversion efficiency of the solar cell is increased, as they can produce several electron-hole pairs from a single absorbed photon.

In the last few years, large-scale production has increased, and producing high-quality, batch-to-batch reproducible quantum dots remains one of the industry's most difficult objectives. Following the groundbreaking research on the hot injection approach that was published in 1993[16,28] by Bawendi and colleagues, several groups endeavoured to shed light on the mechanisms governing the production of quantum dots[17,28].The majority of these investigations concentrated on synthesis parameters including ligand type and concentration [17,28], reaction mechanisms[18,19,28], and precursor physicochemical characteristics[20,28].

Apart from these synthesis techniques, synthesis of quantum dotsare purely based on trial-and-error[21,28], because of which the pace of advancements is slow down[28].

ML is an effective technique for comprehending chemical systems and for assisting scientists in drawing conclusions from information found in public databases or through experimental work[22,28]. In situations when a human analysis would be impractical, it has been used to analyze data from X-ray spectroscopy, deconvolute components in mixed signals, evaluate spectral data, and produce band gap values from enormous data sets[22,28]. Additionally, machine-learning-based algorithms were able to analyze structure-property connections in materials, extract microscopy images from the literature, measure size distribution, and extract microscopy images from the literature[23,28]. ML can identify patterns, quickly and accurately by using a significant quantity of data that can be produced by experiments and simulations[24,29]. An automated black-box system was developed by Krishnadasan et al. to manage the synthesis of CdSe quantum dots in a micro fluidic reactor[25,28].

Additionally, a global search algorithm (SNOBFIT) was added to boost emission intensity at a specific wavelength. Voznyy and coworkers in the field of quantum dots applied machine learning models to experimental data available from six years in their lab (here the importance of good lab documentation is highlighted)[26,28] to identify regions of the synthetic parameter space that lead to superior PbS monodispersity. Moreover, Li and colleagues created an "on-demand" system to synthesis quantum dots with a specific emission wavelength by fusing an automated response platform with a deep reinforcement learning algorithm[27,28].

Synthesis: After nine hours of refluxing 96mM sodium sulphite (Na_2SO_3) with 24mM selenium (Se) in deionized water at 90°C, sodium selenosulfate was produced (Na_2SeSO_3).Se stock solution was kept in the dark since light makes it unstable.Deionized water was mixed with 40mM of cadmium acetate ($Cd(CH_3C00)_2$) and 20ml of Se stock solution for 15 minutes at 30°C to create CdSe aqueous solution. After 5 minutes, 0.025ml of 2-mercaptoethanol was added. After 10-15 minutes of continuous stirring, an aqueous solution of CdSe was produced.

Results and Discussion

XRD: Figure 1a displays the CdSe quantum dot XRD pattern results. Using a Bruker D8 advance diffractometer with monochromated Cuk$^{\alpha}$ radiation (=1.54056A°), XRD patterns of the thin films were recorded in the 2θ = 20°–60° range. The diffraction peaks attained at 24.4 6°,25°,27.3°,35.1°,41.1°,45.8°and 50° correspond to the planes (100), (002), (101), (102), (110), (103), (201) have been observed. These diffraction peaks are consistent with

JCPDS card no. 08-0459, which a hexagonal (wurtzite) structure of CdSe quantum dots.The expanded peaks are caused by the nanocrystals limited size.

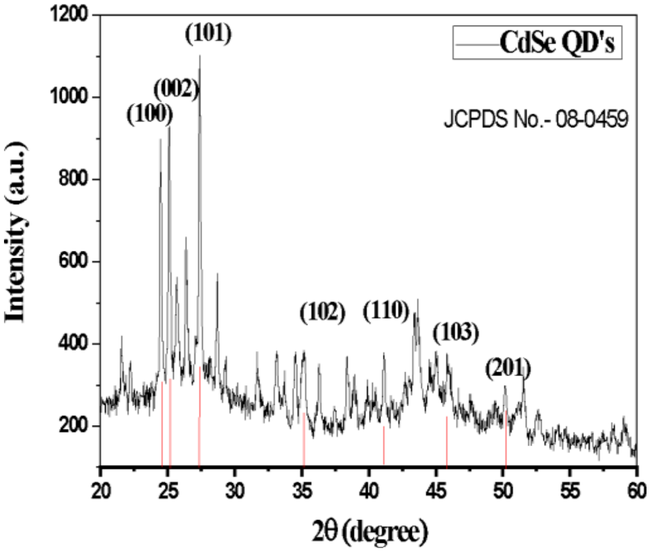

Figure 1a: XRD pattern of CdSe quantum dot

The average particle size of the sample is measured using the Debye scherrer formula described below:-

$d = k\lambda/\beta\cos\theta$

Where λ is the X-ray wavelength (1.54A°), k is a constant of 0.9, and β represents the Full width at half maximum (FWHM). The (101) plane's computed average particle size is about 44 nm.

Photoluminesecence: The optical and electrical characteristics of semiconductors and molecules can be accurately and non-destructively characterized using photoluminescence. Photoluminescence spectra of the CdSe quantum dot are shown by the figure1b. In this the steady state photoluminescence spectra were obtained using a PerkinElmer FS-55 spectrofluorometer. The CdSe sample's emission spectrum's excitation wavelength is 390nm. The luminescence peak for CdSe appears at 565 nm. This has something to do with how electrons in CdSe quantum dots radiatively relax from the lowest energy unoccupied molecular orbital (LUMO) level to the highest energy occupied molecular orbital (HUMO)[29]. The peak intensity decreases as we move to the higher wavelength side. The two causes of the wide emission peak of CdSe quantum dots are trapped states or defect states[30].A subset of trapped states are surface states. Indeed, trapped states can exist at a finite distance from the surface in the bulk or on the surface.

Curiously, the literature establishes that the CdSe luminescence peak is roughly 535nm in wavelength[31]. Despite the fact that the CdSe luminescence peak in our situation is at 565nm. This causes the photoluminescence spectra of polymer nanocomposite for CdSe nanoparticles to shift toward red. Due to a reduction in particle size, the position of the photoluminescence peak is rising in machine learning data. This suggests that by decreasing the size of the particles, the emission peaks can be adjusted from the green to the blue region. Another important component is the FWHM of the ML samples. The FWHMs of the ML samples are greater than synthesized quantum dots which is a significant increase above the FWHM of a typical bulk semiconductor sample. The quantum dots size variations are the primary cause of this phenomena[32]. Because the particle sizes in the CdSe ML samples are the smallest and the quantum confinement effect is most pronounced, these samples have the greatest FWHMs.

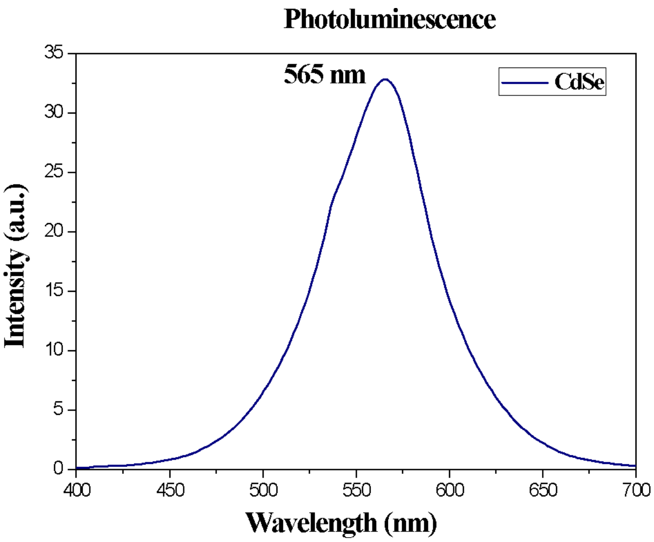

Figure 1b Photoluminescence spectra of CdSe quantum dot

Conclusion

In this paper the luminescence study of CdSe quantum dots for machine learning is studied. We analyse the structure of CdSe quantum dot X-ray diffraction method is used.Particle size is calculated by Debye scherrer formula and it came out to be 44nm for CdSe quantum dot. Additionally, we examine the photoluminescence peak for CdSe quantum dots, which occurs at 565 nm in addition to the wide emission of the PL peak of the CdSe quantum dot caused by trapped states or defect states. The PL peak increasing position in ML samples indicates that particle size reduction can tune emission peaks from the green region to the blue region. Additionally, due to quantum confinement, the FWHM of ML samples of PL is greater.

Conflict of Interest: None

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Ethicial Clearance: Not Required

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