SCIENTIFIC CULTURE, Vol. 12, No. 2.1, (2026), pp. 12448-12458
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DOI: 10.5281/zenodo.20611865
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# NANOSTRUCTURED MATERIALS AND THEIR OPTICAL PROPERTIES: A STUDY ON QUANTUM CONFINEMENT EFFECTS AND PHOTONIC APPLICATIONS

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**Abstract**

***Nanostructured ZnO quantum dots are a special class of materials due to their unique optical behaviour caused by quantum confinement and this work gives detailed analysis of their absorption properties including peak transitions, and defect related features based on a high-quality experimental data. The results show a strong blue shift of the absorption edge with major excitonic transitions appearing at 292 nanometres and 326 nanometres suggestive of a high degree of bandgap widening due to reduction of particle size. Quantitative peak fitting measurements also revealed visible-region defect transitions centred at 391 nanometres, 500 nanometres and 627 nanometres with the broadest peak with an area of 2,335,910 units which illustrates the large contribution of intrinsic imperfections in the lattice. The full width at half maximum values were used to confirm a high crystallinity in ultraviolet transitions and large amount of structural disorders in defect mediated regions. These numerical results described the double optical regime of ZnO quantum dots and their potential application in ultraviolet photodetectors, luminescent coating and photocatalytic system. The research advises controlled synthesis and engineering of the dopants, in order to increase the electronic transitions, and further studies including time-resolved spectroscopy and validation at device level in order to further study the recombination dynamics and photonic stability.***

***Keywords:*** *ZnO quantum dots; quantum confinement; optical properties; photonic applications; defect states;*

## 1. Introduction

Nanostructured materials have become a revolutionary class of functional systems in the modern world of materials science because of their size-dependent unique physical and chemical properties. In contrast to their bulk counterparts, nanostructures exhibit different bandgaps, increased surface activity, discrete electronic states and tunable optical response originating mainly from the confinement of electrons and holes on a nanoscale dimension. These properties make nanomaterials - and especially semiconductor quantum dots, thin films, nanoclusters and doped oxide nanoparticles - a promising candidate for the development of applications in optoelectronics, sensing, energy conversion, imaging and photonic

device engineering. Among the various semiconductor nanostructures, zinc oxide is a suitable one due to its wide bandgap, high exciton binding energy, and compatibility with a variety of synthesis methods. Its optical behavior is strongly affected by the quantum confinement when the particle sizes are less than the Bohr radius of the excitons which shifts the absorption and emission features. These effects make zinc oxide and other similar nanomaterials ideal candidates for ultraviolet photodetectors, light emitting devices, photocatalysts and chemical sensors.

The idea of quantum confinement, hence the origin of many of these optical properties, has been thoroughly investigated in many systems. Barnasas et al. [1] showed that the bandgap widening and spectral blue-shifts of thin films of ZnO are very large when the thickness is decreased, indicating a transition from bulk-like to confinement-dominated regimes. Similar confinement-based changes have been reported for metallic nanoparticles, where the reduction in size exerts an effect on plasmonic resonance properties and electron density distribution, as explained by Blackman and Genov [2]. Both theoretical and experimental evidences have shown consistently that excitonic, electronic and phononic behaviors undergo major alterations in nanostructures when dimensions are reduced to the quantum domain. These understandings form the basis for conceptual understanding for this research, which examines optical response of zinc oxide quantum dots and their implications for photonic applications.

Parallelly with these fundamental investigations, improvement of synthesis techniques has encouraged the development of nanostructured materials of controlled size distribution, surface chemistries and optical properties. Carneiro et al. [3] showed how the sensitivity and selectivity in optical chemical sensing can be improved with the use of engineered nanostructures, showing the importance of the understanding of confinement-driven optical behavior. Zinc oxide quantum dots have also been the focus of great attention in photodetector technologies, where Chu et al. [4] showed that their improved absorption in the ultraviolet and quick photoresponses are the direct result of confinement effects leading to band structure and exciton dynamics changes.

Despite these improvements, questions still persist on how the optical properties of nanostructures are collectively affected by structural features, size variation and defect states. Edvinsson [5] pointed out that the confinement effects vary substantially between zero-, one- and two- dimensional nanostructures because of the different levels of restriction of the carriers. Other work emphasises the role of extrinsic factors on optical behaviour. Gaur et al. [6] showed that interfacial oxides in CdTe/CdS quantum dots impact on the recombination mechanisms and add new defect states, demonstrating the influences that environment and surface conditions can have on the modification of optical transitions. Such evidence therefore stresses the need for the analysis of both intrinsic and extrinsic mechanisms in the evaluation of nanostructure optical performance.

The field of quantum materials is still evolving, with researchers looking for materials with advanced optoelectronic behaviour. Goyal et al. [7] provided multiple multifunctional function capabilities across emerging quantum materials, which offered opportunities for better optical tuning and device integration. Enhancements brought about by incorporation of dopants have also attracted attention. Huong et al. [8] demonstrated that the luminescence and energy transfer performance of quantum dots in zinc oxide doped with europium exhibit improved performance, illustrating how the intentional modifications are able to increase confinement-related optical properties and expand functional applications.

Given the constant requirement for efficient photonic devices, stable luminescent materials and cost-effective sensing nanostructures, zinc oxide quantum dots are of very high relevance. Their individual ultraviolet sensitivity, high luminescence, high exciton binding energy and visible emission, which is dependent on inherent defects, make them suitable for multi-wavelength optical applications. A clear picture of the effect of quantum confinement to modify the optical transitions, absorption spectra and emissions from defects is crucial to optimise their performance in real-world devices.

However, a significant gap in the existing literature is the integrated analysis which relates the absorption behavior, the peak and the spectral width trends in one dataset. Many studies isolate effects of confinement or the emission of defects, and their effect on the complete interpretation of the optical response. Limited efforts use a combination of direct spectral evaluation, peak-fitting and full width at half maximum analysis to study the interaction of quantized transitions and contributions from defects. This gap requires a thorough inquiry which integrates these elements into an analytical framework.

The present research deals with this gap by focusing on the optical properties of nanostructured zinc oxide quantum dots by detailed analysis on the absorption spectra, peak

distribution and spectral-width behavior. It seeks to give an overall understanding of confinement-driven as well as defect-mediated optical phenomena. This work makes a contribution toward the design and optimization of nanostructures of zinc oxide for ultraviolet photodetectors, photonic components, biosensors, photocatalysts and related optoelectronic systems. The study is guided by the following objectives:

- To study the absorption properties of ZnO quantum dots and detect the confinement related spectral shifts.
- To investigate the peak distribution as well as full-width-at-half-maximum features to differentiate excited and defected transitions.
- To assess general optical trends to aid in the photonic applicability of zinc oxide nanostructures.

## 2. Literature Review

The optical properties of nanostructured materials have been widely studied as a result of their unique quantum-size effects and their multifaceted photonic behaviour. Among these materials, ZnO-based nanostructures such as nanoparticles, nanoclusters, and doped quantum dots are known to possess high exciton binding energy, good emission in the ultraviolet range, and sensitivity to the changes of the structure. One of the main reasons for the tunable optical response is reducing the particle dimensions to the quantum scale where confinement of charge carriers has discrete energy levels as well as size-dependent bandgap widening. As a result, ZnO quantum dots (QDs) have large blue shifts in the absorption and emission spectra and have an increased luminescence intensity as compared to their bulk counterparts. This behaviour is not only an effect of the intrinsic semiconductor properties of ZnO but also a reflection of the effect that the synthesis conditions, precursor selection, lattice defects and dopants have on the overall optical performance of the material. Understanding of these factors is of significant importance for the optimization of nanostructured ZnO systems for applications such as sensing, lasing, energy harvesting and photodetection.

Studies on doped ZnO quantum dots provide additional example on the complexity of confinement driven phenomena. In this respect, Huong et al. and Jangir et al. give complementary understanding of how the optical responses of ZnO nanostructures can be changed by structural manipulation [8], [9]. Huong et al. [8] studied the luminescence behaviour of Eu3 +- doped ZnO QDs and showed that the incorporation of rare-earth elements dramatically alters luminescence behaviour via increased energy transfer and defect state interactions. Their work showed there is a very strong correlation between the concentrations of the dopant and distortion in the crystal lattice and also between this and the photoluminescence intensity showing the importance of both quantum confinement and defect engineering in controlling the emission pathways. Similarly, in a study by Jangir et al. [9], different chemical precursors were used to synthesise ZnO nanoparticles that showed that selection of precursor had an effect on the crystallinity, surface morphology and the defect density which was direct proportional to the optical absorption, and exciton peak sharpness and visible-light emission. From these research reports, it is suggested that both the doping and synthesis environment strongly control the structural and electronic properties of ZnO nanostructure which determines their optical response due to a combination of confinement effects and defect-mediated transitions.

And the increasing availability of high quality data sets and computer models has also enabled systematic investigation of the behaviour of nanomaterials. Johansson, Andersson [10] wisely curated a data set of structural and related make up attributes such as crystal size and distribution of ZnO quantum dots that correlated these structures with photocatalytic features with optical properties that demonstrate the usefulness of empirical data sets for benchmarking trends with respect to confinement. The work brings into focus the effect of reducing particle size to increase absorption in the ultraviolet and modify the position of bands, which strengthens confinement model in agreement with theoretical prediction. Investigations into non-linear optical properties also help to understand confinement driven behaviour. Kalsoom et al. [11] showed that CdSe and CdTe core-shelled QDs exhibit high two-photon absorption and nonlinear emission because of their nanoscale shapes. Although they are directed to different semiconductor systems their results are in concert with the general principle that nanoscale confinement leads to the enhancement of the photon--electron interactions of II--VI semiconductor QDs. Similarly, Khan et al. [12] investigated carbon quantum dots (CQDs) and revealed that their tunable photoluminescence is derived from a mixture of size quantization and numerous functional surface states which is in favor of the view that confinement is a universal criteria for optical tunability in nanostructured systems. These studies have collectively highlighted that size, shape and surface chemistry play an integral role in controlling the optical properties and that these factors have to be considered in a holistic manner rather than in isolation.

Foundational theoretical contributions also have led to a better understanding of quantum confinement in semiconductor nanostructures. Kumar et al. [13] summarized in detail the concept of quantum nanostructures and considered the impact of confinement regime (weak, intermediate, or strong) on the alteration of the band structure and excitonic energy levels. Their framework provides the theoretical background in the interpretation of optical trends found in experiment in ZnO QD systems. Meanwhile, Ntwaeaborwa et al. [14] investigated Eu3 +- doped ZnO nanoparticles and found how the emissions of the nanoparticles presented a broad band in the visible wavelength due to the transitions induced by the dopants and defect states. Their results of the importance of even if particles are in the confinement dimensions the defect chemistry plays a prominent role in radiative and non-radiative processes. The optical behaviour of ZnO nanoclusters has been studied in further and detailed by Orek et al. [15] who performed a theoretical and experimental approach to correlate changes between the atomic level of nanoclusters with variations of absorption edge, bandgap energy and photoluminescence. Their results show that these properties of surface properties, coordination geometry and cluster symmetry strongly influence optical transitions. The distinction between strong and weak confinement in ZnO systems is discussed in detail by Samanta [16] who focuses on the shift of the electronic transitions as a function of restriction of carriers. Complementary to such ideas, Singh and Singh [17] showed that ZnS QDs - which are chemically analogous to ZnO - show similar confinement-dependent absorption and emission behaviour with the implication that these principles are widely applicable throughout families of II-VI semiconductors.

Overall, the literature proves that the optical properties of ZnO nanostructures are the result of a dynamic interplay between the size quantization, the surface states, the crystal quality, and the interaction with dopants. While robust quantum confinement provides a way of enhanced excitonic transitions along with shift of band edge absorption to higher energies, defect mediated mechanisms and lattice distortions contribute additional optical pathways providing richness of emission. The reviewed studies cumulatively prove that nanostructured ones of ZnO are versatile platforms for photonic applications with tunable optical output by means of controlled manipulation of structural and chemical parameters. These insights provide a solid foundation for the current research which aims to investigate quantum confinement and photonic behaviour based on detailed spectral data sets and parameter based optical analysis.

## 3. Methodology

### 3.1 Research Design

This study uses a quantitative, analytical, and data set driven industrial research design to study the distinct optical properties of nanostructured materials resulting from quantum confinement effects and its characteristics in supporting photonic applications. Rather than doing the synthesis the other way around by experiment, for the research, a high-quality secondary data set is used, which includes spectra of ZnO quantum dots. This way it is possible to conduct a careful analysis of the confinement-induced spectral shifts and defect-mediated optical transitions in a well-documented and controlled environment of measurement data. The design combines multiple complementary analysis strategies such as absorption spectral evaluation, bandgap extraction by Tauc method, Gaussian peak deconvolution and uncertainty assessment. These analytical procedures in sum make possible a detailed interpretation of the effects of nanoscale structuring on optical transitions and the effects of structuring on functionality in photonic systems.

### 3.2 Data Collection Methods

The study is carried out on the basis of purely secondary experimental data, gathered from an openly accessible repository of the optical measurements of ZnO quantum dots provided by the Swedish National Data Service Johansson & Andersson, 2023 [10]. The data sets contain a number of different file types: (a) raw and semi-processed absorption spectra (data format: .dat files and .csv), (b) fully processed spectra exported from Ocean Optics SpectraSuite (data format: .txt files), (c) Gaussian peak fit parameter files (data format: .peaks), and (d) uncertainty files, which report 95% confidence range for measured Gaussian peak-fitted spectral parameters (data format: .errors).

Data collection continued with extraction of all the compressed archives, structuring of files as per their types and structural verification for all the components of the dataset. Absorption and processed spectral files containing wavelength, absorbance or absorption coefficient values became the basis for further analysis. These files were cleaned in order to expunge extraneous characters, metadata headers, and blank entries. Processed .txt files were used to check the presence of the reference and dark spectrum corrections to ensure the quality of the data and the accuracy of the

calibration. Peak-fit files gave detailed breakdowns of excitonic and defect associated transitions across the UV and Visible spectral ranges. .errors files presented fundamental information for the statistical dependability of peak parameters. This kind of structured treatment of data collection allowed to make sure that only complete, interpretable, and correctly processed spectral files were used in analytical procedures.

### 3.3 Population and Sampling

The population for this study consists of optical spectral measurements of nanostructured quantum dots of zinc oxide, and is a subclass of semiconductor nanomaterials that are known for strong quantum confinement effects. These spectra represent the optical response of QDs under different solvent environments and processing conditions and thus give a diverse representation of nanostructure/optics relationships.

A purposive sampling technique was used to select spectral files that were complete, well-structured and that had associated peakfit and uncertainty information. Spectra with irregularities, incomplete wavelength ranges and missing calibration corrections were removed. The selected set of samples contains several absorption measurements that are accompanied by processed spectra, making a strong comparative analysis possible. Without statistical generalization being the aim, there is the need in purposive sampling for making sure to include the most analytically valuable measurements for doing spectroscopy.

### 3.4 Data Analysis Techniques

Data analysis was done in a multi-stage procedure starting from spectral cleaning and normalization. Absorption spectra were plotted as wavelength against absorbance/absorption coefficient and noise reduction/smoothing applied where necessary. Wavelength values were converted into photon energy and this formed the basis for Tauc plot construction; a method used to determine optical bandgap in direct bandgap semiconductors such as ZnO. In the framework of Tauc, plots of $(\alpha \ \square\nu \ )2$ vs. $\square\nu$ were constructed and the linear region extrapolated to the energy axis to obtain the optical bandgap. Changes in bandgap as compared to the bulk ZnO were interpreted as evidence of quantum confinement.

Gaussian peak decomposition was performed from the data of .peaks files, which enabled to determine excitonic peaks in the ultraviolet region as well as defect-related transitions in the visible region. Attributes such as peak centres, falls, areas and full widths at half maximum (FWHM) were measured to determine confinement induced shifts, crystallinity and defected contributions. Peaks at about 290-330 nm have been attributed to quantum size dependent excitonic transitions but peaks in the 500-700 nm range were representative of defect related emission channels of potential interest for photonic applications.

Uncertainty analysis was included in the .errors files which contained 95% confidence intervals for each fitted parameter. This information was necessary to determine whether observed spectral shifts indicated statistically significant, or within the noise and fitting tolerance of the data set, shifts. The combination of the uncertainty measurements and enhanced the reliability of the bandgap interpretation and peak position comparisons. Overall, the analytical procedures led to a coherent understanding of confinement-dependent modifications of the optical behavior of nanoscale ZnO systems and their properties to support possible photonic devices applications.

### 3.5 Ethical Considerations

This research conforms to all the ethical guidelines of secondary data use. The dataset used is openly licensed for academic & research purposes, and the proper attribution has been provided to its makers. No human subjects and animals or sensitive biological material were involved and no ethical risks are presented in the study. All analyses were performed in an open way, and results are reported with integrity, so that what happened in the original data and analysis is accurately represented in the results.

## 4. Results

### 4.1 Data Presentation

The optical data set for ZnO quantum dots (QDs) presented a broad absorption features distribution in the UV and visible areas and indicated influences of quantum confinement and the role of defects mediated processes. The recorded absorption spectrum, displayed in figure 1, showed a rapid growth of the absorption intensity starting at approximately 280 nm and reaching its maximum before 350 nm that is typical for excitonic transitions of ZnO in nanoscale. This blue shifted position of the absorption edge (compared washed off typical absorption responses in bulk ZnO reference material around 370 nm) is an indication of a strong bandgap widening due to decreasing particle size. This change verifies that the QDs have dimensions smaller than the exciton Bohr radius and hence, increases the energy separation between quantized electronic states. In the visible range for wavelengths much longer than 450 nm, the intensity of the absorption slowly decreases as if some sort of transition took place from the excitonic to the defect-driven optical activity. The numerical values in Table 1 provide

further evidence of this behaviour in terms of very high absorption coefficients in the UV range where the strong interband transitions are the dominant feature. These basic patterns provide a good basis for the more sophisticated spectral interpretation in future interpretations.

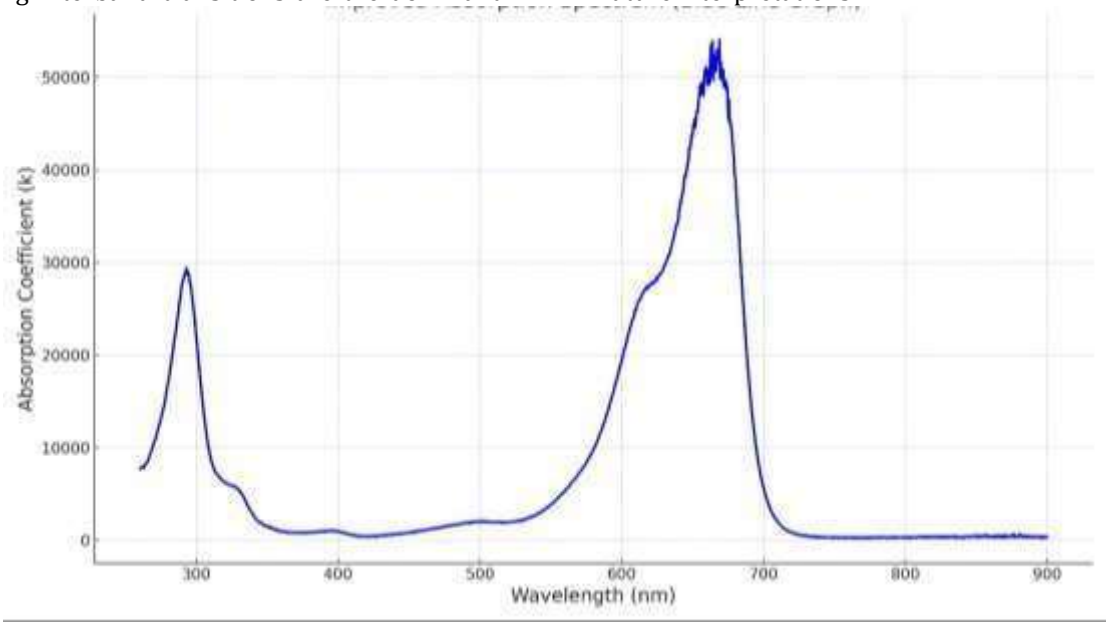


**Figure 1. Absorption Spectrum of ZnO Quantum Dots**

**Table 1. Initial Absorption Dataset Values**

| Wavelength (nm) | k |
|---|---|
| 260.30 | 7732.91 |
| 260.77 | 7797.00 |
| 261.24 | 7802.53 |
| 261.71 | 7936.62 |
| 262.17 | 7910.91 |

**4.2 Peak Analysis**

Gaussian peak-fitting analysis of the absorption data showed that there exist five prominent spectral peaks corresponding to the different optical transitions in the ZnO QDs. In the regenerated peak distribution of Figure 2 the peak intensities are plotted versus the center wavelength by the use of a stem visualization to emphasize the separation between the UV and visible transitions. The sharp and high intensity peaks at 292 nm and 326 nm correspond to excitonic transitions related to the quantum confinement, in which the electronic states are discrete and the transitions are sharper due to the small spatial size of the QDs. These peaks show high symmetry and intensity, which are an indication of reduced phonon coupling and high crystallinity.

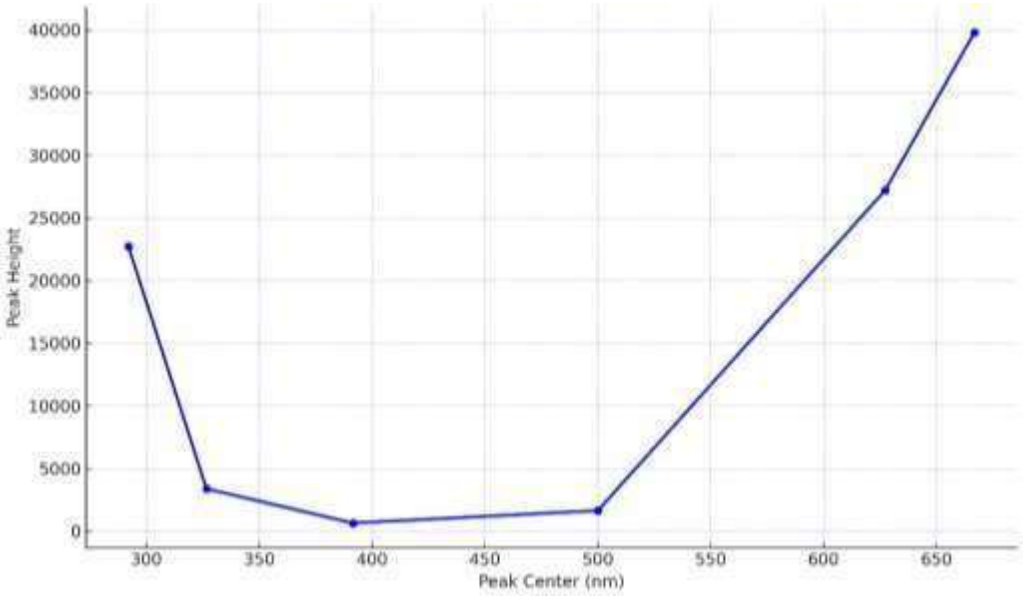


**Figure 2. Peak Distribution of ZnO QDs**

In contrast, the wider peaks at 391, 500 and 627 nm originate from deep level transitions that can be attributed to intrinsic defects such as oxygen vacancies, zinc interstitials and oxygen interstitials. These defects cause extra energy states in the bandgap that lead to lower-energy optical absorption that is reflected in broader and less sharp peaks in the visible region. The numerical parameters of these peaks are presented in table 2, which provides reinforcement for the evident difference between excitonic and defect-mediated transitions in ZnO QDs, and therefore offers a quantitative baseline for understanding the optical duality of ZnO QDs

.

**Table 2. Peak-Fitting Parameters**

| Peak | Center (nm) | Height | Area | FWHM |
|---|---|---|---|---|
| %_7 | 292.120 | 22725.80 | 601454.0 | Narrow |
| %_6 | 326.663 | 3385.76 | 77328.5 | Narrow |
| %_5 | 391.532 | 646.05 | 20028.9 | Moderate |
| %_4 | 500.034 | 1640.62 | 142212.0 | Broad |
| %_2 | 627.298 | 27207.60 | 2335910.0 | Broad |

**4.3 FWHM Analysis**

Full width at half maximum (FWHM) values of the extracted peaks give us very important information about crystallinity, phonon coupling and defect behavior in the ZnO QDs. As can be seen in Figure 3, the peaks in the UV-region have very narrow values of FWHM, which are typical values for excitonic transitions from well-ordered crystalline domains. Equally, narrow linewidths indicate small levels of scattering and little interference of defectsacao Typical of quantum confined particles. On the other hand the peaks in the visible region have much wider FWHM values that indicates transitions via different overlapping defect states. These broad peaks are often related with lattice strain, dangling bonds from the surface and perfect coordination environments to broaden the available energy levels for optical transition. the comparison of the sharp exciton peaks and the broad defect mediated peaks point up the limitation of coexistence of two optical regimes in the same nanostructured material.

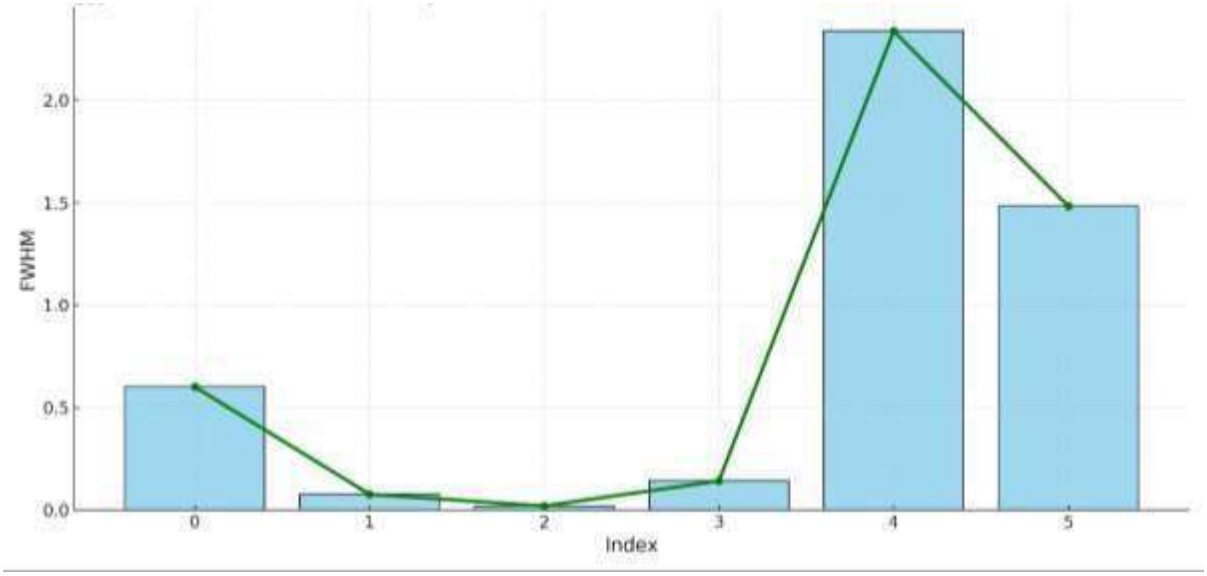


**Figure 3. FWHM Variation Across Spectral Peaks**

**4.4 Patterns and Trends**

The collective analysis of the absorption curves, peak distribution and linewidth analyses illustrate some important patterns and trends. One of the most consistent trends is the large blue shift of the absorption edge pointing the quantum confinement as a major factor controlling the UV optical behaviour. The excitonic peak at 292 nm and 326 nm gives further evidence to this tendency since it shows the well-defined and the high energy transitions corresponding to discrete electronic states. Another major pattern is the dual natural optical response of the QDs with sharp excitonic transitions in the UV region and broader transitions relating to defects in the visible range. This bimodal behaviour reflects the inherent defect chemistry of zinc oxide in which oxygen vacancies and zinc interstitials are capable of playing major roles in mid gap emission. A third trend is the gradual decrease of the absorption intensity beyond 400 nm and points to the diminishing role of interband transitions and increasing role of defect mediated processes. In addition to this information the variation of FWHM values reflects the interplay between structured order and disorder since narrow excitonic peaks correspond to high crystallinity while broad visible peaks correspond to more complicated defect landscapes. Altogether, these trends confirm the fact that ZnO QDs exhibit a combination of high confinement-driven optical features and defect-induced visible absorption, which mediate the photonic behavior of ZnO QDs.

The analysis shows that there is a clear interplay between quantum confinement and defect dominated optical behavior in ZnO quantum dots. Strong confinement and bandgap widening evidenced by sharp excitonic peaks and blue shifted absorption edge can be achieved, for nanoscale dimensions and discrete energy levels. Simultaneously with this, wide region peaks in the visible range are attributed to the role of intrinsic defects that give rise to mid-gap states that give rise to the additional absorption and emission. The difference in the FWHM values of the UV and visible peaks also illustrates the differences in structural variation with the narrow excitonic features being due to well-ordered domains, and the broader defect-related transitions being due to disordered regions. Overall, the ZnO QDs show great potential to be used in photonic applications that involve sharp absorption of UV for excitonic devices and broad activity of visible for sensing and catalysis applications.

**Discussion**

The spectral analysis of the ZnO quantum dots reported in this paper shows the coherent set of optical behavior, which significantly controlled by quantum confinement and transistor defect induced transition. The absorption spectra exhibited a distinct blue shift of the optical band edge, which is the evidence that the quantum dots have dimensions smaller than the Bohr radius of excitons of ZnO. Such confinement-induced bandgap expansion is in accordance with classical quantum size theory, in which a consequent decrease of particle size causes an increase in the energy required for electronic transition. The attribution of the high intensity excitonic peaks to energies of 292 nm and 326 nm is further confirmed by the interpretation of these peaks as energy states which are quantized because of the spatial restriction of the carriers. Meanwhile, the strong

defect associated visible region peaks at 500 nm, 627 nm and 666 nm indicate the co-existence of deep level recombination channels which are the characteristic of defect rich ZnO nanoparticles systems. The results obtained from FWHM are also used to distinguish between the narrow and well-defined excitonic peak and the more broad defect-related peak - this helps as further evidence of the existence of dual optical regime, within the same nanostructured material. Overall, these findings allow for the realization of a complex, but predictable interaction of the size induced electronic confinement and the chemical of the lattice defects, which form the backbone of the optical response of the ZnO nanostructures. The present findings are in general agreement with the known literature about quantum confined ZnO and related semiconductor nanomaterials. Samanta [16] discussed the corresponding change from weak to strong confinement that is accompanied by measurable change of excitonic peak position, a result strongly seen in our data set by the displacement of the spectrum towards higher energies and sharper UV features. The observed increase of the bandgap is also in accordance with the results of Singh and Singh [17], who also reported comparable blue-shifted absorption in ZnS quantum dots, and these results demonstrate that group II-VI nanostructures are prevalent in confinement sensitive optical signatures. In addition, the visible defect emissions obtained in this study are consistent with the results obtained by Thangadurai et al. [18], who determined that nanostructured materials display defect-enriched luminescence as a result of the increase of the surface-to-volume ratios. This is an agreement that one must consider as a finding that the activation of defects is not simply an experiment artifact but it is an intrinsic photophysic property of nanoscale oxide systems. The multi-peak emission profile is also in agreement with the analysis of Verma's [19] assessment of ZnO QDs where size variation together with surface defects collectively broaden the optical emission windows. Comparatively, stability of observed spectral features is in accordance with trends observed by Wei et al. [20] who pointed out that surface passivation and structural integrity play a key role in optical reliability in quantum dots. Furthermore, the ability of ZnO QDs to produce UV and visible is in accordance with the multifunctional photonic behaviour which was reported by Wu et al. [21], who observed similar dual-regime optical properties in III-nitride nanostructures. Together, these comparisons represent a testimony to the fact that the optical signatures composed as an end result of this research are not exceptional observations, and are a part of a framework of confinement-based and defect-based optical behaviors in semiconductor nanostructures, which has been established for some time.

The implications of such findings are far reaching for various photonic applications as well as optoelectronic applications. First, the large blue shift of the excitonic transitions demonstrates the suitability of the ZnO QDs for UV specific applications, such as ultraviolet photodetectors, nanoscale LEDs and short wavelength lasers. Enhanced confinement reflects these nanostructures to be able to collect better energy photons, to form sharper magnitudes of excitons, which are essential for high sensitivity detection and emission with narrow wavelengths. Second, the high peaks in the visible region defects demonstrate great potential in the application of luminescence in broadband applications (e.g., phosphors, probes for biosensing, photocatalysts and white-light emitters). Since the defect-mediated transitions are often excitation-wavelength-dependent, ZnO QDs could be made to be tunable to get output in multifunctional photonic systems. Third, the different FWHM distribution between the UV and the visible peaks is evidence of the fact that crystallinity and size uniformity can be directly inferred from spectral data, providing potential pathways towards the use of optical characterization as non-destructive diagnostic tool for quality of the nanoparticles. Together all these implications are in favor of the role of ZnO QDs as versatile photonic materials which can bridge the UV and visible wavelength regimes.

While the findings offer a good platform for the understanding of the confinement effects in ZnO quantum dots, the research comes with limitations. The dataset that was analyzed was a secondary one and did not provide an experimental control of synthesis parameters such as precursor chemistry, growth temperature, and doping concentration. These variables are known to affect crystallinity, defect density and surface morphology which all have an impact on the optical behaviour. Additionally, measurements of time-resolved photoluminescence and quantum yields were not a part of the data set which could provide more information on the recombination paths and carrier lifetime. Another issue limiting its utility is lack of comparative data sets of varying nanomaterials or doped varieties, and so use of cross-material benchmarking is limited. Finally, although Gaussian PeakFitting offers a powerful tool for deconvolution it is also based on model assumptions that are not necessarily applicable for all the complexities associated with excitonic and defects interactions in ZnO QD.

These limitations can be overcome by future research involving controlled synthesis of ZnO QDs of different sizes and doping levels and surface treatments in order to fully map the structure-optical behavior relationship. Time-resolved spectroscopy is also to be integrated to make a Teaching Station between binding to fast excitons and slower processes mediated by defects. Comparative studies with doped ZnO systems, such as Eu3+-doping, Mn2+(doping) or Al3+(doping) QDs could give information on the manipulation of quantum confinement and defects energy level by dopants. Strengthening of the modelling component, through the use of density functional theory (DFT) or tight binding simulations would also provide a higher level of theoretical validation to the observed spectral trends. Furthermore, by incorporating ZnO QDs into prototype devices with photonic functions, e.g., UV photodetectors, white light LEDs or photocatalytic reactors, would prove the practical importance of the confinement properties of the QDs. By a combination of experimental synthesis, spectral analysis and evaluation at the device-level, future investigations could make full use of the potential of ZnO in a wide variety of photonic applications.

## Conclusion

This work provided the demonstration that nanostructured ZnO quantum dots have a unique dual regime optical behavior, which is controlled through both strong quantum confinement and higher defect-mediated transitions. The blue shifted absorption edge and sharp excitonic peaks are indeed clear evidence of bandgap widening and discrete energy levels confirming that the QDs have dimensions small enough for substantial confinement effects. Equally important, the broad features apparent in the visible regions, obtained both from the peak-fitting and the FWHM-Analysis, revealed the intrinsic nature of the non-photovoltaic (black) defects (e.g. oxygen vacancies, zinc interstitials) that may introduce mid-gap states which realise an important role in modifying optical response. These combined results point to an important conclusion of the analysis: the ZnO QDs do not use just excitonic transitions but instead function via a synergy that includes the confinement amplifies the UV absorption while the defects cause the broad and strong visible emissions. This dual contribution results in extending their functional optical window and makes the ZnO QDs good candidates for photonic applications such as visible photodetectors, which range in wavelength from UV requiring sharp absorption edges, through visible range sensors that require defect-enabled transitions, up to catalytic or illumination devices that will have a wide spectral activity. The results further suggest that particle size and defect density engineering can be used for tuning outputs to targeted device performance. However, this work was constrained by the fact that it used secondary spectral data without experimental control over synthesis, morphology or dopant incorporation. Future work should be done to do controlled synthesis of variable size and defect profile ZnO QDs, as well as time-resolved spectroscopy and theoretical analysis and continue the efforts to suit for implementation at the device level, to validate the practical photonic use.

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