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Relationship between Nanostructure, Band Gap, and Optoelectronic Performance of Semiconductor Nanomaterials

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Abstract: *Semiconductor nanomaterials exhibit electronic and optical properties that differ substantially from those of their bulk counterparts because their dimensions approach characteristic length scales such as the exciton Bohr radius. Among the most important structure–property relationships is the dependence of the effective band gap on nanostructure size, dimensionality, morphology, composition, surface chemistry, and interfacial architecture. In quantum-confined semiconductor nanocrystals, decreasing particle size generally increases the energy separation between the confined electron and hole states, producing a wider effective band gap and a shift of absorption and photoluminescence toward shorter wavelengths. Conversely, increasing nanocrystal dimensions generally reduces confinement and shifts optical transitions toward longer wavelengths. The relationship is not controlled by size alone: nanowire diameter, nanoplatelet thickness, aspect ratio, crystal quality, surface defects, strain, dielectric environment, doping, and core–shell structures also influence carrier dynamics and optical response.*

Keywords: Semiconductor Nanomaterials, Nanostructure, Quantum Confinement, Band Gap, Quantum Dots, Photoluminescence

I. INTRODUCTION

Semiconductor nanomaterials have become an important research area because reducing the dimensions of a semiconductor to the nanometer scale can produce substantial changes in its electronic structure, optical response, charge transport, and surface-related properties. In bulk semiconductors, electrons and holes occupy nearly continuous bands, whereas confinement at the nanoscale can produce discrete or quasi-discrete electronic states. Quantum dots provide the strongest example because charge carriers are confined in three dimensions, while nanowires and quantum wells experience confinement in fewer dimensions.

Consequently, nanostructural dimensions can become a direct design parameter for controlling the effective band gap and optical transition energies. The band gap is one of the most important parameters governing semiconductor optoelectronic behavior. It determines the minimum photon energy required for intrinsic electronic excitation and strongly influences the wavelength range in which a material absorbs or emits light.

When semiconductor crystals are reduced to dimensions comparable with or smaller than the exciton Bohr radius, quantum confinement modifies the energy of electron and hole states. In quantum dots, reduction in particle size generally increases the effective band gap, causing a blue shift in absorption and photoluminescence. This size-dependent behavior has enabled semiconductor nanocrystals to provide wavelength-selectable optical properties.

The relationship between structure and optoelectronic performance, however, is more complicated than a simple particle-size dependence. Nanostructure dimensionality, shape, crystallinity, surface-to-volume ratio, defects, strain, interfaces, doping and composition can alter carrier generation, recombination and transport. For example, one-dimensional

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nanowires provide directional pathways for carrier transport while simultaneously offering quantum confinement when their diameter becomes sufficiently small. Heterostructured nanorods can independently exploit the dimensions and compositions of different semiconductor regions to manipulate charge separation and optical transitions.

Therefore, understanding the relationship between nanostructure, band gap and optoelectronic performance is essential for rational materials design. The present paper examines this relationship by considering quantum confinement, dimensionality, size, morphology, defects, surface effects, heterostructures and composition. Particular attention is given to how these structural parameters influence absorption, photoluminescence, carrier transport, photodetection, light emission and photovoltaic applications.

RELATIONSHIP BETWEEN NANOSTRUCTURE SIZE AND BAND GAP

Particle size is one of the most effective parameters for controlling the optical properties of semiconductor nanomaterials. As the size of a quantum dot decreases, spatial confinement becomes stronger and the energy separation between allowed electron and hole states increases. The resulting increase in effective band gap causes absorption and emission to move toward higher photon energies and shorter wavelengths. Conversely, larger nanocrystals generally show weaker confinement and optical transitions closer to the bulk band gap.

The relationship between photon energy and wavelength is:

$$E = \frac{hc}{\lambda}$$

where E is photon energy, h is Planck's constant, c is the speed of light and λ is wavelength.

Consequently,

$$\lambda_g = \frac{hc}{E_g}$$

or, when Eg is expressed in electron volts,

$$\lambda_g(nm) \approx \frac{1240}{E_g(eV)}$$

Thus, increasing the nanostructure band gap produces a reduction in the corresponding absorption/emission wavelength. This provides a direct connection between nanoscale structural engineering and optical color.

Experimental research has demonstrated that this relationship can be exploited to tune semiconductor nanocrystals across ultraviolet, visible and near-infrared spectral regions. The ability to control emission wavelength by changing nanocrystal size is one of the central advantages of quantum-dot materials.

EFFECT OF DIMENSIONALITY ON BAND STRUCTURE

Nanostructure dimensionality strongly affects electronic states. Zero-dimensional quantum dots confine carriers in three dimensions, one-dimensional nanowires confine carriers primarily in two dimensions, and two-dimensional quantum wells confine carriers in one dimension. Consequently, the density of states changes substantially with dimensionality.

Nanostructure	Main confinement	Electronic states	Typical optical characteristic	Major optoelectronic relevance
Quantum dot (0D)	3D confinement	Discrete	Strongly size-tunable absorption/emission	LEDs, displays, lasers, photovoltaics
Nanowire (1D)	2D confinement	Quasi-discrete/subband	Directional optical and electrical response	Photodetectors, LEDs, lasers

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Nanoplatelet/quantum well (2D)	1D confinement	Quasi-continuous in plane	Thickness-dependent optical transitions	LEDs, photonics
Thin film (2D/3D-like)	Weak confinement	Nearly continuous	Near-bulk band structure	Solar cells, photodetectors
Bulk semiconductor	Negligible confinement	Continuous bands	Fixed material-dependent band gap	Conventional electronics/optoelectronics

The dimensionality-dependent behavior is particularly evident in CdSe systems. Experimental studies of semiconductor nanostructures have shown that optical band gaps can vary with dimensionality even when structures have comparable characteristic dimensions. For example, one-dimensional CdSe nanowires can exhibit different optical band gaps from zero-dimensional structures because confinement is distributed differently among the spatial directions.

Nanowires additionally provide an important combination of confinement and directional transport. Their geometry creates a high surface-to-volume ratio and can provide efficient pathways for carrier collection. These characteristics make one-dimensional nanostructures attractive for photodetectors, light-emitting devices and nanoscale lasers.

NANOSTRUCTURE MORPHOLOGY AND OPTICAL PROPERTIES

Morphology influences the electronic structure through particle dimensions, aspect ratio, crystal facets and surface states. Two nanostructures made from the same semiconductor composition can exhibit different optoelectronic behavior if their morphologies differ.

For example, spherical quantum dots have approximately isotropic confinement, whereas nanorods exhibit stronger anisotropy. In nanorods, the longitudinal and transverse dimensions can be independently controlled, producing anisotropic electronic and optical behavior. Heterostructured nanorods provide additional control because the spatial arrangement of different semiconductor components determines carrier localization and charge-transfer pathways.

Surface-to-volume ratio also increases dramatically with decreasing particle size. Consequently, surface defects become increasingly important in small nanostructures. Surface traps can capture electrons or holes and introduce non-radiative recombination pathways, reducing photoluminescence efficiency. Surface passivation and core–shell structures are therefore widely used to reduce surface-related losses. Research on giant semiconductor nanocrystals has demonstrated that shell growth can isolate photogenerated carriers from surface defects and influence carrier lifetime and mobility.

PHOTOLUMINESCENCE AND NANOSTRUCTURAL DEPENDENCE

Photoluminescence (PL) is one of the most widely used methods for investigating semiconductor nanomaterials. When photons with sufficient energy excite electrons from the valence band to the conduction band, electron–hole pairs are generated. Radiative recombination produces photons whose energy reflects the relevant electronic transition.

The photoluminescence quantum yield can be expressed as:

$$PLQY = \frac{N_{\text{emitted photons}}}{N_{\text{absorbed photons}}} \times 100$$

A high PLQY generally indicates efficient radiative recombination relative to non-radiative pathways. Nanostructural defects can reduce PLQY by introducing trap-assisted non-radiative recombination. Conversely, surface passivation, controlled shell growth and optimized crystal quality can suppress these pathways.

Core–shell quantum dots are particularly useful because a wider-band-gap shell can surround a lower-band-gap core. Such structures can improve carrier confinement and protect the active core from surface-related defects.

Recent research has also emphasized the importance of emission linewidth. Narrow photoluminescence is desirable for applications requiring high color purity and spectrally precise emission. Structural uniformity is important because variations in nanocrystal size and composition can produce ensemble spectral broadening.

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EFFECT OF SURFACE DEFECTS AND PASSIVATION

At the nanoscale, the surface constitutes a significant fraction of the total material volume. Unsaturated bonds, vacancies, impurities and surface reconstruction can therefore introduce localized electronic states within the band gap.

These states may act as:

electron traps,

hole traps,

recombination centers,

non-radiative relaxation pathways, or

charge-transfer sites.

Consequently, two nanomaterials having similar particle sizes and nominal band gaps may exhibit substantially different optical and electrical performance because of differences in surface chemistry.

Surface passivation can reduce these effects. Ligand treatment, shell growth and controlled chemical modification are common approaches. In core–shell quantum dots, the shell can provide both electronic confinement and physical protection of the core. Structure–property studies of core–shell systems have shown that shell thickness and composition can strongly influence carrier lifetime, emission properties and charge transport.

NANOSTRUCTURE–BAND GAP–PERFORMANCE RELATIONSHIP

The overall relationship can be summarized in the following table.

Structural parameter	Change at nanoscale	Effect on electronic structure	Optical consequence	Expected device influence
Particle size	Decrease	Stronger quantum confinement	Band-gap increase and blue shift	Wavelength tunability
Nanowire diameter	Decrease	Increased radial confinement	Shift in absorption/emission	Tunable photodetection
Nanoplatelet thickness	Decrease	Stronger vertical confinement	Spectral shift	Narrow-band optical emission
Aspect ratio	Increase	Anisotropic states/transport	Polarization-dependent response	Directional optoelectronics
Surface area	Increase	More surface states	Trap-related PL changes	Can improve or reduce sensitivity
Crystal quality	Improve	Fewer defect states	Higher PL efficiency	Better carrier transport
Shell thickness	Increase appropriately	Better carrier confinement/passivation	Improved emission stability	Higher optical efficiency
Composition	Change	Band-edge modification	Tunable spectral range	Customized optoelectronic response
Strain	Increase/control	Band-edge shifts	Modified optical transitions	Band-gap engineering
Doping	Controlled	Fermi-level and carrier-density changes	Modified absorption/emission	Improved conductivity
Interface quality	Improve	Reduced interfacial recombination	Better carrier separation	Improved photovoltaic/detector performance

The table demonstrates that the band gap should be considered as a structural and electronic property rather than an isolated material constant. In nanoscale systems, it can be engineered through size, shape, dimensionality, composition and interfaces.

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NANOSTRUCTURES FOR LASERS AND OPTICAL AMPLIFIERS

Semiconductor nanocrystals are also attractive for nanoscale lasers because quantum confinement can produce discrete energy levels and size-dependent optical transitions. Colloidal semiconductor nanostructures offer solution processing together with tunable optical gain and emission wavelengths.

Research during the 2010–2023 period has demonstrated significant development of colloidal nanocrystal lasers, with size-dependent emission, optical gain and engineered nanostructures providing opportunities for wavelength-selectable laser systems.

The lasing threshold is influenced not only by the band gap but also by radiative efficiency, carrier lifetime, optical gain, surface passivation and optical confinement. Consequently, an optimized nanostructure must simultaneously control electronic and photonic properties.

NANOSTRUCTURES FOR PHOTOVOLTAIC APPLICATIONS

In photovoltaic devices, semiconductor nanomaterials can be engineered to absorb specific regions of the solar spectrum. Quantum confinement provides a method for tuning the absorption edge, while heterostructures can facilitate charge separation.

The theoretical photon-to-energy relationship indicates that photons satisfying

$$h\nu \geq E_g$$

can generate electron–hole excitations across the semiconductor band gap.

However, increasing the band gap is not automatically beneficial. A larger band gap may reduce absorption of lower-energy photons, while a smaller band gap may increase spectral absorption but potentially increase energy losses through thermalization. Therefore, the useful design objective is to balance spectral absorption, carrier separation, transport and recombination.

Nanostructured photovoltaic systems can also exploit high absorption coefficients, multiple excitonic effects and heterostructure interfaces. Semiconductor nanocrystals have consequently been studied extensively for solar-energy conversion.

II. CONCLUSION

The relationship between nanostructure, band gap and optoelectronic performance represents a fundamental principle of semiconductor nanomaterials research. When semiconductor dimensions approach characteristic carrier length scales, quantum confinement modifies the electronic energy structure and creates size-dependent optical properties. In quantum dots, decreasing size generally increases the effective band gap and produces a blue shift, while increasing size reduces confinement and shifts optical transitions toward longer wavelengths. The effect is complemented by dimensionality, morphology, surface chemistry, composition, strain, defects and heterostructure architecture.

The evidence from research published between 2010 and 2023 demonstrates that nanostructural engineering provides multiple routes for controlling semiconductor optical and electronic properties. Quantum dots enable size-tunable emission, nanowires provide directional carrier transport, nanoplatelets provide strong thickness-dependent confinement, and core–shell structures provide improved carrier confinement and surface passivation. These characteristics support applications in LEDs, displays, photodetectors, lasers, photovoltaics and integrated photonics.

Ultimately, high optoelectronic performance cannot be attributed to band gap alone. The most effective semiconductor nanomaterials require coordinated optimization of band structure, carrier transport, surface states, recombination, optical absorption and structural stability. Thus, the central principle is that nanostructure controls electronic structure, electronic structure determines optical transitions and carrier behavior, and the combination determines optoelectronic performance.

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