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Review of Morphology and Surface Structure on the Optoelectronic Properties of Nanomaterials

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Abstract: *Nanomaterials exhibit optical and electronic properties that are strongly influenced not only by their chemical composition but also by their morphology, dimensions, crystallinity, surface structure, and interfacial chemistry. At the nanoscale, reduction in particle size produces quantum-confinement effects, while the increasing surface-to-volume ratio makes surface atoms, defects, dangling bonds, vacancies, ligands, and interfaces increasingly important. These structural factors influence the band gap, absorption coefficient, photoluminescence, charge-carrier generation, carrier transport, recombination, and light-emission efficiency. This review examines the relationship between morphology and surface structure and the optoelectronic properties of semiconductor nanomaterials, with emphasis on quantum dots, nanowires, nanorods, nanosheets, nanoplates, nanoparticles, and hierarchical structures*

Keywords: Nanomaterials, Morphology, Surface Structure, Quantum Confinement, Surface Defects, Nanostructures

I. INTRODUCTION

Nanomaterials have attracted extensive scientific interest because their physical and chemical properties can differ substantially from those of the corresponding bulk materials. When at least one dimension of a material is reduced to the nanoscale, surface-to-volume ratio increases and quantum effects may become significant.

Consequently, parameters such as particle size, aspect ratio, morphology, crystallographic orientation, surface roughness, porosity, defect density, and interface structure can modify electronic and optical behavior. The nanoscale morphology is therefore not simply a geometrical characteristic; it is an important determinant of functional performance. Reviews of nanomaterials have emphasized that high surface area and quantum-size effects are among the principal reasons for the unusual electrical and optical characteristics of nanoscale materials.

For semiconductor nanomaterials, the relationship between morphology and optoelectronic behavior is particularly important. Quantum dots, for example, confine charge carriers in three dimensions, whereas nanowires and nanorods can provide strong confinement in two dimensions while allowing comparatively extended carrier transport along their longitudinal direction. Semiconductor nanocrystals therefore provide opportunities for tuning electronic energy levels and optical transitions through size and shape control.

Morphology also determines the manner in which light interacts with a nanostructured material. Particle size and shape can modify absorption and scattering, while nanowire arrays and porous structures can increase light trapping and provide directional pathways for charge transport. A review of semiconductor morphologies for photoelectrochemical applications reported that morphology can influence light absorption, charge-carrier transport, charge recombination, and light scattering.

Surface structure is equally significant because a large proportion of atoms in a nanomaterial are located at or near the surface. Surface atoms may possess incomplete coordination, dangling bonds, vacancies, strain, reconstruction, or adsorbed species. These features can introduce electronic states within the band gap and consequently influence carrier trapping, recombination and emission. Studies of quantum dots have demonstrated that surface trap states can strongly

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affect their optical and electronic properties, while appropriate ligand or shell passivation can reduce these detrimental effects.

MORPHOLOGY OF NANOMATERIALS

Morphology refers to the size, shape, dimensionality, aspect ratio, crystallographic orientation, surface roughness and spatial organization of a nanomaterial. Nanomaterials are commonly classified as zero-dimensional (0D), one-dimensional (1D), two-dimensional (2D), and three-dimensional (3D) structures.

Table 1. Relationship Between Nanomaterial Morphology and Optoelectronic Behavior

Morphology	Representative structures	Major structural feature	Main optoelectronic influence	Typical applications
0D	Quantum dots, nanoparticles	Confinement in three dimensions	Tunable band gap and emission	LEDs, displays, bioimaging
1D	Nanowires, nanorods, nanotubes	High aspect ratio and directional transport	Improved carrier transport and light absorption	Photodetectors, solar cells
2D	Nanosheets, nanoplates, quantum wells	Strong lateral dimensions with nanoscale thickness	Quantum confinement and large interfaces	Photodetectors, transistors
3D	Nanoflowers, porous networks, hierarchical structures	Interconnected nanoscale building blocks	Light trapping and high active surface area	Photocatalysis, photovoltaics
Core–shell	Core/shell quantum dots	Radial heterostructure	Carrier confinement and surface passivation	LEDs, lasers
Oriented arrays	Nanowire/nanoplate arrays	Controlled orientation	Directional carrier and photon transport	Solar cells, sensors

The dimensionality of a nanostructure controls the number of directions in which charge carriers are confined. Consequently, changing morphology can alter the density of electronic states, exciton behavior and optical transitions. Modern reviews of nano-confinement emphasize that 1D, 2D and 3D confinement can produce distinct electronic behavior and that rational control of nanomorphology is increasingly important for optoelectronic materials.

SIZE AND QUANTUM CONFINEMENT

One of the most important relationships between morphology and optoelectronic properties is quantum confinement. When the dimensions of a semiconductor nanocrystal become comparable to or smaller than the exciton Bohr radius, the motion of electrons and holes becomes spatially restricted. This confinement modifies the energy spectrum and generally increases the effective optical band gap as particle dimensions decrease.

A simplified expression for the size-dependent band gap of a semiconductor quantum dot can be represented by the effective-mass approximation:

$$E_g(R) \approx E_{g,bulk} + \frac{\hbar^2\pi^2}{2R^2}\left(\frac{1}{m_e^*} + \frac{1}{m_h^*}\right) - \frac{1.8e^2}{4\pi\varepsilon_0\varepsilon_r R}$$

where:

Eg(R) = size-dependent band gap,

Eg, = bulk band gap,

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R = nanocrystal radius,
$\hbar$ = reduced Planck constant,
me and mh = effective masses of electrons and holes,
e = elementary charge,
ε_0 = vacuum permittivity,
εr = relative dielectric constant.
The first confinement term increases strongly as R decreases, whereas the Coulomb term partially offsets this increase. Semiconductor nanocrystals therefore provide size-tunable electronic states and optical transitions.
The importance of quantum confinement is also observed in nanowires. A review of quantum confinement in nanowires reported a relationship between nanowire diameter and band gap and highlighted the interaction between confinement, surface reconstruction and surface-related structural effects.

NANOWIRES AND NANORODS

One-dimensional nanostructures such as nanowires and nanorods are particularly attractive for optoelectronics because their high aspect ratio provides a natural pathway for directional carrier transport. Compared with randomly oriented nanoparticles, aligned nanowires can reduce the number of grain boundaries encountered during carrier transport.
The morphology of a nanowire can be characterized using parameters such as diameter d, length L, and aspect ratio:

$$AR = \frac{L}{d}$$

A larger aspect ratio generally indicates a more strongly elongated structure. However, the relationship between aspect ratio and device performance is not necessarily linear because extremely thin structures can have a high surface-defect density. Thus, optimization requires balancing carrier confinement, surface-to-volume ratio, crystallinity and surface passivation.
Semiconductor nanowires have been investigated extensively for photonics, solar cells and electronic applications. Their ability to provide controlled carrier transport and nanoscale light–matter interactions has made them important building blocks for optoelectronic systems.

SURFACE-TO-VOLUME RATIO AND SURFACE STRUCTURE

The surface-to-volume ratio increases rapidly as particle dimensions decrease. For a spherical nanoparticle:

$$\frac{S}{V} = \frac{4\pi R^2}{\frac{4}{3}\pi R^3} = \frac{3}{R}$$

where S is surface area and V is volume.
Thus, decreasing the radius increases the surface-to-volume ratio. This simple relationship explains why surface chemistry becomes progressively more important as nanomaterials become smaller.
Surface atoms can possess dangling bonds and reduced coordination. These sites may generate electronic states inside the band gap. Depending on their energetic position and concentration, such states can either promote or inhibit optical emission and charge transport.
In colloidal quantum dots, surface dangling bonds can act as charge-carrier traps and reduce luminescence efficiency. Experimental studies of InP quantum dots, for example, have shown that surface defects are associated with trap states that influence optical characteristics.

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SURFACE DEFECTS AND ELECTRONIC TRAP STATES

Surface defects include vacancies, interstitials, antisites, dangling bonds, under-coordinated atoms and reconstructed surface sites. These defects can introduce localized electronic levels within the forbidden band gap.

A simplified carrier-recombination pathway can be represented as:

$$e^- + h^+ \rightarrow h\nu$$

for radiative recombination, whereas surface-trap-assisted recombination can be represented conceptually as:

$$e^- \rightarrow E_{trap} \rightarrow h^+$$

where Etrap represents a defect-related electronic state.

The presence of trap states can reduce radiative efficiency by providing non-radiative recombination pathways. In quantum dots, surface electronic states can dominate optical and electronic properties because of the large fraction of atoms located at the surface.

However, not every surface state is necessarily detrimental. Controlled surface states can contribute to sensing, charge transfer, photodetection and other functionalities. The critical factor is therefore the controlled engineering of surface-state density, energy and spatial distribution.

SURFACE PASSIVATION

Surface passivation is one of the principal methods for controlling the influence of surface defects. It involves chemically or physically modifying surface sites to reduce dangling bonds and trap states.

For quantum dots, organic ligands, inorganic ligands and semiconductor shells can be employed for surface passivation. Core–shell structures are particularly effective because the shell can spatially isolate photogenerated carriers from surface defects. Studies of giant semiconductor quantum dots have shown that shell engineering can modify carrier lifetimes, surface-defect interactions and optical behavior.

A simplified representation of passivation is:

$$S^* + L \rightarrow S - L$$

where S∗ represents an unpassivated surface site and L represents a passivating ligand.

Passivation can therefore reduce the density of electronically active surface states:

$$N_{trap,passivated} < N_{trap,unpassivated}$$

leading, under appropriate conditions, to reduced non-radiative recombination and increased photoluminescence efficiency.

MORPHOLOGY AND PHOTOLUMINESCENCE

Photoluminescence is highly sensitive to morphology and surface structure. In an ideal nanocrystal, excitation generates electron–hole pairs that subsequently recombine radiatively. The emitted photon energy is related approximately to the transition energy:

$$E_{photon} = h\nu \approx E_g$$

where h is Planck's constant and ν is the emitted photon frequency.

When particle size decreases, quantum confinement can increase the transition energy and shift emission toward shorter wavelengths. Surface defects, on the other hand, can introduce lower-energy emission pathways or suppress band-edge emission.

The photoluminescence quantum yield can be expressed as:

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$$PLQY = \frac{k_r}{k_r + k_{nr}}$$

where kr is the radiative recombination rate and knr is the non-radiative recombination rate.
Surface passivation can improve PLQY when it decreases knr. This principle is particularly important for quantum dots and perovskite nanocrystals. Surface-treatment studies on $CsPbCl_3$ nanocrystals, for example, demonstrated substantial changes in emission intensity following surface treatment, illustrating the sensitivity of optical performance to surface chemistry.

MORPHOLOGY AND CHARGE TRANSPORT

Morphology affects charge transport through crystallinity, grain boundaries, orientation, connectivity and dimensionality. In randomly arranged nanoparticles, charge carriers may encounter numerous interfaces and grain boundaries. In aligned nanowires, the transport pathway can become more directional.
A simplified relation between carrier mobility and conductivity is:

$$\sigma = q(n\mu_n + p\mu_p)$$

where:
σ = electrical conductivity,
q = elementary charge,
n and p = electron and hole concentrations,
μn and μp = electron and hole mobilities.
Morphological optimization can affect both carrier density and mobility indirectly by changing defect concentrations, interfaces and crystallographic orientation.
For photovoltaic and photodetector devices, morphology can therefore influence not only absorption but also the distance carriers travel before recombination.

COMPARATIVE REVIEW OF REPRESENTATIVE NANOMATERIALS

Table 4. Representative Nanomaterials and Morphology–Property Relationships

Nanomaterial	Typical morphology	Important surface feature	Main optical/electronic effect	Application
CdSe	Quantum dots	Ligand-controlled surface	Size-tunable emission	QD-LEDs
InP	Quantum dots	Dangling bonds and surface traps	Surface-dependent PL	Displays, LEDs
PbS/CdS	Core–shell QDs	Shell passivation	Improved carrier confinement	NIR devices
$CsPbX_3$	Nanocubes/nanocrystals	Halide vacancies	Tunable PL and carrier trapping	LEDs
ZnO	Nanorods/nanowires	Oxygen-related surface states	UV emission and transport	UV photodetectors
Si	Nanocrystals/nanowires	Surface reconstruction/passivation	Quantum-confined emission	Photonics
III–V semiconductors	Nanowires	Surface states	Directional transport	Photonics

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2D halide perovskites	Nanoplates/thin films	Interfaces and defects	Excitonic optical response	LEDs/photovoltaics
C60	1D/2D/3D micro/nanostructures	Morphology-dependent interfaces	Charge transport and optical behavior	Organic electronics

The literature indicates that morphology is particularly important in systems where carrier confinement, surface states and interfaces are closely coupled. For example, silicon nanomaterials exhibit emission mechanisms related to both quantum confinement and surface states, while different C_{60} nanostructures can exhibit different optoelectronic characteristics because of morphology-dependent organization.

II. CONCLUSION

Morphology and surface structure are fundamental determinants of the optoelectronic behavior of nanomaterials. Reduction of dimensions produces quantum confinement, while increasing surface-to-volume ratio makes surface chemistry, defects and interfaces increasingly influential. Particle size controls quantum-confinement-induced band-gap changes; shape and aspect ratio affect carrier and photon transport; dimensionality determines confinement and density of electronic states; crystallinity influences carrier mobility; and surface defects can introduce trap states that modify recombination and emission.

The reviewed literature from 2010–2023 demonstrates that no single structural parameter independently determines optoelectronic performance. Instead, size, shape, dimensionality, crystal orientation, surface defects, ligands, interfaces and passivation interact to determine the final optical and electronic response. Quantum dots illustrate the importance of size and surface passivation, nanowires demonstrate the value of directional morphology, two-dimensional materials demonstrate the role of thickness and interfaces, and perovskite nanostructures demonstrate the strong coupling between morphology, surface defects and optical performance.

REFERENCES

1. Asha, A. B., & Narain, R. (2020). Nanomaterials properties. In *Polymer Science and Nanotechnology: Fundamentals and Applications* (pp. 343–359). Elsevier.
2. Blancon, J.-C., Even, J., Stoumpos, C. C., Kanatzidis, M. G., & Mohite, A. D. (2020). Semiconductor physics of organic–inorganic 2D halide perovskites. *Nature Nanotechnology, 15*, 969–985.
3. Bodnarchuk, M. I., Boehme, S. C., (2018). Rationalizing and controlling the surface structure and electronic passivation of cesium lead halide nanocrystals. *ACS Energy Letters, 3*, 1994–2001.
4. Cho, E., Kim, T., Choi, S.-m., Jang, H., (2018). Optical characteristics of the surface defects in InP colloidal quantum dots for highly efficient light-emitting applications. *ACS Applied Nano Materials, 1*(12), 7106–7114.
5. Esmaili, H., Kowsari, E., & Ramakrishna, S. (2021). Significance of nanostructure morphologies in photoelectrochemical water splitting cells: A brief review. *Journal of Molecular Structure, 1224*, 129856.
6. Jang, E., & Jang, H. (2023). Review: Quantum dot light-emitting diodes. *Chemical Reviews, 123*(8), 4663–4692.
7. Ko, J., Berger, R., Lee, H., Yoon, H., Cho, J., & Char, K. (2021). Electronic effects of nano-confinement in functional organic and inorganic materials for optoelectronics. *Chemical Society Reviews, 50*, 3585–3628.
8. Mak, C. H., Huang, X., Liu, R., Tang, Y., Han, X., Ji, L., Zou, X., Zou, G., & Hsu, H.-Y. (2020). Recent progress in surface modification and interfacial engineering for high-performance perovskite light-emitting diodes. *Nano Energy, 73*, 104752.
9. Nozik, A. J. (2010). Nanoscience and nanostructures for photovoltaics and solar fuels. *Nano Letters, 10*, 2735–2742.
10. Singh, M., Rana, S., & Agarwal, S. (2020). Light induced morphological reforms in thin film of advanced nano-materials for energy generation: A review. *Optics & Laser Technology, 129*, 106284.

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11. Talapin, D. V., Lee, J.-S., Kovalenko, M. V., & Shevchenko, E. V. (2010). Prospects of colloidal nanocrystals for electronic and optoelectronic applications. *Chemical Reviews, 110*, 389–458.
12. Yang, P., Yan, R., & Fardy, M. (2010). Semiconductor nanowire: What's next? *Nano Letters, 10*(5), 1529–1536.
13. Yang, L., Zhang, S., (2023). I–III–VI quantum dots and derivatives: Design, synthesis, and properties for light-emitting diodes. *Nano Letters, 23*(7), 2443–2453.