

Article

A Unified Axisymmetric BenDaniel–Duke Effective Mass Model for Investigating Strain-Engineered Optical Properties of Core–Shell Quantum Dots under Uniform External Electric Fields

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Abstract: A unified axisymmetric model based on the BenDaniel-Duke effective-mass approach is proposed to study the effect of lattice-mismatch induced strain on the electronic structure and optical properties of CdSe/CdS core-shell quantum dots. The formulation also permits the presence of a uniform external electric field. The model takes into account the continuum elastic strain, the shifts of the band edges due to the deformation potential, the position-dependent effective mass of the carriers, the quantum confinement, and the first-order direct Coulomb interaction between the electrons and holes, within a two-dimensional axisymmetric configuration. Numerical calculations were performed for a CdSe core of radius 4.0 nm and CdS shell of thickness 2.0 nm. The lattice mismatch was estimated to be 4.022%, giving rise to a compressive hydrostatic strain of -2.298% in the core and a tensile strain of +0.817% in the shell, with a maximum elastic displacement of 0.130 nm. Thus, the strain-modified band gap of the CdSe core was 1.876 eV. The confinement energies for the ground state were found to be 0.0717 eV for electrons and 0.0390 eV for holes. The corresponding effective confinement potentials were about 0.081 and 0.420 eV, respectively. Accounting for the direct electron-hole Coulomb interaction leads to a binding-energy correction of 49.85 meV, and reduces the optical transition energy from the single-particle value of 1.986 eV to an excitonic value of 1.936 eV. This transition corresponds to an emission line at about 640.3 nm. The calculated ground-state wavefunction overlap of 0.904 and relative oscillator strength of 0.817 indicate a significant spatial overlap between the confined electron and hole states and a strong fundamental optical transition. The numerical implementation demonstrated good convergence in the ten lowest eigenstates, preservation of matrix symmetry within numerical precision, and errors in wavefunction normalisation of order 10^{-16} . Overall, the results demonstrate that the axisymmetric BenDaniel-Duke formulation is a numerically stable and physically consistent approach to describe strain-dependent carrier confinement and optical transitions in CdSe/CdS core-shell quantum dots. The developed framework also provides a basis for future investigations of electric-field-induced modifications to their electronic and optical behavior

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1. Introduction

Semiconductor quantum dots (QDs) have attracted much attention because of their size-dependent electronic and optical properties, which are mainly due to quantum confinement. By controlling the size, composition, morphology and interfacial properties of nanocrystals, it is possible to tune their electronic energy levels and optical response for a broad set of applications. Core-shell heterostructures provide further opportunities to tune these properties, as the spatial confinement of electrons and holes is defined by the band offsets, the effective masses of the carriers, the dielectric properties and the lattice parameters of the involved semiconductors. Among the II-VI semiconductor heterostructures the CdSe/CdS core-shell quantum dots are of special interest, because the relatively narrow band gap of CdSe combined with the wider band gap of CdS creates favourable conditions for optical transitions and controlled carrier delocalization. Depending on the size of the core and shell, the electron wavefunctions may penetrate into the CdS region, whereas the holes tend to be more strongly confined in the CdSe core. This variation in the localisation of the carriers makes these nanostructures sensitive to changes of their geometrical and strain properties, as well as to the application of external fields, thus providing potential for their use in light-emitting devices, electro-absorption devices, photodetectors and field-controlled excitonic processes [1-7]. The experimental basis for the understanding and control of their size-dependent optical behaviour was laid by early studies of semiconductor nanocrystals. In particular, the advances in synthesis of nearly monodisperse II-VI nanocrystals have allowed for the investigation of the relationship between nanocrystal dimensions and electronic properties. Later studies on CdSe/ZnS core-shell structures showed that the existence of proper shell could improve photoluminescence through passivation of the surface and change of electronic environment around the QDs. These developments have provided an important basis for further studies of CdSe/CdS heterostructures [8-10]. Further advances in controlled nanocrystal growth yielded more complex geometries, such as seeded nanorods, tetrapods and branched nanocrystals. Such developments also highlighted the need to consider nanocrystal geometry and heterointerface location in the interpretation of quantum confinement and carrier distributions [11,12].

Besides the conventional band-edge emission, optical gain and stimulated emission of semiconductor nanocrystals have been investigated and potential electronic and optoelectronic applications have been explored [13,14]. We have advanced our understanding of the relationship between carrier localisation and optical properties by optimising the synthesis of high quality CdSe/CdS nanocrystals and by performing time-resolved photoluminescence measurements capable of discriminating between emission processes from the core and those from the shell [15,16]. These studies focus on different aspects of semiconductor nanocrystals, but together they show the importance of the knowledge of the effect of structural properties on confined electronic states. One of the crucial factors that affects the electronic structure of CdSe/CdS quantum dots is the lattice mismatch between CdSe and CdS. In the case of a coherent interface between materials with different equilibrium lattice parameters the resulting elastic deformation leads to a spatially varying strain field. This strain through the deformation-potential coupling shifts the conduction- and valence-band edges and affects carrier confinement energies and optical transitions. The effect of strain on the properties of spherical CdSe/CdS/ZnSe core-shell-shell quantum dots was studied by Rodriguez-Magdaleno et al. [17] by using an effective-mass model combined with continuum elasticity theory. Their results showed that strain modifies the electronic energy spectrum and intraband optical absorption, while the magnitude of these changes depends on the dimensions of the constituent layers. This finding, together with related investigations, indicates that lattice-mismatch strain must be considered when modeling the electronic and optical properties of II-VI semiconductor heterostructures [17-19]. The distribution of confined carriers is also strongly influenced by the relative alignment of the conduction and valence bands.

Studies of inverted and type-II core-shell nanostructures have shown that changing the constituent materials or their arrangement can substantially alter electron and hole localization [20,21]. Experimental investigations of carrier quenching and wavefunction engineering in CdSe/CdS systems have provided further evidence that shell composition and interfacial band alignment influence carrier delocalization [22,23]. Although carrier extraction is not explicitly considered in the present model, these findings emphasize the need to account for both conduction- and valence-band offsets when describing carrier confinement. The importance of strain engineering in CdSe/CdS nanostructures has also been demonstrated experimentally. Different anisotropic strain distributions were achieved by Kim et al. [19] by varying the position of the CdSe core in the CdSe/CdS dot-in-rod nanocrystals. Their observations showed significant changes in the absorption and emission characteristics of the nanocrystals. Such optical changes under rather strong strain conditions are related to the modifications of the valence-band states and to the strain-induced internal electrostatic effects affecting the electron-hole separation. These results, together with related studies [18,19], suggest that strain can be used as a way of tailoring the optoelectronic properties of CdSe/CdS heterostructures rather than being just an unavoidable consequence of lattice mismatches.

In addition to the structural modification, the external electric field provides an extra way to tune the carrier confinement and optical response after the nanocrystal synthesis. [23] Gollner et al. investigated ultrafast electro-absorption switching in colloidal CdSe/CdS core-shell quantum dots subjected to intense terahertz electric fields [24]. Their theoretical model modelled the field interaction via an additional electrostatic potential acting on the confined electron and hole states, while the Coulomb effects were treated in the effective Hartree approach. The experiments performed in conjunction showed remarkable modulation of visible light transmission proving that the optical response of CdSe/CdS quantum dots can be altered by externally applied fields on ultrafast time scales. These results are in agreement with the general understanding of field-induced carrier redistributions and quantum-confined Stark effects in semiconductor nanostructures [24–26]. Furthermore, experiments have detected permanent dipole moments and non-uniform charge distributions in colloidal semiconductor nanocrystals [27]. These observations provide a more detailed insight into the microscopic origin of the field-sensitive optical behaviour. However, the present investigation does not resolve permanent microscopic dipoles explicitly. It is focused on the influence of an externally applied electrostatic potential. The electric field induced modifications are not restricted to the optical transition energies, but can also influence the excitonic recombination processes. Tang et al. [28] studied single giant CdSe/CdS nanocrystals under applied electric fields and observed an average ~40% reduction of the biexciton Auger recombination rate and an average ~10% reduction of the single-exciton radiative recombination rate. Some of these changes were attributed to the redistribution of the electron and hole wavefunctions and the corresponding modification of the interactions between the carriers. Their results show that an external electric field can affect both the carrier localisation and the excitonic dynamics of recombination.

Carrier interactions have also been found to be important in further studies on Auger recombination, multiexciton dynamics and optical gain in semiconductor quantum dots [29–33]. Studies of highly emissive multiexciton states, reduced blinking in giant CdSe-based nanostructures, and the mechanisms responsible for fluorescence intermittency have also provided important insights into excited-state and charge-state behaviour [34–36]. These phenomena are outside the single-exciton ground-state description treated in the present work, but point to the general importance of carrier localisation and electron-hole interactions in determining nanocrystal optical properties. Recent theoretical studies have further examined the combined effect of external fields, material composition and quantum confinement. Doped CdTe/CdS core-shell quantum dots embedded in dielectric oxide matrices were studied by Ed-Dahmouny et al. [37] with the effective-mass

approximation and finite-element calculations. Their analysis showed that linear and nonlinear optical absorption and refractive-index changes can be controlled by external electric fields. The calculated optical features showed red-shift/blueshift depending on the dielectric environment and the configuration of impurities. The material system is different from CdSe/CdS but their results show the sensitivity of core-shell quantum dots. Baghdasaryan et al. [38] studied the excitonic states of CdSe nanoplatelets under the influence of a uniform in-plane electric field, taking into account the combined effects of confinement, dielectric environment, and electric fields. It is shown that the applied field affects the exciton energy spectrum, spatial probability distributions and quantum-confined Stark shift, and that sufficiently strong fields can compromise the exciton stability. These observations indicate that the electric field not only shifts the optical transition energy but also changes the spatial relationship between electrons and holes. In a similar work, Jaouane et al. [39] studied the excitons in spherical ZnS/CdS/ZnS core-shell-shell quantum dots by means of the effective mass approximation and the finite-element method. Their calculations show that changes in electric-field strength and structural dimensions affect the excitonic energies, oscillator strengths, and radiative lifetimes. The electron-hole Coulomb interaction was included by means of first-order perturbation theory, which offers a convenient way of accounting for excitonic corrections within an effective mass approximation [38,39].

Localised and delocalized charged excitons as well as bright and grey emission states have been also observed in experimental photoluminescence studies of single CdSe/CdS nanocrystals [40,41]. These observations further illustrate the diversity of optical behavior associated with carrier localization. Related studies on fluorescence blinking suppression and theoretical multiexciton generation have broadened the understanding of semiconductor nanocrystal photophysics [42,43]. However, these processes involve additional charge-state or many-body mechanisms and therefore do not directly establish the accuracy of a single-particle model supplemented by a first-order excitonic correction. An additional consideration is the fine structure of band-edge excitons. Previous theoretical and experimental studies have examined bright and dark exciton states, valence-band coupling, size-dependent energy-level splitting, and dark-exciton emission in CdSe nanocrystals [44-47]. Such effects require a more detailed treatment of electronic band structure and carrier interactions than that provided by a single-band, spin-independent approximation. Previous theoretical studies of finite semiconductor crystallites also indicated the importance of the electron-hole interactions and the nanoscale charging effects in the determination of the electronic energy levels [48]. Later, more elaborate many-body pseudo-potential calculations have given a more complete description of the excitonic correlations in semiconductor nanocrystals [49]. These approaches provide useful points of comparison, while also pinpointing the physical limitations associated with the simplified Coulomb treatment adopted in the present work.

Despite great progress, a major challenge is the consistent description of the coupled mechanical, electronic and optical properties of strained semiconductor heterostructures. Most of the previous work has considered lattice-mismatch strain, carrier confinement, or electric-field effects separately, often for different material combinations or geometries. Studies on strain have demonstrated the effect of elastic deformation on band edges and optical transition energies. The influence of applied electric fields on Stark shifts, electron-hole separation, oscillator strengths and excitonic recombination has been established. In contrast, a comprehensive axisymmetric analysis of CdSe/CdS core-shell quantum dots incorporating these coupled physical phenomena in a single computational framework has been paid less attention. The need for such a formulation is evident when one considers the relationship between strain and carrier localisation. Elastic deformation modifies the local conduction and valence band edges resulting in modifications of the confinement potentials experienced by electrons and holes. These changed potentials

determine the spatial distribution of carrier wavefunctions. An externally applied electric field can additionally redistribute the carriers along the direction of the field. The field induced displacement of the electrons and the holes with opposite charges can change the spatial wavefunction overlap, the exciton binding energy, the oscillator strength and the optical transition energy. Therefore, treating these effects independently may ignore aspects of their combined influence on the quantum-confined Stark response. A physically consistent description requires a numerical method able to deal with spatially varying effective masses and appropriate boundary conditions at the semiconductor heterointerfaces [17,18,24-26,28,50].

The BenDaniel-Duke effective-mass formalism provides an appropriate basis for such an approach. As opposed to constant effective mass descriptions, it explicitly allows for variations of the carrier effective mass at material interfaces, satisfying the probability current continuity conditions for the latter. When applied to a 2-D axisymmetric geometry, the formulation preserves the essential radial and axial dependence of the heterostructure without the necessity of a fully 3-D computational treatment. This provides a computationally efficient basis to explore the influences of core radius, shell thickness, strain distribution and carrier localisation, with the possibility of extending the calculations to externally applied electric fields [6,51,52]. Here, it develops a unified axisymmetric BenDaniel-Duke effective-mass model for CdSe/CdS core-shell quantum dots. This model includes continuum elasticity, deformation-potential-induced band-edge shifts, position-dependent electron and hole effective masses, finite heterostructure confinement potentials, and the direct electron-hole Coulomb interaction. The uniform external electric field is also included in the theoretical formulation via the electrostatic potential. Numerical analysis is performed on the confined carrier states, probability density distributions, electron-hole wavefunction overlap, excitonic transition energies, emission wavelengths and relative oscillator strengths. The study establishes the relationship between strain-induced changes in the confinement landscape and the resulting electronic and optical properties, providing a consistent zero-field reference for subsequent studies of field-induced carrier redistribution and optical modulation in CdSe/CdS core-shell quantum dots.

2. Materials and Methods

2.1. Mathematical Models: Physical Description

A semiconductor CdSe/CdS core-shell quantum dot is considered as an axisymmetric heterostructure composed of a CdSe spherical core surrounded by a CdS shell and embedded in an insulating host medium. The lattice mismatch between the core and shell materials generates an intrinsic strain field throughout the heterointerface, while a uniform static electric field is applied along the symmetry axis. The electronic structure is described within the framework of the single-band effective mass approximation, where the charge carriers are confined by finite conduction- and valence-band offsets and experience spatially varying material parameters across the heterostructure [5,6,53].

2.2. Envelope Function Approximation

The electronic states of the heterostructure are described within the envelope function approximation (EFA), which separates the rapidly varying crystal-periodic component of the wave function from its slowly varying macroscopic envelope. Accordingly, the total carrier wave function can be written as [4,54].

$$\Psi(\mathbf{r}) = F(\mathbf{r})u_{nk}(\mathbf{r}) \dots (1)$$

where $u_{nk}(\mathbf{r})$ is the Bloch function associated with the periodic crystal potential, whereas $F(\mathbf{r})$ denotes the envelope function describing the spatial confinement of the carrier inside the quantum dot.

The validity of the envelope function approximation relies on the fact that the envelope function varies on a characteristic length scale much larger than the crystal periodicity. Consequently, the rapidly oscillating lattice potential can be incorporated into

a set of effective material parameters, allowing the carrier dynamics to be described without explicitly solving the microscopic crystal potential [4,54]. Within this approximation, the influence of the underlying crystal lattice is represented by the effective carrier mass, while the heterostructure itself is introduced through spatially varying material parameters and finite confinement potentials [4,54].

2.3. Single-Band Effective Mass Approximation

Since the present work is primarily concerned with the ground and low-lying confined states responsible for the optical response, the single-band effective mass approximation is adopted for both electrons and heavy holes. Under this assumption, interband coupling, spin-orbit interaction, and band-mixing effects are neglected, and each carrier is described independently by an effective one-particle Hamiltonian [51,52,54]. Unlike homogeneous semiconductors, a core-shell quantum dot consists of different semiconductor materials, each possessing distinct effective masses. Therefore, the carrier effective mass cannot be considered constant throughout the computational domain but must be treated as a spatially dependent material parameter [5,51,52]. The position-dependent effective mass is therefore defined as [51,52].

$$m^*(\mathbf{r}) = \begin{cases} m_{\text{CdSe}}, & \mathbf{r} \in \Omega_c \\ m_{\text{CdS}}, & \mathbf{r} \in \Omega_s \end{cases} \dots (2)$$

where Ω_c and Ω_s denote the core and shell regions, respectively. Similarly, the conduction- and valence-band edge potentials are described as piecewise continuous functions, reflecting the finite band discontinuities at the heterointerface. Accordingly, the confinement potential experienced by electrons is expressed as [3,5,6,53].

$$V_c(\mathbf{r}) = \begin{cases} 0, & \mathbf{r} \in \Omega_c \\ \Delta E_c, & \mathbf{r} \in \Omega_s \end{cases} \dots (3)$$

where ΔE_c is the conduction-band offset between CdSe and CdS. Likewise, the hole confinement potential is given by

$$V_v(\mathbf{r}) = \begin{cases} 0, & \mathbf{r} \in \Omega_c \\ \Delta E_v, & \mathbf{r} \in \Omega_s \end{cases} \dots (4)$$

where ΔE_v denotes the valence-band offset. The CdSe/CdS core-shell heterostructure is formed by joining two semiconductor materials with different equilibrium lattice constants. Owing to the lattice mismatch at the heterointerface, the shell is elastically deformed in order to maintain crystallographic coherence with the core. Assuming coherent epitaxial growth and neglecting plastic relaxation, the strain distribution can be accurately described within the framework of linear continuum elasticity [17,18,19,55]. Under static equilibrium conditions and in the absence of body forces, the displacement field [17,55].

$$\mathbf{u}(\mathbf{r}) = (u_r, u_\phi, u_z)$$

satisfies the equilibrium equation

$$\nabla \cdot \boldsymbol{\sigma} = 0 \dots (5)$$

Where denotes the Cauchy stress tensor. Since the present quantum dot possesses axial symmetry

$$\frac{\partial}{\partial \phi} = 0, u_\phi = 0 \dots (6)$$

and the displacement field reduces to

$$\mathbf{u}(r, z) = (u_r(r, z), u_z(r, z)) \dots (7)$$

Consequently, the mechanical problem becomes two-dimensional in the meridional plane. Within the infinitesimal strain approximation, the strain tensor is defined as [17,55].

$$\varepsilon_{ij} - \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \dots (8)$$

where

$$i, j = r, \phi, z$$

For an axisymmetric structure, the non-zero strain components become

$$\varepsilon_{rr} - \frac{\partial u_r}{\partial r} \dots (9)$$

$$\varepsilon_{\phi\phi} - \frac{u_r}{r} \dots (10)$$

$$\varepsilon_{zz} - \frac{\partial u_z}{\partial z} \dots (11)$$

and

$$\varepsilon_{rz} - \varepsilon_{zr} - \frac{1}{2} \left(\frac{\partial u_r}{\partial z} + \frac{\partial u_z}{\partial r} \right) \dots (12)$$

These four components completely characterize the strain state of the axisymmetric quantum dot. For semiconductor heterostructures described within the effective mass approximation, the hydrostatic component of the strain tensor is primarily responsible for shifting the conduction and valence band edges. The hydrostatic strain is therefore defined as the first invariant of the strain tensor [17,18,19,55].

$$\varepsilon_h - \varepsilon_{rr} + \varepsilon_{\phi\phi} + \varepsilon_{zz} \dots (13)$$

which represents the local volumetric deformation induced by lattice mismatch. The hydrostatic strain constitutes the fundamental quantity through which the elastic field couples to the electronic structure, the intrinsic strain alters the electronic band structure through the deformation potential mechanism. Accordingly, the conduction-band edge is shifted by [17,18,19,55].

$$\Delta E_c^{(\text{strain})} - a_c \varepsilon_h \dots (14)$$

Where a_c is the hydrostatic deformation potential of the conduction band. Similarly, the valence-band edge is modified according to

$$\Delta E_v^{(\text{strain})} - a_v \varepsilon_h \dots (15)$$

Where a_v denotes the hydrostatic valence-band deformation potential. Unlike simplified formulations in which strain is introduced as an independent potential term, the present formulation modifies the electronic band edges directly. Consequently, strain affects carrier confinement through the effective confinement potential rather than through an additional external interaction term. The effective confinement potentials therefore become

$$V_c^{\text{eff}}(\mathbf{r}) - V_c(\mathbf{r}) + a_c \varepsilon_h(\mathbf{r}) \dots (16)$$

and

$$V_v^{\text{eff}}(\mathbf{r}) - V_v(\mathbf{r}) + a_v \varepsilon_h(\mathbf{r}) \dots (17)$$

These effective potentials simultaneously account for both the finite band offsets and the strain-induced modification of the semiconductor band structure [17,18,19]. To investigate the quantum-confined Stark effect, a uniform static electric field is applied along the symmetry axis [24,25,26,28,50].

$$\mathbf{E} - E_0 \hat{\mathbf{z}} \dots (18)$$

Where E_0 denotes the field magnitude. The electrostatic potential associated with the applied field is obtained from

$$\mathbf{E} = -\nabla\Phi, \dots (19)$$

which yields

$$\Phi(z) = -E_0 z \dots (20)$$

after choosing the zero reference potential at the center of the quantum dot. The corresponding electrostatic interaction energy for a carrier having charge q is therefore

$$V_E(\mathbf{r}) = q\Phi = -qE_0 z \dots (21)$$

For electrons

$$q = -e,$$

Giving

$$V_E^{(e)} = eE_0 z \dots (22)$$

whereas for holes

$$q = +e,$$

the interaction becomes

$$V_E^{(h)} = -eE_0 z \dots (23)$$

Consequently, the applied electric field introduces an asymmetric perturbation along the axial direction, breaking the spatial inversion symmetry of the confinement potential and producing the quantum-confined Stark effect [24,25,26,28,50]. Having established the material distribution, strain-induced band-edge modification, and electrostatic potential, the complete quantum-mechanical description of the confined carriers can now be formulated. Unlike homogeneous semiconductors, the effective mass in a core-shell heterostructure varies discontinuously across the material interface. Consequently, the conventional Schrodinger Hamiltonian with a constant effective mass is no longer applicable because it does not satisfy the continuity conditions of the probability current at heterointerfaces. To overcome this limitation, the present work adopts the BenDaniel-Duke Hamiltonian, which explicitly incorporates the spatial variation of the effective mass while preserving the Hermitian nature of the operator and ensuring current conservation across material interfaces [51,52]. The generalized Hamiltonian for a confined carrier is therefore written as

$$\hat{H} = -\frac{\hbar^2}{2} \nabla \cdot \left(\frac{1}{m^*(\mathbf{r})} \nabla \right) + V_{\text{eff}}(\mathbf{r}) + V_E(\mathbf{r}) \dots (24)$$

Where denotes the position-dependent effective mass $m^*(\mathbf{r})$, represents the strain-modified confinement potential $V_{\text{eff}}(\mathbf{r})$ is the electrostatic potential induced by the external electric field $V_E(\mathbf{r})$. Equation (24) constitutes the fundamental governing equation of the present theoretical model and serves as the basis for all subsequent numerical calculations [51,52]. The confinement potential entering Eq. (24) is not limited to the conduction- or valence-band discontinuity. Instead, it also incorporates the stridence modification of the electronic band structure [17,18,51,52]. For electrons, the effective potential is expressed as

$$V_{\text{eff}}^{(e)}(\mathbf{r}) = V_c(\mathbf{r}) + a_c \varepsilon_h(\mathbf{r}) \dots (25)$$

whereas for heavy holes

$$V_{\text{eff}}^{(h)}(\mathbf{r}) = V_v(\mathbf{r}) + a_v \varepsilon_h(\mathbf{r}) \dots (26)$$

The total potential experienced by each carrier therefore becomes

$$U^{(e)}(\mathbf{r}) = V_{\text{eff}}^{(e)} + eE_0 z \dots (27)$$

And

$$U^{(h)}(\mathbf{r}) = V_{\text{eff}}^{(h)} - eE_0 z \dots (28)$$

Accordingly, the Hamiltonian for electrons becomes

$$\hat{H}_e = -\frac{\hbar^2}{2} \nabla \cdot \left(\frac{1}{m_e^*(\mathbf{r})} \nabla \right) + U^{(e)}(\mathbf{r}) \dots (29)$$

while the hole Hamiltonian is written as

$$\hat{H}_h = -\frac{\hbar^2}{2} \nabla \cdot \left(\frac{1}{m_h^*(\mathbf{r})} \nabla \right) + U^{(h)}(\mathbf{r}) \dots (30)$$

Both Hamiltonians possess identical mathematical structures but differ in their effective masses, confinement potentials, deformation potentials, and electrostatic interaction [51,52]. The stationary electronic states are obtained solving the time-independent Schrödinger equation [51,52,54].

$$\hat{H}\Psi = E\Psi \dots (31)$$

Substituting the BenDaniel-Duke Hamiltonian into Eq. (31) yields

$$-\frac{\hbar^2}{2} \nabla \cdot \left(\frac{1}{m^*(\mathbf{r})} \nabla \Psi \right) + U(\mathbf{r})\Psi = E\Psi \dots (32)$$

Equation (32) represents the fundamental eigenvalue problem governing the confined electronic states within the strained core-shell quantum dot [51,52,54].

The corresponding eigenvalues define the quantized carrier energies, whereas the associated eigenfunctions determine the spatial localization of electrons and holes inside the heterostructure. The CdSe/CdS core-shell quantum dot exhibits rotational symmetry around the z-axis. Consequently, all physical quantities are independent of the azimuthal coordinate [51,55].

$$\frac{\partial}{\partial \phi} = 0 \dots (33)$$

Under cylindrical coordinates (r, ϕ, z) the divergence operator appearing in Eq. (32) becomes

$$\nabla \cdot \left(\frac{1}{m} \nabla \Psi \right) = \frac{1}{r} \frac{\partial}{\partial r} \left(\frac{r}{m} \frac{\partial \Psi}{\partial r} \right) + \frac{\partial}{\partial z} \left(\frac{1}{m} \frac{\partial \Psi}{\partial z} \right) \dots (34)$$

Substituting Eq. (34) into Eq. (32) leads to the axisymmetric Schrödinger equation

$$-\frac{\hbar^2}{2} \left[\frac{1}{r} \frac{\partial}{\partial r} \left(\frac{r}{m^*(r, z)} \frac{\partial \Psi}{\partial r} \right) + \frac{\partial}{\partial z} \left(\frac{1}{m^*(r, z)} \frac{\partial \Psi}{\partial z} \right) \right] + U(r, z)\Psi = E\Psi \dots (35)$$

Equation (35) is the central governing equation of the present study. It simultaneously incorporates the finite confinement potential, spatially varying effective

masses, strain-induced band-edge modification, and the externally applied electric field [50,51,52]. All subsequent numerical formulations, including the finite-difference discretization, sparse matrix assembly, and eigenvalue solution, will be derived directly from this equation.

2.4 Finite Difference Formulation

The governing equation derived in the previous section cannot be solved analytically because of the simultaneous presence of spatially varying effective masses, finite confinement potentials, strain-induced band-edge modification, and the externally applied electric field. Therefore, the governing equation is transformed into a discrete algebraic eigenvalue problem using the finite difference method (FDM). In the present work, the conservative form of the BenDaniel-Duke operator is discretized directly in order to preserve the Hermitian property of the Hamiltonian and ensure numerical stability [51,52]. Unlike the conventional Laplacian operator, the BenDaniel-Duke kinetic operator contains a spatially varying coefficient inside the divergence operator. Consequently, the differential operator is discretized without expanding its derivatives.

2.4.1. Computational Grid

The computational domain is discretized using a uniform axisymmetric mesh. The radial coordinate is divided into N_r grid points whereas the axial coordinate is divided into N_z points. The mesh spacings are: -

$$\Delta r = \frac{R_{\max}}{N_r - 1} \dots (36)$$

$$\Delta z = \frac{Z_{\max} - Z_{\min}}{N_z - 1} \dots (37)$$

Each computational node is therefore located at

$$(r_i, z_j)$$

Where

$$\begin{aligned} r_i &= i\Delta r \\ z_j &= Z_{\min} + j\Delta z \end{aligned}$$

The envelope wave function is evaluated only at these nodal locations

$$\Psi_{i,j} = \Psi(r_i, z_j) \dots (38)$$

The envelope wave function is sampled only at the computational nodes, and all spatial derivatives appearing in the governing equation are subsequently approximated using second-order central finite differences.

2.4.2 Midpoint Effective Mass

Because the effective mass changes discontinuously at the heterointerface, evaluating it directly at the computational nodes produces inaccurate carrier fluxes. Instead, the effective mass is evaluated at the midpoint between adjacent nodes using the harmonic average [51,52]

$$m_{i+\frac{1}{2},j} = \frac{2m_{i,j}m_{i+1,j}}{m_{i,j} + m_{i+1,j}} \dots (39)$$

$$m_{i-\frac{1}{2},j} = \frac{2m_{i,j}m_{i-1,j}}{m_{i,j} + m_{i-1,j}} \dots (40)$$

Similarly,

$$m_{i,j+\frac{1}{2}} = \frac{2m_{i,j}m_{i,j+1}}{m_{i,j} + m_{i,j+1}} \dots (41)$$

and

$$m_{i,j-\frac{1}{2}} = \frac{2m_{i,j}m_{i,j-1}}{m_{i,j} + m_{i,j-1}} \dots (42)$$

The harmonic averaging is consistent with the BenDaniel-Duke interface conditions and provides a conservative approximation of the carrier flux across material interfaces. [51,52]

2.4.3 Radial Kinetic Operator

The radial part of Eq. (35) is

$$\frac{1}{r} \frac{\partial}{\partial r} \left(\frac{r}{m} \frac{\partial \Psi}{\partial r} \right)$$

Using second-order central differences

$$\left. \frac{\partial \Psi}{\partial r} \right|_{i+\frac{1}{2}} \approx \frac{\Psi_{i+1,j} - \Psi_{i,j}}{\Delta r} \dots (43)$$

the radial operator becomes

$$\mathcal{L}_r(\Psi) = \frac{1}{r_i} \frac{1}{\Delta r} \left[\frac{r_{i+\frac{1}{2}}}{m_{i+\frac{1}{2},j}} \frac{\Psi_{i+1,j} - \Psi_{i,j}}{\Delta r} - \frac{1}{2} \frac{\Psi_{i,j} - \Psi_{i-1,j}}{m_{i-\frac{1}{2},j} \Delta r} \right] \dots (44)$$

At the symmetry axis ($r = 0$), the apparent singularity introduced by the $1/r$ term is removed by imposing the axisymmetric Neumann boundary condition

$$\left. \frac{\partial \Psi}{\partial r} \right|_{r=0} = 0,$$

which guarantees a finite radial flux and preserves the regularity of the solution. Notice that the conservative form is preserved exactly. No derivative of the effective mass appears explicitly.

2.4.4. Axial Operator

The axial contribution is discretized similarly,

$$\mathcal{L}_z(\Psi) = \frac{1}{\Delta z} \left[\frac{1}{m_{i,j+\frac{1}{2}}} \frac{\Psi_{i,j+1} - \Psi_{i,j}}{\Delta z} - \frac{1}{m_{i,j-\frac{1}{2}}} \frac{\Psi_{i,j} - \Psi_{i,j-1}}{\Delta z} \right] \dots (45)$$

Again, the conservative form of the operator is preserved

2.4.5. Complete Discrete Schrödinger Equation

Substituting Eqs. (44) and (45) into Eq. (35) yields

$$\left(-\frac{\hbar^2}{2} [\mathcal{L}_r + \mathcal{L}_z] + U_{i,j} \right) \Psi_{i,j} - E \Psi_{i,j} \dots (46)$$

Equation (46) represents the discrete form of the axisymmetric BenDaniel-Duke equation

Unlike the continuous formulation, Eq. (46) is defined only at the computational nodes and constitutes a sparse linear eigenvalue problem [51,52].

2.4.6 Matrix Representation

ecting the unknown nodal values into a single vector

$$\Psi = [\Psi_1, \Psi_2, \dots, \Psi_N]^T \dots (47)$$

where

$$N = N_r N_z$$

the discrete problem is transformed into the matrix equation

$$\mathbf{H}\Psi = E\Psi \dots (48)$$

The matrix $\mathbf{H}$ is real, sparse, and symmetric. Furthermore, because the conservative BenDaniel-Duke operator has been discretized directly using harmonic interface masses, the Hamiltonian remains Hermitian, ensuring real eigenvalues and orthogonal eigenfunctions [51,52].

2.5 BenDaniel-Duke Boundary Conditions

The mathematical formulation developed in the previous sections is valid only when appropriate boundary conditions are imposed at the interfaces separating different semiconductor materials. Unlike homogeneous media, semiconductor heterostructures

are characterized by abrupt changes in effective mass and band-edge potentials. Consequently, the conventional continuity conditions used for constant-mass Schrödinger equations are no longer sufficient. Instead, the carrier wave function must satisfy the BenDaniel-Duke interface conditions, which ensure conservation of probability current across every material interface [51,52]. Accordingly, the envelope wave function remains continuous

$$\Psi_1 = \Psi_2 \dots (49)$$

where the subscripts denote the two semiconductor regions located on opposite sides of the heterointerface. The probability current continuity requires:

$$\frac{1}{m_1^*} \frac{\partial \Psi_1}{\partial n} = \frac{1}{m_2^*} \frac{\partial \Psi_2}{\partial n} \dots (50)$$

where

$\frac{\partial}{\partial n}$ denotes the outward normal derivative at the interface. Equations (49) and (50) completely describe the interface behavior of confined carriers in the present CdSe/CdS heterostructures. These conditions are automatically satisfied through the conservative finite-difference discretization employing harmonic interface masses [51,52]. Consequently, no additional interface equations are required during the numerical implementation. The computational domain is truncated by an artificial external boundary sufficiently far from the quantum dot to avoid numerical interaction between the confined carrier states and the outer computational limits. Since the surrounding insulating medium presents a very high potential barrier, the carrier envelope function rapidly decays outside the quantum dot. Therefore, homogeneous Dirichlet boundary conditions are imposed

$$\Psi = 0 \dots (51)$$

along the external computational boundary. This approximation accurately represents carrier confinement provided that the computational domain is chosen sufficiently larger than the physical dimensions of the quantum dot. The eigenfunctions obtained from Eq. (48) must satisfy the normalization condition in order to preserve their probabilistic interpretation [4,54]. For an axisymmetric structure, the normalization integral becomes

$$2\pi \int_{\Omega} |\Psi(r, z)|^2 r dr dz = 1 \dots (52)$$

The additional factor $2\pi r$ originates from the cylindrical coordinate transformation and accounts for the rotational symmetry around the z -axis.

In the discrete formulation, Eq. (52) becomes

$$2\pi \sum_{i=1}^{N_r} \sum_{j=1}^{N_z} |\Psi_{ij}|^2 r_i \Delta r \Delta z = 1 \dots (53)$$

The normalized eigenfunctions obtained from Eq. (53) are subsequently employed in all optical calculations. The spatial localization of the confined carriers is described by the probability density [4,56].

$$P(r, z) = |\Psi(r, z)|^2 \dots (54)$$

The probability density provides direct information regarding carrier localization inside the core-shell structure and constitutes one of the principal quantities used to investigate electric-field-induced carrier redistribution. The normalization condition guarantees

$$2\pi \int_{\Omega} P(r, z) r dr dz = 1 \dots (55)$$

Solving the discrete eigenvalue problem,

$$\mathbf{H}\Psi = E\Psi$$

produces two independent eigenvalue spectra. The electron energy levels are denoted by

$$E_e^{(n)}, n = 1, 2, \dots, N_e \dots (56)$$

whereas the heavy-hole energy levels are

$$E_h^{(m)}, m = 1, 2, \dots, N_h \dots (57)$$

The lowest eigenvalues correspond to the confined ground states, while the higher eigenvalues describe excited electronic states [4,57,58]. The associated normalized eigenfunctions are written as

$$\Psi_e^{(n)}(r, z)$$

and

$$\Psi_h^{(m)}(r, z),$$

Respectively. These eigenstates constitute the complete quantum-mechanical basis required for the evaluation of the optical properties, within the single-particle approximation adopted in present work, the optical transition energy between the electron state n and the heavy-hole state m is given by [4,57,59].

$$E_{nm} = E_e^{(n)} - E_h^{(m)} \dots (58)$$

Equation (58) represents the fundamental optical transition responsible for photon absorption and emission. The corresponding optical wavelength is determined from

$$\lambda_{nm} = \frac{hc}{E_{nm}} \dots (59)$$

Where h , is Planck's constant and c is the speed of light in vacuum

2.6 Electric Dipole Transition Matrix

The optical response of the quantum dot is determined by the overlap between the confined electron and hole wave functions. Within the electric dipole approximation, the transition matrix element between the electron state n and the hole state m is defined as [4,60,61,62].

$$M_{nm} = \int_{\Omega} \Psi_e^{(n)*}(r, z) \hat{\mathbf{e}} \cdot \mathbf{r} \Psi_h^{(m)}(r, z) d\Omega \dots (60)$$

where $\hat{\mathbf{e}}$ denotes the polarization direction of the incident electromagnetic wave, For the axisymmetric formulation adopted in the present work

$$d\Omega = 2\pi r dr dz,$$

therefore Eq. (60) becomes

$$M_{nm} = 2\pi \int_{\Omega} \Psi_e^{(n)*}(r, z) (\hat{\mathbf{e}} \cdot \mathbf{r}) \Psi_h^{(m)}(r, z) r dr dz \dots (61)$$

The transition matrix element quantifies the probability amplitude of an optical transition and directly determines the optical strength of the corresponding electronic transition. The oscillator strength is adopted as the principal quantity describing the transition probability between confined carrier states [56,60,61,62,63]. It is defined as

$$f_{nm} = \frac{2m_0 E_{nm}}{\hbar^2} |M_{nm}|^2 \dots (62)$$

Where m_0 is the free-electron mass. The oscillator strength provides a direct measure of the optical activity of each electronic transition. Large values of f_{nm} indicate highly allowed transitions, whereas weak oscillator strengths correspond to optically forbidden or weakly allowed transitions. The linear optical absorption spectrum is evaluated using the Lorentz broadening model. The absorption coefficient is therefore expressed as [17,60,64].

$$\alpha(\omega) = A \sum_{n,m} f_{nm} \frac{\Gamma}{(E_{nm} - \hbar\omega)^2 + \Gamma^2}, \dots (63)$$

where , is a proportionality constant A , is the phenomenological broadening parameter Γ .denotes the angular frequency of the incident radiation ω - Equation (63) predicts the complete optical absorption spectrum of the quantum dot by summing all .allowed electron-hole transitions

2.7 Optical Absorption Spectrum

The photon energy is related to the angular frequency through

$$E_{ph} = \hbar\omega \dots (64)$$

Consequently, the absorption spectrum can be represented as a function of either photon energy or wavelength

$$\lambda = \frac{hc}{E_{ph}} \dots (65)$$

The peak positions of the absorption spectrum correspond directly to the transition energies determined .from the calculated eigenvalue spectrum [17,60,64].

3. Results

The numerical analysis of the CdSe/CdS core-shell quantum dot was carried out using the structural, electronic, dielectric, and elastic properties listed in Table 1. The modeled nanostructure comprises a CdSe core with a radius of 4.0 nm and a surrounding CdS shell with a thickness of 2.0 nm , giving an overall radius of 6.0 nm. Within the single-band effective-mass approximation, the material parameters were defined as spatially dependent quantities to account for the distinct physical properties of the core and shell regions. Particular attention was given to the differences in electron and heavy-hole effective masses across the CdSe/CdS interface, which were incorporated explicitly using the position-dependent effective-mass formulation. This approach accounts for the mass discontinuities at the heterointerface and provides a more physically consistent description of carrier confinement and electronic states than a model based on a uniform effective mass throughout the nanostructure [3,5,6,53].

Table 1. Structural and material parameters used in the numerical modeling of the CdSe/CdS coreshell quantum dot.

Parameter	Symbol	CdSe core	CdS shell	Unit
Core radius	R_{core}	4.0	-	nm
Shell thickness	t_{shell}	-	2.0	nm
Electron effective mass	m_e^*/m_0	0.13	0.21	-
Hole effective mass	m_h^*/m_0	0.45	0.80	-
Band gap energy	E_g	1.74	2.42	eV
Relative dielectric constant	ϵ_r	9.50	8.90	-
Lattice constant	a	6.052	5.818	Å
Elastic constant	C_{11}	74.1	90.7	GPa
Elastic constant	C_{12}	45.2	52.1	GPa
Elastic constant	C_{44}	13.4	15.0	GPa
Conduction-band deformation potential	a_c	-4.90	-4.50	eV
Valence-band deformation potential	a_v	1.00	0.80	eV
Conduction-band offset	ΔE_c	0.23 (interface)	-	eV
Valence-band offset	ΔE_v	0.45 (interface)	-	eV

Note: m_0 denotes the free-electron mass. The total nanocrystal radius is 6.0 nm, corresponding to a 4.0 nm CdSe core radius and a 2.0 nm CdS shell thickness. The conduction-band offset ($\Delta E_c = 0.23\text{eV}$) and valence-band offset ($\Delta E_v = 0.45\text{eV}$) refer to the CdSe/CdS heterointerface rather than to the individual materials.

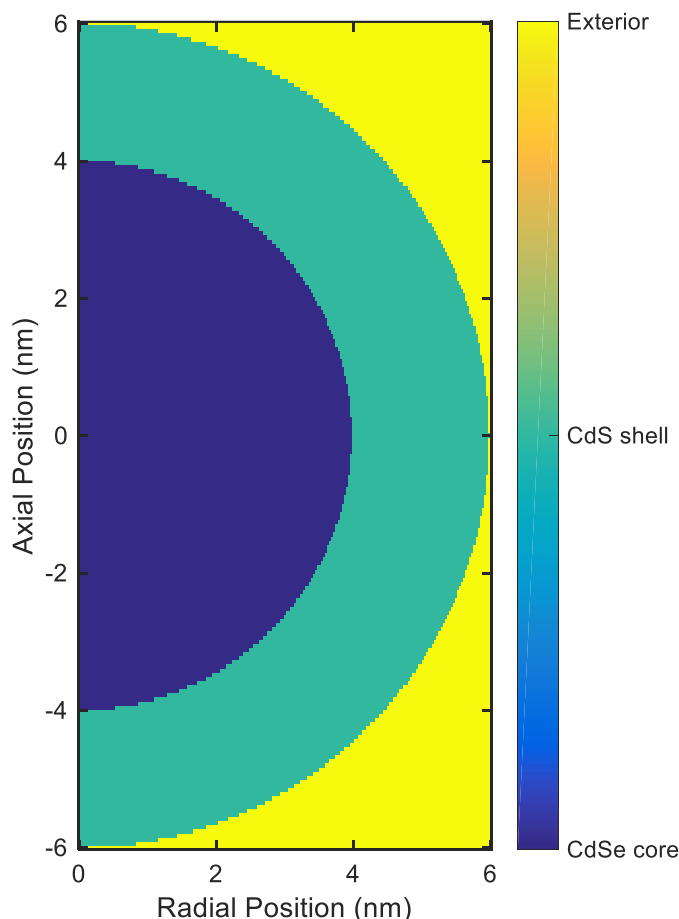


Figure 1. Spatial distribution of the constituent materials in the axisymmetric CdSe/CdS core-shell quantum dot, illustrating the CdSe core, CdS shell, and surrounding exterior computational region.

The spatial structure of the CdSe/CdS core-shell quantum dot used for the numerical calculations is shown in Figure 1. The heterostructure is described by an axisymmetric geometry, with the CdSe core and CdS shell differentiated by their material properties. The interface between the two semiconductors controls the spatial variation of effective masses, lattice parameters, deformation potentials, dielectric constants and carrier confinement potentials. The three-dimensional effective-mass problem is reduced to a two-dimensional problem in the radial and axial coordinates by using the rotational symmetry of the system and not neglecting the spatial dependence of the carrier envelope functions within the assumed symmetry class. The equation which governs the system is written in terms of the axisymmetric BenDaniel-Duke Hamiltonian of Eq. (35), which takes into account the position dependence of the carrier effective mass and provides a consistent description of quantum confinement at the semiconductor heterointerface [5,6,53].

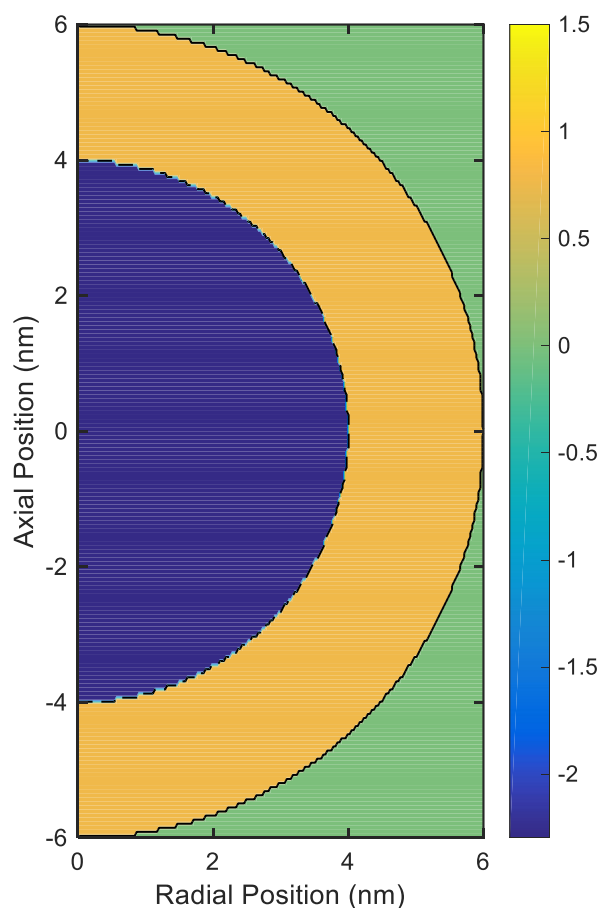


Figure 2. Calculated spatial distribution of hydrostatic strain in the CdSe/CdS core-shell quantum dot. Dashed and solid contours represent the CdSe/CdS interface and the outer nanocrystal boundary, respectively. The compressive deformation of the core and the tensile strain developed in the surrounding shell are evident.

Fig. 2 shows the strain distribution resulting from the lattice mismatch between CdSe and CdS. The lattice parameters used for CdSe and CdS are 6.052 Å and 5.818 Å, respectively, which corresponds to a lattice mismatch of about 4.022%. This difference in equilibrium lattice parameters forces coherent structural continuity at the core-shell interface, inducing elastic deformation. The calculated hydrostatic strain has opposite signs in the two regions, with the CdSe core being compressed and the CdS shell being deformed in tension. In particular, the hydrostatic strain is about -2.298 % in the core and +0.817 % in the shell. This behaviour is due to rearrangement of elastic deformation needed to accommodate the lattice mismatch and to keep interfacial compatibility. [17,18,19]. Moreover, the elastic solution predicts a maximum displacement of about 0.130 nm, which is small when compared to the total radius of the nanocrystal, 6.0 nm. This observation agrees with the small-displacement assumption taken in the numerical formulation. However, the maximum equivalent strain reaches about 5.96% while the hydrostatic strain is limited to a maximum absolute magnitude of about 2.3%. Although the displacement is small relative to the entire structure, the magnitude of the local equivalent strain should be taken into account when assessing the limits of linear elasticity[17,18]. No undefined or infinite values are found in the numerical strain field, which means the implemented calculation yields a finite solution over the entire computational domain. In the employed deformation-potential approximation the calculated hydrostatic strain directly shifts the local conduction- and valence-band edges

according to the relations .Consequently, the effects of lattice mismatch are incorporated into the electronic confinement problem through physically defined band-edge modifications rather than through an independently prescribed strain-related potential [19,55].

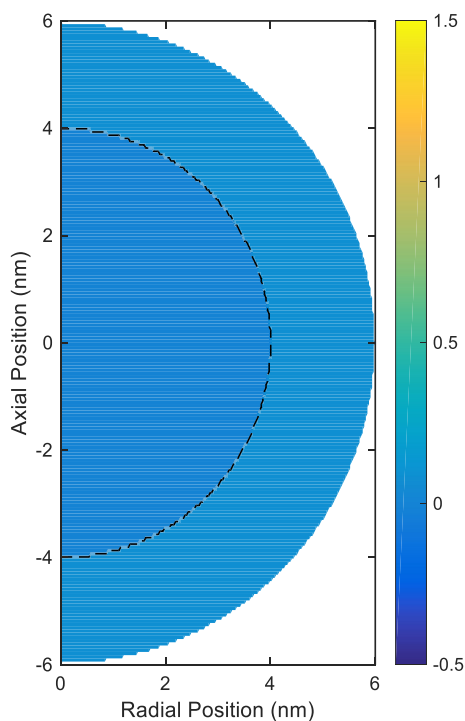


Figure 3. Strain-modified electron confinement potential in the CdSe/CdS core-shell quantum dot, incorporating the conduction-band offset and hydrostatic-strain-induced band-edge shifts.

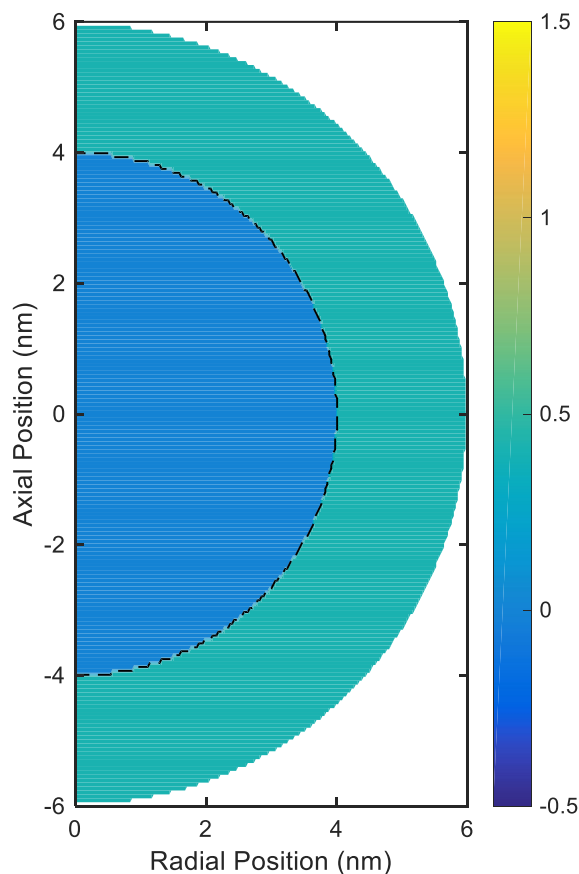


Figure 4. Strain-modified heavy-hole confinement potential in the CdSe/CdS core-shell quantum dot, showing the combined contributions of the valence-band offset and strain-induced changes in the valence-band edge.

The influence of the calculated strain distribution on carrier confinement is demonstrated in Figs. 3 and 4, which present the effective potential profiles for electrons and heavy holes, respectively. The range of the electron confinement potential is about 0.0807 eV and that of the heavy-hole confinement potential is about 0.4205 eV. These possible scales differ by a large factor due to the different conduction- and valence-band offsets and their different response to the deformation induced by lattice mismatch. The effective potentials entering the electron and heavy-hole Hamiltonians consist of the intrinsic band alignment and the strain-induced shifts of the band edges as formulated in model . These contributions together account for the spatial confinement environments experienced by the two carrier species [17,18,19]. The electron confinement potential is rather shallow, so that the electron envelope function can extend further spatially into the CdS shell. In contrast, the much larger heavy-hole potential barrier favours more localisation of the hole on the CdSe core. The difference in confinement behaviour is also due to the contrast in effective-mass of the two carriers. The electron effective masses are $0.13 m_0$ and $0.21 m_0$ in CdSe and CdS, respectively, and the corresponding heavy-hole effective masses are $0.45 m_0$ and $0.80 m_0$ as reported in Table 1 [22,23]. The contribution of the kinetic energy related to the spatial confinement varies inversely as the effective mass, so the lighter electrons have larger confinement energies than the heavier holes, when the geometric conditions are similar. The asymmetric electron and hole localisation observed in the calculated states is thus physically explained by the combined effects of band-edge alignment, strain induced potential modification and spatially dependent carrier masses [56,61].

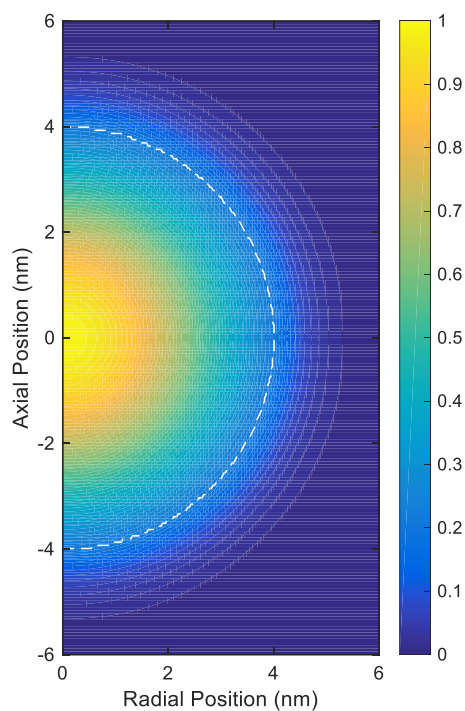


Figure 5. Normalised ground state electron probability density in the CdSe/CdS core-shell quantum dot, illustrating the localisation of the electron in the core and the penetration of the wavefunction into the surrounding CdS shell.

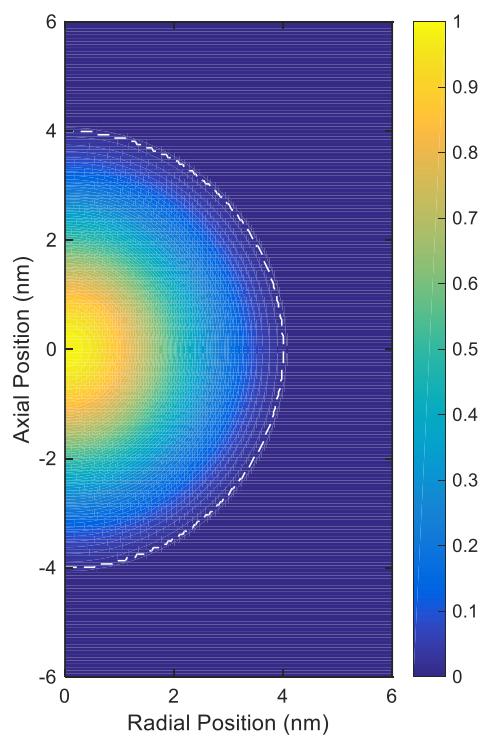


Figure 6. Heavy-hole probability density of the ground state of a CdSe/CdS core-shell quantum dot in normalised units, demonstrating a stronger spatial localisation of the hole compared to the electron ground state.

Figures 5 and 6 illustrate the normalized ground-state probability densities obtained for the electron and heavy hole, respectively. The corresponding envelope functions were obtained by solving the stationary eigenvalue problem of Eq. (48) after discretizing the axisymmetric BenDaniel-Duke Hamiltonian by finite differences. The conservative numerical treatment given in Eq. (46) is based on harmonic averaging of the position dependent effective masses at the material interfaces. This expression is constructed to preserve the necessary symmetry properties of the discrete Hamiltonian, and the discretized operator describes the BenDaniel-Duke interfacial matching conditions. This approach is particularly important in core-shell heterostructures as the discontinuities of the effective masses of the carriers affect both the eigenenergies and the spatial behaviour of the envelope functions [51,52,56,61]. The confinement energies of the ground state are 0.07168 eV and 0.03899 eV for the electron and the heavy hole respectively. The ground-state energy of the heavy hole is lower than that of the electron, although the confinement barrier is much larger. The difference in their effective masses can explain the behaviour, as the kinetic energy contribution from spatial localisation is reduced by the heavier heavy-hole mass. The numerical results thus indicate that the carrier confinement cannot be explained by the potential-barrier height only, but is determined by the combined effect of the confinement shape, local band-edge profile and position-dependent effective mass. The calculated energy difference between the two carriers is therefore consistent with the expected mass dependence of the quantum confinement in semiconductor nanostructures [4,57,58]. This interpretation is consistent with the probability-density distributions shown in Fig. 5 and Fig. 6. The electron ground state is characterised by a relatively broader spatial distribution from the CdSe core to the CdS shell, while the heavy-hole probability density is more localised in the core region. However, the two distributions show a large spatial coincidence, indicating that the electron-hole overlap is large, although the localisation characteristics are different. The carrier envelope functions were normalised according to the axisymmetric normalisation condition of Eq. (52) and its discrete version of Eq. (53). The maximum reported normalization error is approximately 4.44×10^{-16} for both carrier states, indicating that the discrete normalization condition is satisfied to near machine precision. This result verifies the numerical normalization procedure, although it does not independently establish convergence with respect to spatial discretization [22,23,56,61].

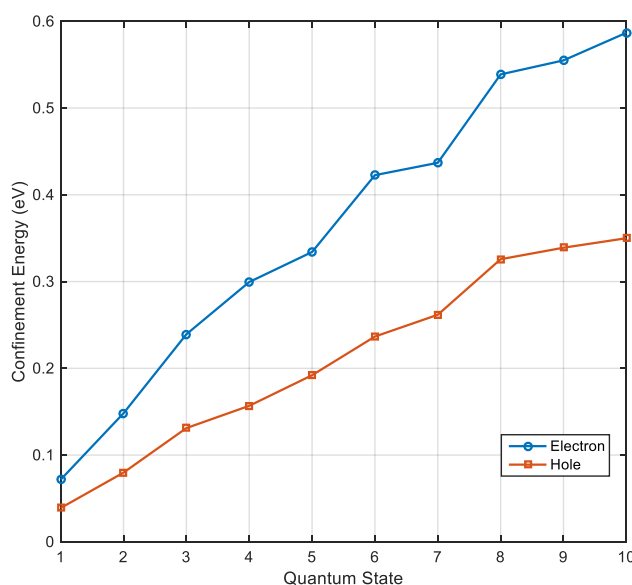


Figure 7. Calculated low-lying electron and heavy-hole confinement-energy spectra of the CdSe/CdS core-shell quantum dot obtained from the axisymmetric BenDaniel-Duke effective-mass Hamiltonian.

The low-lying confinement-energy spectra calculated for electrons and heavy holes are presented in Fig. 7. The electron energies increase from 0.07168 eV for the ground state to approximately 0.58677 eV for the tenth computed state. In comparison, the heavy-hole spectrum extends from 0.03899 to approximately 0.34997 eV over the corresponding set of states. The larger energy separation in the electron spectrum is consistent with the smaller electron effective mass, which enhances the kinetic-energy contribution due to the spatial confinement. In contrast, the heavy-hole mass is larger, so the energy spectrum is more dense. These results demonstrate the combined effect of quantum confinement and of the carrier-dependent effective masses on the electronic structure of the CdSe/CdS heterostructure [4,57,58]. The resulting numerical eigenvalue problem was formulated in terms of a sparse 40401×40401 dimensional Hamiltonian matrix, with 198803 nonzero elements. This sparsity reduces the computational storage requirements of the finite-difference discretization, and facilitates the evaluation of low-lying eigenstates. The reported relative symmetry error is essentially zero indicating that the assembled matrix preserves the expected discrete symmetry. Furthermore, the first shift-invert calculation converged all ten requested eigenstates, with the solver convergence flag being zero. The numerical values show that the discretized eigenvalue problem has been solved successfully and the computed eigenpairs satisfy the convergence criteria of the solver. Nevertheless, an independent mesh-refinement analysis [51,52] would be needed for a full verification of the spatial discretization accuracy.

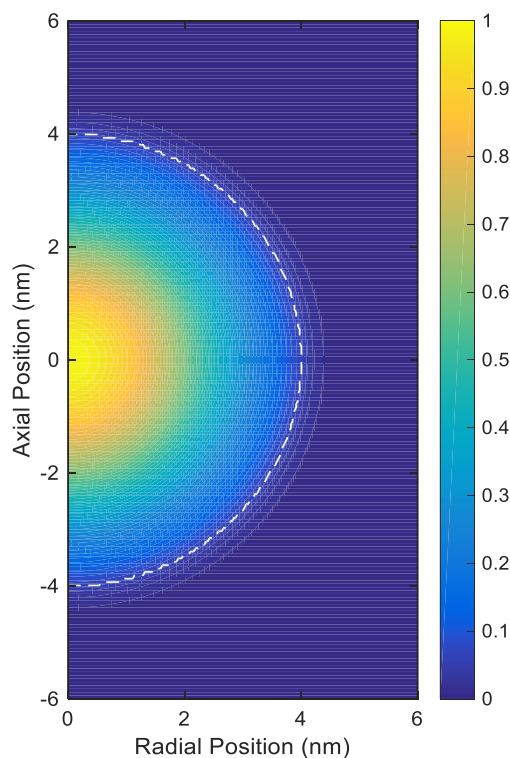


Figure 8. Spatial overlap density associated with the ground-state electron-hole transition in the CdSe/CdS core-shell quantum dot. The squared overlap integral, $|\langle \Psi_e | \Psi_h \rangle|^2$, characterizes the spatial coincidence of the normalized carrier envelope functions.

Figure 8 presents the spatial overlap associated with the fundamental electron-hole transition. The calculated overlap integral is approximately 0.904, corresponding to a

squared overlap of approximately 0.817. This relatively high value indicates that the electron and heavy-hole ground-state wavefunctions retain substantial spatial coincidence despite the greater penetration of the electron state into the CdS shell. The result demonstrates that the asymmetric confinement potentials do not lead to pronounced separation of the carrier distributions under the zero-field conditions considered here. Within the envelope-function approximation, the electron-hole overlap contributes directly to the interband transition matrix element introduced in Eq. (60). Accordingly, the calculated overlap provides an important indication of the relative optical-transition strength associated with the ground-state excitonic transition [56,60,61,62].

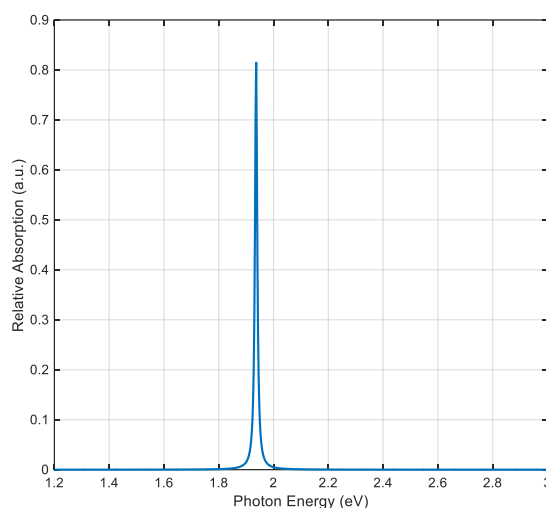


Figure 9. Calculated relative optical absorption spectrum of the CdSe/CdS core-shell quantum dot, including the first-order direct electron-hole Coulomb correction. The fundamental excitonic transition occurs at approximately 1.936 eV, corresponding to an equivalent photon wavelength of 640.3 nm.

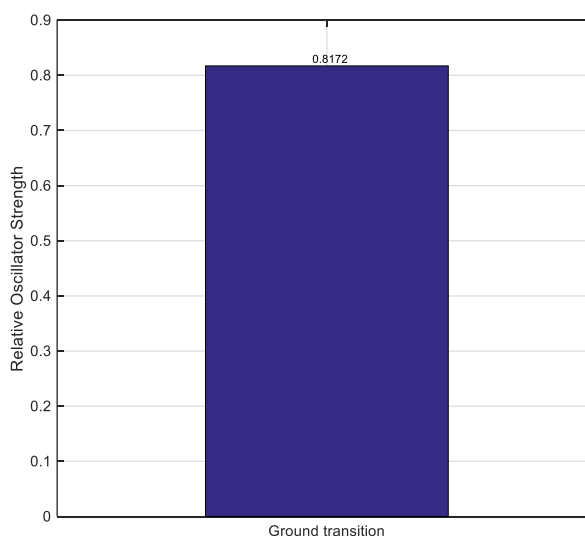


Figure 10. Calculated relative ground-state oscillator strength of the CdSe/CdS core-shell quantum dot. The value of approximately 0.817 reflects the squared spatial overlap between the electron and heavy-hole envelope functions within the adopted normalization scheme.

The substantial electron-hole overlap obtained from the ground-state wavefunctions is reflected in the calculated optical-transition strength. As shown in Fig. 10, the relative oscillator-strength measure reaches approximately 0.817, consistent with the squared envelope-function overlap reported in Fig. 8. This correspondence follows from the adopted optical formulation, in which the relative transition strength is evaluated from the overlap contribution to the interband transition matrix element. Therefore, the overlap distribution and relative oscillator strength provide complementary descriptions of the same underlying carrier-localization behavior. The result indicates that the fundamental transition remains optically active despite the unequal confinement characteristics of electrons and heavy holes. The relationship between the transition matrix element and oscillator strength is defined [56,60,61,62,63]. The calculated strain-modified band gap of the CdSe core is 1.87556 eV. Incorporating the ground-state electron and heavy-hole confinement energies according to the transition-energy expression associated with Eq. (58) gives an independent-particle optical transition energy of 1.98624 eV. To account for the attractive interaction between the confined carriers, the direct electron-hole Coulomb contribution was subsequently evaluated, yielding an energy correction of approximately 0.04985 eV. Inclusion of this interaction reduces the transition energy to 1.93639 eV. The calculated excitonic transition energy thus reflects the competing contributions of quantum confinement, which increases the transition energy, and electron-hole Coulomb attraction, which lowers it relative to the independent-particle value [17,18,19].

The direct Coulomb interaction produces a redshift of approximately 49.9 meV relative to the calculated independent-particle transition. This shift represents a non-negligible contribution to the optical transition energy for the nanocrystal dimensions considered in the present study. The resulting fundamental excitonic transition corresponds to a photon wavelength of approximately 640.3 nm, within the red region of the visible spectrum. These findings emphasize the importance of including electron-hole attraction when evaluating the optical properties of strongly confined semiconductor heterostructures. However, the predicted wavelength should be interpreted as the spectral position of the calculated optical transition rather than as an independently determined photoluminescence maximum, since emission dynamics and associated relaxation processes are not explicitly evaluated in the present model [49,57,59].

The Coulomb correction was calculated using the ground-state carrier probability densities within a first-order direct-interaction approximation. The adopted treatment therefore accounts for the electrostatic attraction between the electron and hole but does not include the full range of electron-hole correlations accessible through a configuration-interaction or many-body formulation. The effective dielectric constant employed in the Coulomb calculation is approximately 9.435, consistent with an intermediate dielectric response between the constituent CdSe and CdS regions. Numerical evaluation of the interaction employed 1271 effective quadrature points and a cell-scale regularization length of approximately 0.168 nm. Within these computational assumptions, the resulting 49.85 meV correction provides an estimate of the direct electron-hole binding contribution to the fundamental optical transition. The calculated relative optical absorption spectrum is presented in Fig. 9. Its principal spectral feature occurs near the fundamental excitonic transition energy of 1.936 eV, in agreement with the transition energy obtained after incorporating the direct Coulomb correction. The absorption response was constructed from the allowed interband transitions using the Lorentzian broadening function specified in Eq. (63), with a phenomenological linewidth parameter of 5 meV. The maximum calculated normalized absorption intensity is approximately 0.815. The optical calculation provides a relative spectral response, but not an absorption coefficient calibrated in absolute physical units, so the intensity reported is a dimensionless relative quantity within the normalisation procedure used. Therefore, the spectral peak position is more directly correlated to the predicted excitonic transition energy than an absolute absorption magnitude [17,60,64].

The correlation of Figs. 8-10 displays how the calculated carrier states determine the optical response of the heterostructure. The large spatial overlap between the electron and heavy-hole ground states enhances the envelope-function contribution to the optical transition matrix element, which leads to a large relative oscillator strength and a pronounced fundamental absorption feature[56,60]. Such behaviour connects the electronic and optical properties via a common physical mechanism: the strain-tuned band alignment defines the effective confinement potentials which control the spatial distribution of the electron and hole wavefunctions and therefore their overlap and the strength of the optical transitions. Thus, the computed optical response directly follows from the carrier states determined in the same effective-mass framework, rather than from an optical-transition model proposed separately [61,62].

4. Discussion

The global results can be understood in the frame of the unified theoretical framework of Eq. (66), which provides a systematic relation between the mechanical, electronic and optical properties of the CdSe/CdS core-shell quantum dot. The distribution of strain caused by the lattice mismatch at the heterointerface is determined by the material parameters given in Table 1. The resulting hydrostatic strain changes the local conduction- and valence-band edges via the deformation-potential interaction, which defines the effective confinement potentials used in the BenDaniel-Duke Hamiltonian [6,17]. The resulting sparse eigenvalue problem is solved to obtain the confined electron and hole energy levels and the corresponding envelope wavefunctions, from which the excitonic transition energy, oscillator strength and optical absorption characteristics are obtained. This formulation allows a consistent description of these coupled physical processes and serves as a reasonable basis to investigate the effect of structural deformation on the carrier confinement and optical transitions in semiconductor heterostructures [18,51,52]. The obtained results for the structural and material parameters, given in Table 1, demonstrate that the CdSe/CdS heterostructure possesses a moderate strain induced by a lattice mismatch, different confinement characteristics for electrons and holes, and a substantial spatial overlap of the envelope wavefunctions. The lowest electron and hole confinement energies are calculated as $E_{(e,1)}=0.07168$ eV and $E_{(h,1)}=0.03899$ eV, respectively, and the direct electron-hole Coulomb correction is 49.85 meV [15]. The contributions give an excitonic transition energy of 1.93639 eV, corresponding to an emission wavelength of approximately 640.3 nm. The calculated relative oscillator strength of 0.817 also indicates a strong optical transition of the ground state exciton. Overall, these results indicate that the chosen core-shell dimensions offer good conditions for electron-hole coupling and radiative optical transitions, highlighting the combined effect of strain, band alignment and quantum confinement on the electronic and optical behaviour of the nanostructure [16,56,61]. Another feature of the proposed model is the possibility of introducing a uniform external electric field via the electrostatic potential terms and included in the electron and hole Hamiltonians. Owing to their opposite electric charges, electrons and holes respond differently to the applied field, producing an asymmetric modification of their confinement potentials along the symmetry axis. The results presented in the preceding analysis were obtained under zero-field conditions ($F=0$) and therefore provide a reference state for evaluating the influence of an external electric field. According to Eq. (35), applying a finite electric field modifies the spatial potential profiles experienced by the charge carriers and may lead to a redistribution of their probability densities[24,25]. These changes are expected to affect the electron-hole spatial overlap and oscillator strength, together with the excitonic transition energy and the corresponding emission wavelength. Such behavior is consistent with the physical mechanism underlying the quantum-confined Stark effect, in which the applied electric field alters the electronic states and optical transitions of a quantum-confined system [28,50]. The zero-field calculations therefore provide a reference configuration for the

subsequent investigation of electric-field-dependent optical properties. Within the scope of the present study a systematic examination of the ground-state electron and hole energies, electron-hole overlap, excitonic transition energy, emission wavelength, and relative oscillator strength as functions of the applied electric field would allow the predicted field-induced modifications to be quantified. In particular, comparison of these quantities with their zero field values would shed light on the relative contributions of carrier redistribution, confinement asymmetry and electron-hole interaction to the resulting optical response [26,28]. The advantage of the unified approach is that lattice-mismatch strain, position dependent effective masses, heterointerface band discontinuities, quantum confinement, Coulomb interaction and electric-field effects can be described within a common axisymmetric computational scheme. Such a combined treatment offers a proper theoretical framework to study the coupled structural, electronic and optical properties of strained core-shell quantum dots under external electric fields [38,39].

5. Conclusion

In this work, it is developed a unified axisymmetric BenDaniel-Duke effective mass formalism to study the coupled mechanical, electronic and optical properties of strained CdSe/CdS core-shell quantum dots. The model incorporates lattice-mismatch strain, deformation-potential-induced band-edge shifts, position-dependent effective masses, quantum confinement, and electron-hole Coulomb interaction, while allowing the inclusion of a uniform external electric field. For a CdSe core radius of 4.0 nm and a CdS shell thickness of 2.0 nm, the calculated lattice mismatch of 4.022% produced compressive hydrostatic strain of -2.30% in the core and tensile strain of +0.82% in the shell. The resulting strain-modified confinement potentials were approximately 0.0807 eV for electrons and 0.4205 eV for heavy holes, leading to ground-state confinement energies of 0.0717 and 0.0390 eV, respectively. The stronger hole confinement and greater electron delocalization resulted in a substantial electron-hole overlap, with a squared overlap integral of 0.817, indicating a strong fundamental optical transition. Including the direct electron-hole Coulomb interaction reduced the transition energy from 1.9862 to 1.9364 eV, corresponding to an emission wavelength of approximately 640.3 nm. The value of the Coulomb correction of 49.85 meV obtained indicates the importance of excitonic interactions in the optical response. Numerical consistency was shown by the symmetry of the discretized Hamiltonian, convergence of the computed eigenstates and wavefunction-normalization errors of the order of 10^{-16} .

The results together demonstrate that the electronic structure and optical activity of CdSe/CdS core-shell quantum dots are determined by a combination of lattice-mismatch strain and carrier confinement. The proposed framework provides a consistent numerical basis for the study of these coupled effects, and a zero-field reference for future investigations of electric-field-induced carrier redistribution and quantum-confined Stark shifts. Its versatility also makes it suitable to investigate the effect of core size, shell thickness and material composition on the optical properties of semiconductor heterostructures.

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