

Article

Regression-Based Machine Learning Prediction of Electronic and Nonlinear Optical Properties in Coupled GaN/AlN Quantum Dots

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Abstract

This study investigates the electronic and nonlinear optical properties of coupled GaN/AlN quantum dots using a numerical approach based on coordinate transformation combined with the finite difference method (FDM). The Schrödinger equation is solved to determine the electronic energy levels and wave functions of the system, which are subsequently used to evaluate the nonlinear optical rectification (NOR) response. Since numerical simulations become computationally expensive for large quantum dot systems, several regression-based models, including Polynomial Regression, Ridge Regression, LASSO, and Elastic Net, are trained on high-fidelity numerical data. These models learn the relationship between structural parameters and the resulting electronic and optical properties, enabling fast and reliable predictions for larger quantum dot configurations. The predictive performance of the ML models is assessed by comparing their results with the numerical simulations, showing excellent agreement while significantly reducing computational effort. The proposed hybrid physics–machine learning framework therefore provides an efficient and reliable approach for predicting the electronic and nonlinear optical behavior of coupled GaN/AlN quantum dots.

Keywords: quantum dots; electronic structure; nonlinear optical properties; machine learning

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1. Introduction

Group III–nitride wide-bandgap semiconductors, including GaN, AlN, (In,Ga)N, (Al,Ga)N, and (Al,In,Ga)N, have attracted sustained scientific and technological interest owing to their remarkable physical properties and broad applicability in high-performance electronic and optoelectronic devices [1,2]. The continuous advancement of epitaxial growth techniques, particularly Molecular Beam Epitaxy (MBE) and Metal–Organic Chemical Vapor Deposition (MOCVD) [3,4], has enabled the fabrication of compound semiconductor heterostructures with atomic-scale precision. These technological developments have facilitated the controlled realization of semiconductor nanostructures exhibiting complex and finely engineered geometries. Among these nanostructures, GaN/AlN quantum dots

(QDs) have emerged as promising candidates for ultraviolet optoelectronic applications due to their strong carrier confinement and large band offsets [5]. Experimentally, GaN/AlN QDs are commonly observed to adopt truncated pyramidal morphologies, resulting from strain-driven self-assembly during epitaxial growth, as shown in Figure 1 [6].

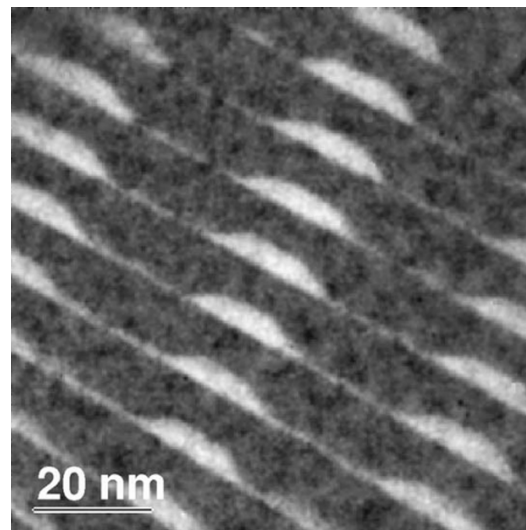


Figure 1. GaN QDs embedded inside an AlN matrix.

To date, considerable research efforts have been dedicated to the investigation of nonlinear properties of semiconductor structures based on intersubband transitions and have grown dramatically in both theoretical and experimental research [4,5]. Grzegorz et al. [7] used the finite element method to model the nonlinear piezoelectricity in wurtzite GaN/AlN QD. Wenjie Yao et al. [5] studied the linear and third order nonlinear absorption coefficients and refractive index changes in strained single quantum dots. Significant efforts have been devoted to the study of nonlinear optical waveguides relying on near-infrared intersubband transitions in GaN/AlN quantum wells [8]. To date, only a limited number of theoretical studies have addressed the comprehensive modeling of self-assembled quantum dots. In this context, Congxin Xia et al. [9] investigated the donor binding energy of a hydrogenic impurity in zinc-blended GaN/AlN coupled quantum dots using a variational approach, assuming a symmetric cylindrical quantum dot geometry with the impurity located at a radial position r . While this idealized geometry facilitates analytical treatment, it does not accurately reflect the truncated pyramidal morphology typically observed in self-assembled GaN/AlN quantum dots grown by epitaxial methods. In this work, we introduce a numerical approach that combines a coordinate transformation with the finite difference method (FDM) to solve the Schrödinger equation in nanostructures of varying dimensionality. In our earlier studies, this approach was successfully applied to a variety of quantum dot configurations, including hexagonal [10,11] and elliptical geometries, concentric and nonconcentric core-shell quantum dots [12–14], as well as isolated and self-assembled QDs with a dome-shaped cross section [15]. The results obtained showed good agreement with available experimental observations.

The novelty of this study lies in the integration of machine learning (ML) techniques with a numerical framework based on coordinate transformation and the finite difference method (FDM) to efficiently predict the electronic and nonlinear optical properties of coupled GaN/AlN quantum dots. ML techniques have recently emerged as powerful tools for tackling various challenges in materials physics [16]. Unlike previous studies that relied exclusively on analytical or numerical approaches applied to relatively simple quantum dot geometries, the present approach introduces several significant advances. First, the electronic structure of the coupled quantum dot system is deter-

mined by solving the Schrödinger equation using a coordinate transformation combined with the finite difference method, enabling an accurate description of realistic nanostructures. Second, the high-fidelity numerical results obtained from these simulations are used to train machine learning models capable of capturing the relationship between structural parameters and the corresponding electronic and optical responses. In this work, several regression-based ML models, including Polynomial Regression [17], Ridge Regression [18–20], LASSO [19,20], and Elastic Net [19], are employed to learn this relationship and predict the electronic energy levels and nonlinear optical properties. Third, the trained ML models are shown to reproduce the numerical results with high accuracy while considerably reducing the computational cost [21,22]. The main objective of this work is therefore to develop a fast, reliable, and generalizable predictive framework for the electronic and nonlinear optical properties of coupled quantum dot systems, facilitating the exploration of larger quantum dot configurations that would otherwise require extensive numerical simulations. To construct the training dataset, the Schrödinger equation is solved using the coordinate transformation–FDM approach to obtain the corresponding energy levels and wave functions. The predictive capability of the ML algorithms is then evaluated by comparing their outputs with the numerical results obtained from the physical simulations.

The remainder of this paper is organized as follows: Section 2 presents the mathematical formulation and the numerical approach based on the coordinate transformation combined with the finite difference method used to solve the Schrödinger equation for truncated pyramidal GaN/AlN quantum dots. Section 3 discusses the obtained numerical results, focusing on the electronic structure and the nonlinear optical properties of coupled quantum-dot systems. It also introduces the machine-learning framework employed to predict the electronic and nonlinear optical properties for larger quantum-dot arrays. Finally, Section 4 summarizes the main findings and presents the conclusions of this work.

2. Mathematical Formulation and Numerical Method

In this section, we present a numerical method based on coordinate transformation combined with the finite difference approach to solve the Schrödinger equation for quantum dots with complex geometries.

$$-\frac{\hbar^2}{2} \left[\frac{\partial}{\partial x} \left(\frac{1}{m^*(x,y,z)} \frac{\partial \psi}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{1}{m^*(x,y,z)} \frac{\partial \psi}{\partial y} \right) + \frac{\partial}{\partial z} \left(\frac{1}{m^*(x,y,z)} \frac{\partial \psi}{\partial z} \right) \right] + V(x,y,z)\psi = E\psi. \quad (1)$$

where m^* denotes the electron or hole effective mass, $V(x,y,z)$ represents the three-dimensional potential profile determined by the conduction or valence band offset, and E and $\psi(x,y,z)$ are the quantized energy levels and their corresponding wave functions, respectively.

In order to reach a realistic approach of self-assembled truncated pyramidal GaN/AlN QD, we have used the method of coordinate transformation. Additional details regarding the proposed method are provided in Refs. [13,14]. The coordinate transformation defining the GaN/AlN nanostructure geometry is introduced as follows:

$$\begin{aligned} x &= Tu \\ y &= T \frac{u^m \sinh(Av) \sin(Ku^p)}{D \cosh(Bw)^q} \\ z &= Tw \end{aligned} \quad (2)$$

This transformation simplifies the geometry of the nanostructure, leading to flat interfaces in the computational domain. The first space corresponds to the real space defined

by the original coordinates $\beta(x, y, z)$, while the second space, $\gamma(u, v, w)$, represents the computational space.

Consequently, the Schrödinger equation can be mapped into the γ -space as:

$$-\frac{\hbar^2}{2} \left[u_x \frac{\partial}{\partial u} \psi^1(u, v, w) + v_x \frac{\partial}{\partial v} \psi^1(u, v, w) + w_x \frac{\partial}{\partial w} \psi^1(u, v, w) \right. \\ \left. + u_y \frac{\partial}{\partial u} \psi^2(u, v, w) + v_y \frac{\partial}{\partial v} \psi^2(u, v, w) + w_y \frac{\partial}{\partial w} \psi^2(u, v, w) \right. \\ \left. + u_z \frac{\partial}{\partial u} \psi^3(u, v, w) + v_z \frac{\partial}{\partial v} \psi^3(u, v, w) + w_z \frac{\partial}{\partial w} \psi^3(u, v, w) \right] + V\psi = E\psi. \quad (3)$$

where $\psi^1(u, v, w)$, $\psi^2(u, v, w)$, and $\psi^3(u, v, w)$ are auxiliary functions, defined as:

$$\psi^1(u, v, w) = \left[\frac{u_x}{m^*} \frac{\partial \psi}{\partial u} + \frac{v_x}{m^*} \frac{\partial \psi}{\partial v} + \frac{w_x}{m^*} \frac{\partial \psi}{\partial w} \right]. \quad (4)$$

$$\psi^2(u, v, w) = \left[\frac{u_y}{m^*} \frac{\partial \psi}{\partial u} + \frac{v_y}{m^*} \frac{\partial \psi}{\partial v} + \frac{w_y}{m^*} \frac{\partial \psi}{\partial w} \right]. \quad (5)$$

$$\psi^3(u, v, w) = \left[\frac{u_z}{m^*} \frac{\partial \psi}{\partial u} + \frac{v_z}{m^*} \frac{\partial \psi}{\partial v} + \frac{w_z}{m^*} \frac{\partial \psi}{\partial w} \right]. \quad (6)$$

Therefore, we describe the two Jacobian matrices J_{xyz} and J_{uvw} :

$$J_{x,y,z} = J_{u,v,w}^{-1} \quad (7)$$

$$J_{u,v,w} = \begin{bmatrix} x_u & x_v & x_w \\ y_u & y_v & y_w \\ z_u & z_v & z_w \end{bmatrix} = \begin{bmatrix} T & 0 & 0 \\ T f_u & T f_v & T f_w \\ 0 & 0 & T \end{bmatrix} \quad (8)$$

$$J_{x,y,z} = \begin{bmatrix} u_x & u_y & u_z \\ v_x & v_y & v_z \\ w_x & w_y & w_z \end{bmatrix} = \begin{bmatrix} \frac{1}{T} & 0 & 0 \\ -\frac{f_u}{T f_v} & \frac{1}{T f_v} & -\frac{f_w}{T f_v} \\ 0 & 0 & \frac{1}{T} \end{bmatrix} = \frac{1}{T} \begin{bmatrix} 1 & 0 & 0 \\ \mu & \rho & \lambda \\ 0 & 0 & 1 \end{bmatrix} \quad (9)$$

The derivatives of $f(u, v, w)$ are f_u , f_v and f_w :

$$\mu = T v_x = -\frac{f_u}{f_v} \quad (10)$$

$$\rho = T v_y = \frac{1}{f_v} \quad (11)$$

$$\lambda = T v_z = -\frac{f_w}{f_v} \quad (12)$$

The Schrödinger equation becomes:

$$-\frac{\hbar^2}{2T^2} \left[\frac{\partial}{\partial u} \left(\frac{1}{m^*} \frac{\partial \psi}{\partial u} + \frac{\mu}{m^*} \frac{\partial \psi}{\partial v} \right) + \frac{\partial}{\partial v} \left(\frac{1}{m^*} \frac{\partial \psi}{\partial v} + \frac{\mu}{m^*} \frac{\partial \psi}{\partial u} \right) \right. \quad (13)$$

$$\left. + \frac{\partial}{\partial v} \left(\frac{\lambda}{m^*} \frac{\partial \psi}{\partial w} + \frac{\rho}{m^*} \frac{\partial \psi}{\partial v} \right) + \frac{\partial}{\partial w} \left(\frac{\lambda}{m^*} \frac{\partial \psi}{\partial v} + \frac{1}{m^*} \frac{\partial \psi}{\partial w} \right) \right] + V\psi = E\psi \quad (14)$$

After discretizing the equation by the (FDM), we obtain:

$$\begin{aligned}
& -\frac{\hbar^2}{2T^2} \left[\left(A_{uu}^1 \left(\frac{1}{m^*} \right)_{i+\frac{1}{2},j,k} - A_{uu}^2 \left(\frac{1}{m^*} \right)_{i-\frac{1}{2},j,k} \right) \right. \\
& + \mu_{i,j,k} \left(A_{uv}^1 \left(\frac{\mu}{m^*} \right)_{i+\frac{1}{2},j,k} - A_{uv}^2 \left(\frac{\mu}{m^*} \right)_{i-\frac{1}{2},j,k} \right) \\
& + \mu_{i,j,k} \left(A_{vu}^1 \left(\frac{1}{m^*} \right)_{i,j+\frac{1}{2},k} - A_{vu}^2 \left(\frac{1}{m^*} \right)_{i,j-\frac{1}{2},k} \right) \\
& + \left(A_{vv}^1 \left(\frac{\mu}{m^*} \right)_{i,j+\frac{1}{2},k} - A_{vv}^2 \left(\frac{\mu}{m^*} \right)_{i,j-\frac{1}{2},k} \right) \\
& + \rho_{i,j,k} \left(A_{vv}^1 \left(\frac{\rho}{m^*} \right)_{i,j+\frac{1}{2},k} - A_{vv}^2 \left(\frac{\rho}{m^*} \right)_{i,j-\frac{1}{2},k} \right) \\
& + \lambda_{i,j,k} \left(A_{vw}^1 \left(\frac{\lambda}{m^*} \right)_{i,j+\frac{1}{2},k} - A_{vw}^2 \left(\frac{\lambda}{m^*} \right)_{i,j-\frac{1}{2},k} \right) \\
& + \left(A_{wv}^1 \left(\frac{\lambda}{m^*} \right)_{i,j,k+\frac{1}{2}} - A_{wv}^2 \left(\frac{\lambda}{m^*} \right)_{i,j,k-\frac{1}{2}} \right) \\
& \left. + \left(A_{ww}^1 \left(\frac{1}{m^*} \right)_{i,j,k+\frac{1}{2}} - A_{ww}^2 \left(\frac{1}{m^*} \right)_{i,j,k-\frac{1}{2}} \right) \right] + V_{i,j,k} \psi_{i,j,k} = E_{i,j,k} \psi_{i,j,k}.
\end{aligned} \tag{15}$$

The finite-difference coefficients are defined as follows:

$$\begin{aligned}
A_{uu}^1 &= \frac{\psi_{i+1,j,k} - \psi_{i,j,k}}{h_u^2}, & A_{uv}^1 &= \frac{\psi_{i+\frac{1}{2},j+\frac{1}{2},k} - \psi_{i+\frac{1}{2},j-\frac{1}{2},k}}{h_u h_v}, \\
A_{vu}^1 &= \frac{\psi_{i+\frac{1}{2},j+\frac{1}{2},k} - \psi_{i-\frac{1}{2},j+\frac{1}{2},k}}{h_u h_v}, & A_{uu}^2 &= \frac{\psi_{i,j,k} - \psi_{i-1,j,k}}{h_u^2}, \\
A_{uv}^2 &= \frac{\psi_{i-\frac{1}{2},j+\frac{1}{2},k} - \psi_{i-\frac{1}{2},j-\frac{1}{2},k}}{h_u h_v}, & A_{vu}^2 &= \frac{\psi_{i+\frac{1}{2},j-\frac{1}{2},k} - \psi_{i-\frac{1}{2},j-\frac{1}{2},k}}{h_u h_v}, \\
A_{vv}^1 &= \frac{\psi_{i,j+1,k} - \psi_{i,j,k}}{h_v^2}, & A_{vw}^1 &= \frac{\psi_{i,j+\frac{1}{2},k+\frac{1}{2}} - \psi_{i,j+\frac{1}{2},k-\frac{1}{2}}}{h_v h_w}, \\
A_{wv}^1 &= \frac{\psi_{i,j+\frac{1}{2},k+\frac{1}{2}} - \psi_{i,j-\frac{1}{2},k+\frac{1}{2}}}{h_w h_v}, & A_{vv}^2 &= \frac{\psi_{i,j,k} - \psi_{i,j-1,k}}{h_v^2}, \\
A_{vw}^2 &= \frac{\psi_{i,j-\frac{1}{2},k+\frac{1}{2}} - \psi_{i,j-\frac{1}{2},k-\frac{1}{2}}}{h_v h_w}, & A_{wv}^2 &= \frac{\psi_{i,j+\frac{1}{2},k-\frac{1}{2}} - \psi_{i,j-\frac{1}{2},k-\frac{1}{2}}}{h_w h_v}, \\
A_{ww}^1 &= \frac{\psi_{i,j,k+1} - \psi_{i,j,k}}{h_w^2}, & A_{ww}^2 &= \frac{\psi_{i,j,k} - \psi_{i,j,k-1}}{h_w^2}.
\end{aligned} \tag{16}$$

In the above matrix, j and k are the discretization-point indices, whereas h_u , h_v , and h_w denote the discretization steps along the u , v , and w coordinates, respectively.

We consider N_u , N_v , and N_w as the number of points in each direction u , v , and w , respectively. The discretization matrix is obtained by taking into account the following boundary conditions:

$$\psi_{0,j,k} = \psi_{N_u+1,j,k} = 0, \quad \psi_{i,0,k} = \psi_{i,N_v+1,k} = 0, \quad \psi_{i,j,0} = \psi_{i,j,N_w+1} = 0. \tag{17}$$

To investigate the influence of the coordinate transformation parameters on the resulting structural shape, the corresponding figures are presented below.

Figure 2a–c illustrate the influence of the parameters A and B on the geometry of the quantum dot. The parameter A mainly affects the dot height h , with increasing A leading to a higher and more pronounced vertical profile. In contrast, the parameter B controls the dot width along the z -direction, modifying the lateral extension of the structure. Variations in B result in either a more confined or a more spread spatial distribution along the z -axis. Together, the parameters A and B provide an effective way to tune the aspect ratio of the quantum dot, allowing independent control of its height and width.

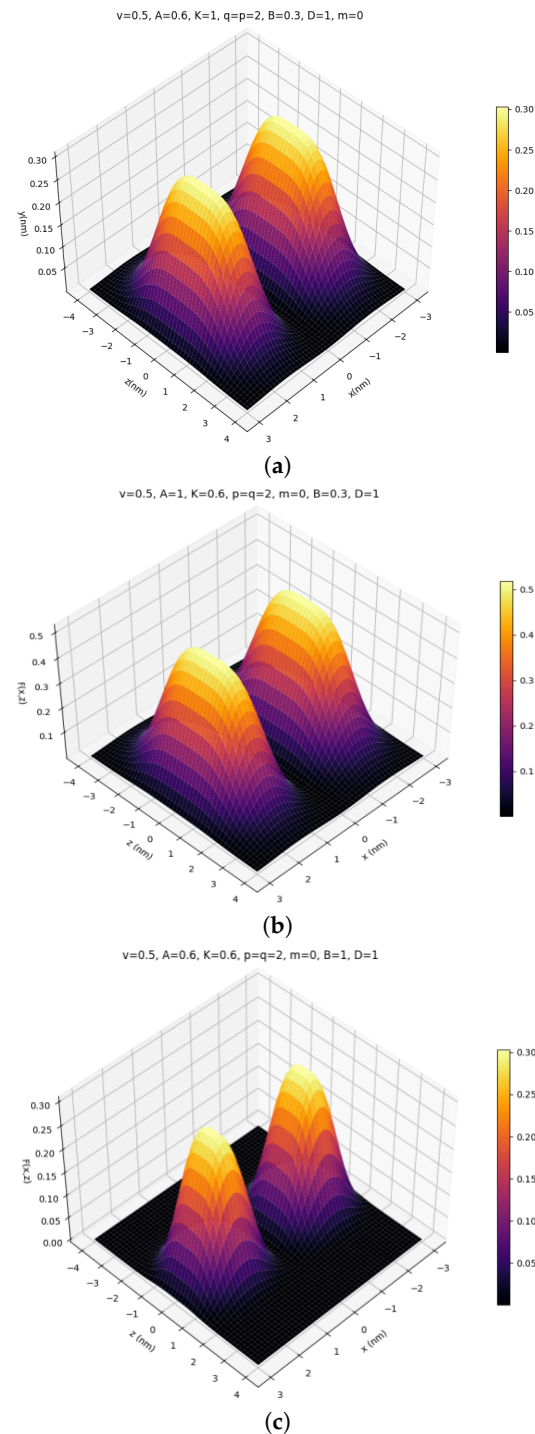


Figure 2. Influence of the parameters on the quantum dot geometry: (a) $v = 0.5, A = 0.6, K = 1, p = q = 2, B = 0.3, D = 1$, and $m = 0$; (b) $v = 0.5, A = 1, K = 0.6, p = q = 2, B = 0.3, D = 1$, and $m = 0$; (c) $v = 0.5, A = 0.6, K = 0.6, p = q = 2, B = 1, D = 1$, and $m = 0$.

To better understand the influence of the geometrical parameters A and B on the quantum dot shape, topographic maps of the coordinate transformation function are presented in Figure 3a,b for different values of these parameters. These maps provide a clearer visualization of how A and B affect the spatial profile of the truncated pyramidal quantum dot geometry. It is clearly observed from Figure 3 that the parameter A mainly affects the height of the quantum dot profile, whereas the parameter B influences the lateral extension.

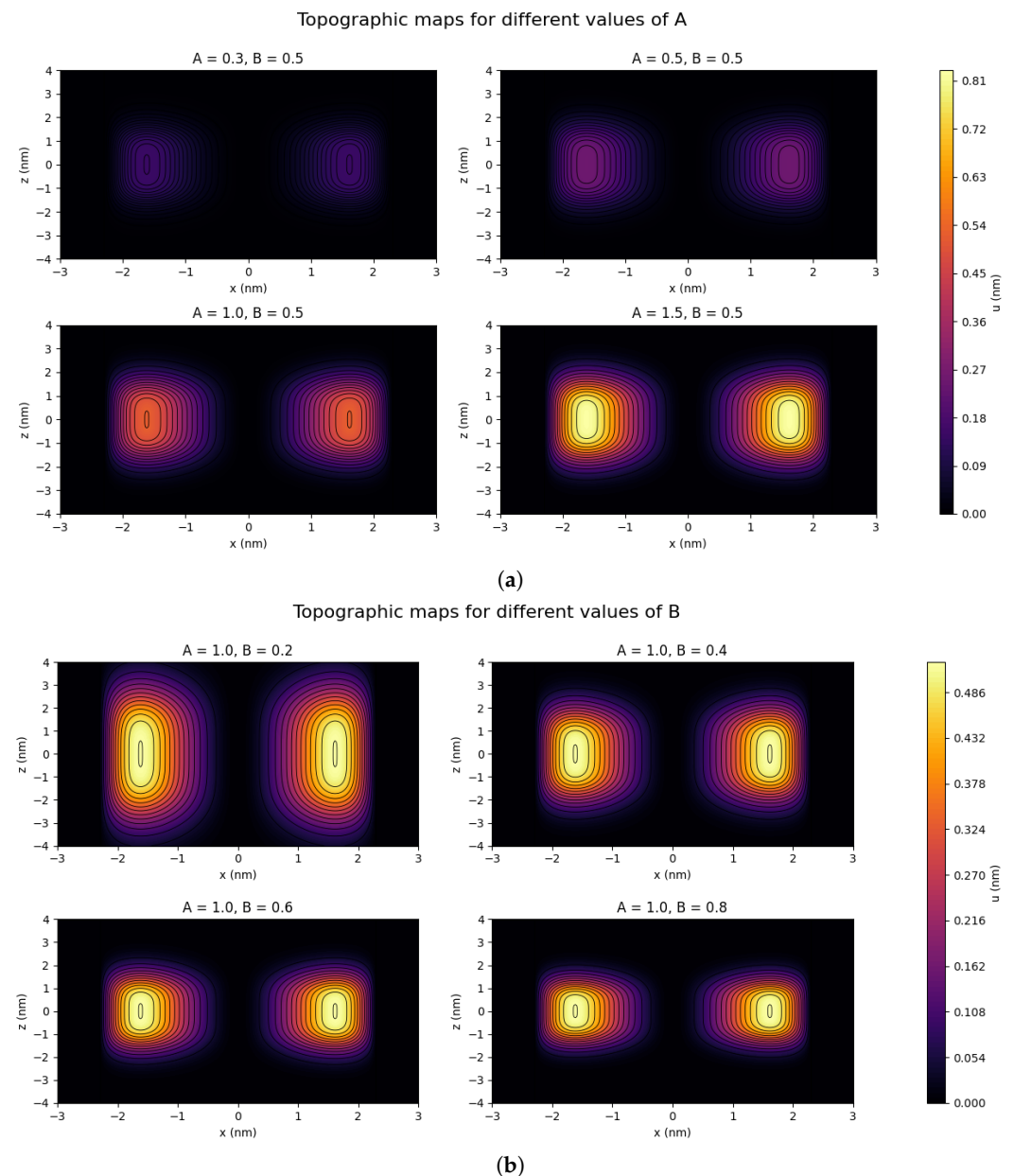


Figure 3. Topographic maps of the quantum dot geometry for different values of (a) A and (b) B and fixed values $v = 0.5$, $K = 0.6$, $p = q = 2$, $D = 1$, $m = 0$ and $T = 1$.

As illustrated in Figures 4–6 the shape of the function is strongly governed by the mathematical parameters. Figure 4b shows that, for $q = 1$, the truncation is cancelled and the quantum dot adopts a non-truncated pyramidal shape. The truncation of the pyramidal quantum dot is mainly governed by the truncation parameter q . This parameter controls the degree of flattening of the pyramid apex and therefore modifies the transition from a sharp pyramidal shape to a truncated pyramidal geometry.

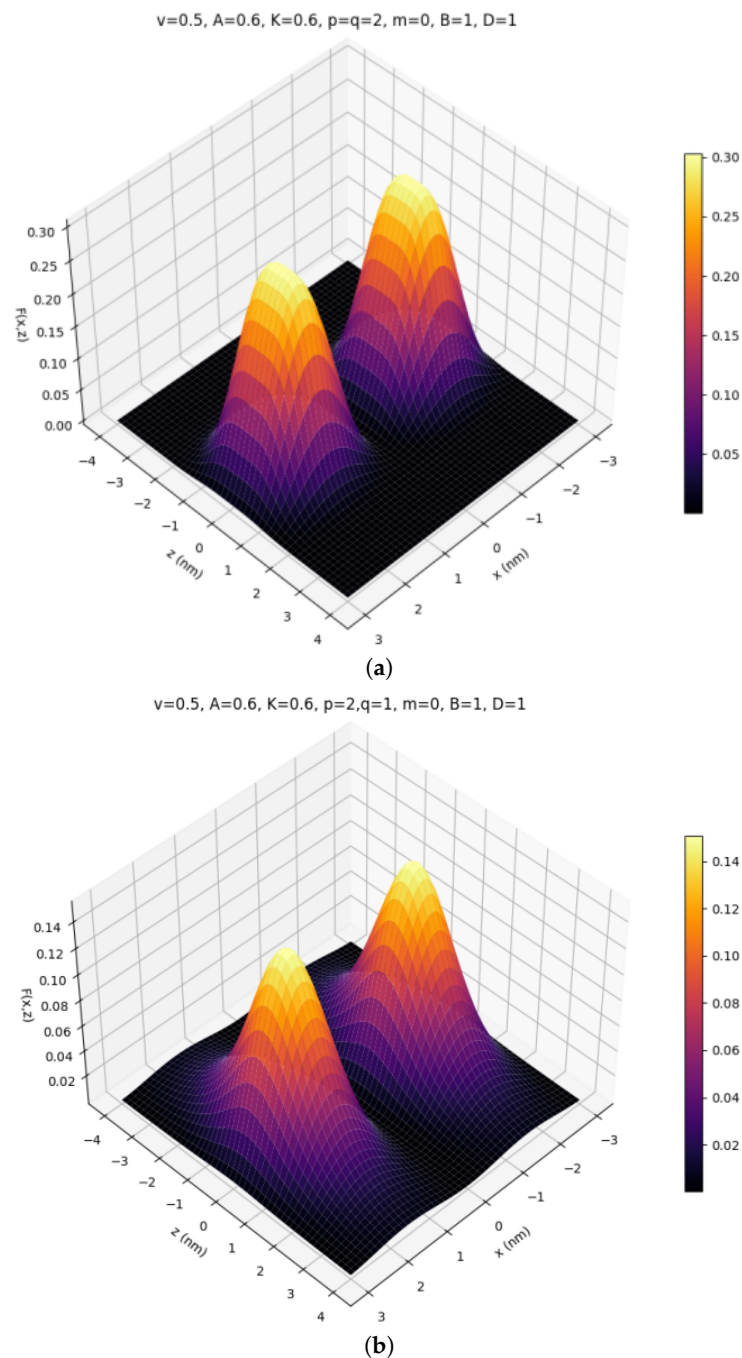


Figure 4. Influence of the truncation parameter q on the quantum dot geometry: (a) quantum dot geometry for $q = 2$; (b) quantum dot geometry for $q = 1$. The other parameters are fixed at $v = 0.5$, $A = 0.6$, $K = 0.6$, $p = 2$, $m = 0$, $B = 1$, and $D = 1$.

Figure 5 shows that the parameter m strongly affects the nanostructure geometry. For even integer values of m , the inter-dot distance is modified. In contrast, for odd values of m , the spatial profile becomes antisymmetric, and the notion of a well-defined inter-dot distance is no longer applicable.

Figure 6 indicates that the parameter K plays a key role in determining the number of coupled quantum dots, with higher values of K resulting in a larger number of dots.

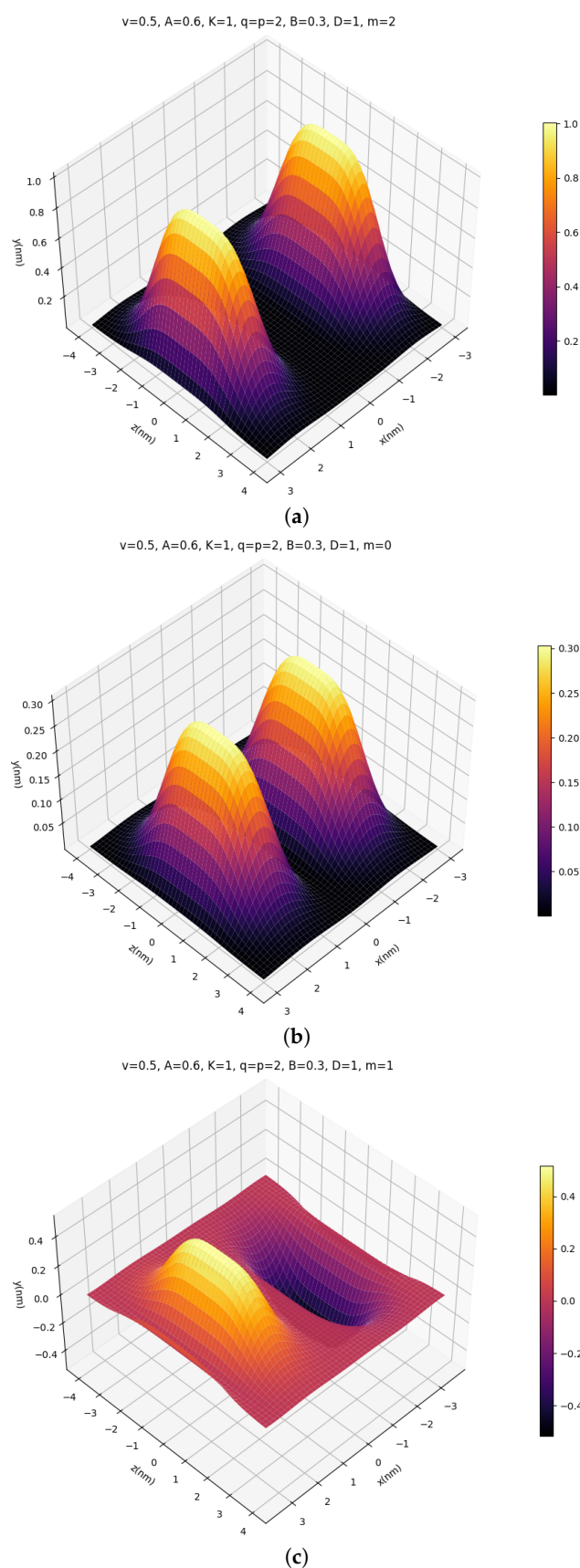


Figure 5. Effect of the parameter m on the nanostructure geometry: (a) nanostructure geometry for $m = 2$; (b) nanostructure geometry for $m = 0$; (c) nanostructure geometry for $m = 1$. The other parameters are fixed at $v = 0.5$, $A = 0.6$, $K = 1$, $p = q = 2$, $B = 0.3$, and $D = 1$.

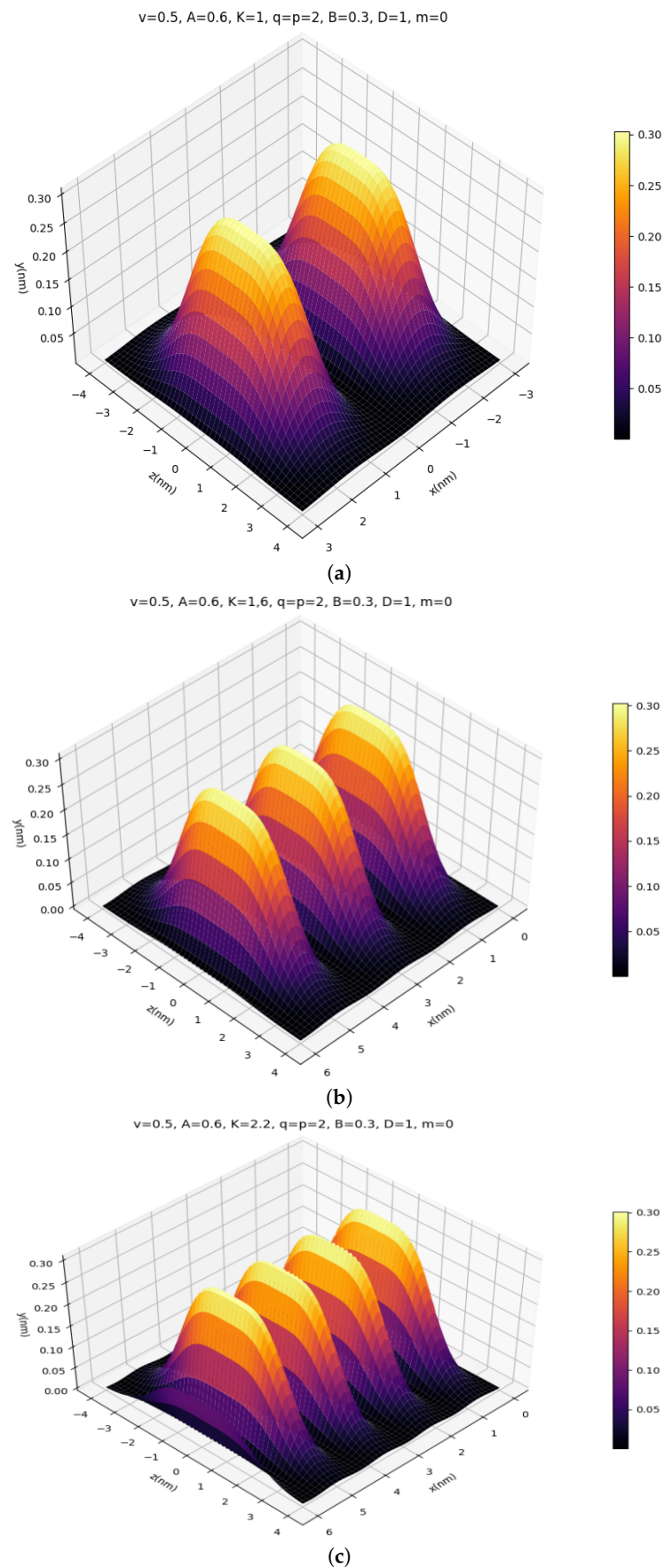


Figure 6. Effect of the parameter K on the nanostructure geometry: (a) nanostructure geometry for $K = 1$; (b) nanostructure geometry for $K = 1.6$; (c) nanostructure geometry for $K = 2.2$. The other parameters are fixed at $v = 0.5, A = 0.6, p = q = 2, B = 0.3, D = 1$, and $m = 0$.

3. Results and Discussion

3.1. Numerical Analysis of Coupled GaN/AlN Double Quantum Dots

Numerical simulations are performed in this section to investigate the electronic and optical properties of laterally coupled GaN/AlN double quantum dots with a truncated pyramidal geometry. The electronic properties are systematically analyzed by calculating the ground and first excited electron states as functions of the quantum dot geometric parameters, namely the height h , lateral dimension (L_x, L_z), and inter-dot separation L_c .

Figure 7 shows the evolution of the ground (E_{11}, E_{12}) and first excited (E_{21}, E_{22}) electron energy levels as a function of the quantum dot height h with fixed value of quantum dot length $L_z = 6.3$ nm, $L_x = 2$ nm and $L_c = 0.5$ nm. All energy levels decrease monotonically with increasing h , indicating a strong dependence of the electronic spectrum on the dot height. These results are in agreement with previously reported results [23–25].

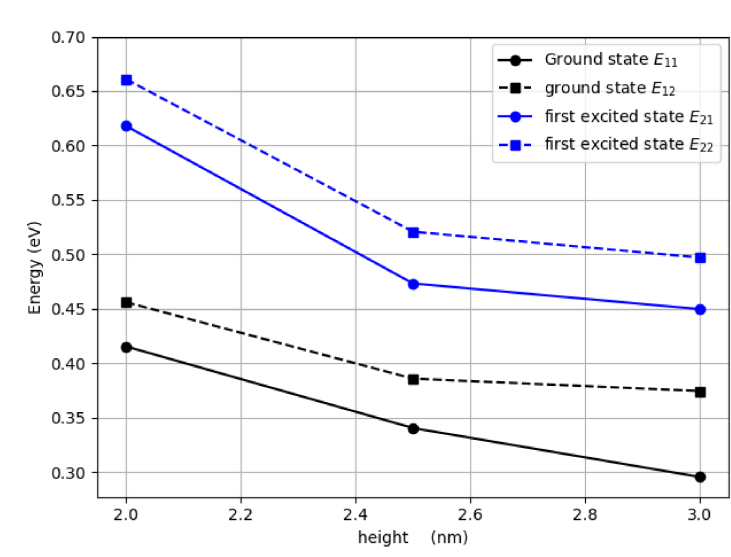


Figure 7. Energy levels E_{11} , E_{12} , E_{21} , and E_{22} as a function of the quantum dot height h for laterally coupled truncated pyramidal GaN/AlN quantum dots.

The decrease is more pronounced for the excited states than for the ground states, showing that higher-energy states are more sensitive to variations in the quantum dot dimensions. In addition, a finite energy splitting persists between the paired levels (E_{11} – E_{12} and E_{21} – E_{22}), suggesting the presence of coupling or symmetry-related effects.

These results demonstrate that the quantum dot height plays an important role in tuning the electronic energy levels of GaN/AlN quantum dots.

For fixed values of the quantum dot height $h = 2$ nm, a lateral base width $L_x = 2$ nm and the inter-dot distance $L_c = 0.5$ nm, Figure 8 illustrates the variation of the ground (E_{11}, E_{12}) and first excited (E_{21}, E_{22}) electron energy levels as a function of the quantum dot length L_z . All energy levels decrease with increasing L_z , indicating a strong dependence of the electronic spectrum on the dot length, a behavior consistent with previous reports by D. Makhoul et al. [26] and L. Zhang et al. [27].

The calculated energy levels E_1 and E_2 for two laterally coupled truncated pyramidal GaN/AlN quantum dots as a function of the inter-dot distance L_c are presented in Table 1. At small separations ($L_c = 0.5$ nm), strong lateral tunnel coupling splits each confined state into bonding and antibonding levels due to the overlap of electron wave functions through the AlN barrier. As the inter-dot distance increases, the splitting rapidly decreases because of the reduced wave-function overlap. For larger separations ($L_c \geq 3$ nm), the energy levels converge toward those of isolated quantum dots, indicating negligible coupling

and independent dot behavior. The obtained results are in good agreement with previous studies reported in the literature [28].

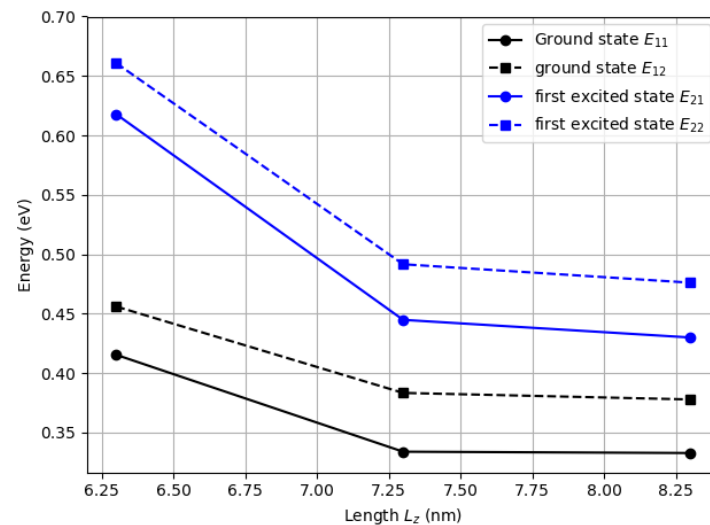


Figure 8. Energy levels E_{11} , E_{12} , E_{21} , and E_{22} as a function of the quantum dot length L_z for laterally coupled truncated pyramidal GaN/AlN quantum dots.

Table 1. Calculated electron energy levels as a function of the inter-dot distance L_c .

Energy Level	Inter-Dot Distance L_c (nm)				
	0.5	2	3	5	6
E_{11} (eV)	0.41536	0.50922	0.84961	0.85159	0.99198
E_{12} (eV)	0.45608	0.51188	0.84965	0.85161	0.99198
E_{21} (eV)	0.61785	0.77909	1.11620	1.12913	1.23030
E_{22} (eV)	0.66085	0.78201	1.11645	1.12918	1.23080

3.2. Impact of the Number of Coupled Quantum Dots on the Electronic and Optical Properties

Table 2 shows the ground (E_1) and first excited (E_2) electron energy levels for different quantum dot numbers calculated for fixed geometrical parameters $h = 1$ nm, $L_x = 2$ nm, $L_z = 8$ nm, and $L_c = 0.5$ nm. Increasing the number of coupled quantum dots leads to a splitting of the confined states and a gradual decrease of the lowest energy levels, indicating enhanced electronic delocalization due to inter-dot coupling [15].

Table 2. Ground (E_1) and first excited (E_2) electron energy levels for different quantum dot numbers.

Quantum Dot Number N	E_1 (eV)	E_2 (eV)
1	0.53497	0.73972
2	0.53201	0.73638
	0.54158	0.74954
3	0.52206	0.72906
	0.53263	0.73759
	0.53615	0.75518
4	0.51390	0.72038
	0.53094	0.73633
	0.53403	0.74151
	0.54746	0.75672

After determining the electron energy levels E and their corresponding envelope wavefunctions ψ , the nonlinear optical rectification (NOR) can be calculated as follows [4,29–31]:

$$\chi_0^{(2)} = \mu_{12}^2 \delta_{12} \frac{q^3 \sigma_v}{\varepsilon_0 \hbar} \frac{2\omega_{12}^2}{[(\omega_{12} - \omega)^2 + \Gamma_0^2][(\omega_{12} + \omega)^2 + \Gamma_0^2]} \quad (18)$$

where $\delta_{12} = |\langle \psi_2 | r | \psi_2 \rangle - \langle \psi_1 | r | \psi_1 \rangle|$, $\hbar\omega_{12} = E_2 - E_1$. Also, $\mu_{12} = |\langle \psi_1 | r | \psi_2 \rangle|$, ω is the incident radiation frequency, ε_0 is the vacuum permittivity, σ_v is the electron density in the system, and $\Gamma_0 = 1/\tau$ is the relaxation rate. In this work, the material parameters adopted in our theoretical calculations are as follows: $\sigma_v = 3 \times 10^{22} \text{ m}^{-3}$, $\Gamma_0 = 0.11 \text{ ps}$ [4,32].

The variation of the nonlinear optical rectification (NOR) coefficient as a function of photon energy $\hbar\omega$ for different numbers of coupled quantum dots N is shown in Figure 9. As the number of coupled quantum dots increases from $N = 1$ to $N = 4$, the amplitude of the NOR coefficient increases significantly. This enhancement can be attributed to stronger electronic coupling between neighboring quantum dots, which increases the overlap of the electronic wave functions and consequently enhances the dipole transition matrix element. In addition, a slight shift of the resonance position is observed as the number of coupled quantum dots increases. This shift results from the modification of the electronic energy levels induced by inter-dot coupling, which slightly changes the energy separation between the involved quantum states.

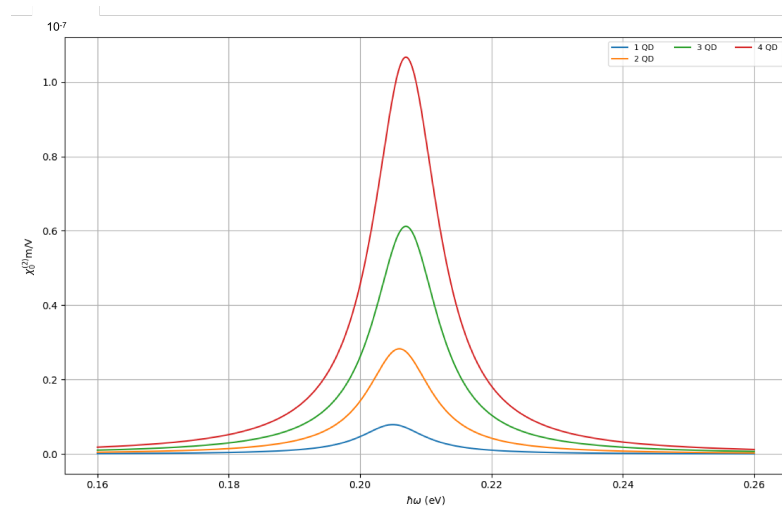


Figure 9. Nonlinear optical rectification versus photon energy for different numbers of coupled GaN/AlN quantum dots.

3.3. Machine Learning-Based Prediction of Electronic and Nonlinear Optical Properties

The numerical simulations presented in the previous sections provide an accurate description of the electronic structure and nonlinear optical rectification of coupled GaN/AlN quantum dots. However, extending these fully numerical calculations to larger numbers of coupled quantum dots requires a significant increase in computational time and memory, making systematic parametric studies impractical. To address this limitation, a machine learning (ML) approach is introduced as an efficient surrogate modeling strategy. The numerical results obtained for systems containing a small number of quantum dots are used as a high-fidelity training dataset, allowing the ML model to learn the underlying relationship between the quantum dot number and the resulting electronic and nonlinear optical properties. Once trained and validated, the ML model is then employed to predict the electronic structure and nonlinear optical rectification for larger quantum dot systems containing 4–10 coupled dots. This combined numerical–ML framework enables

fast and reliable extrapolation to larger systems while preserving the essential physical trends observed in the fully numerical calculations.

3.3.1. Selection of Machine Learning Models

To efficiently predict the electronic properties of larger quantum dot systems, a regression-based machine learning framework is adopted. The physical quantity of interest y , such as the electronic energy levels, is modeled as a function of the number of coupled quantum dots N . As a baseline approach, polynomial regression is employed to describe the nonlinear dependence of the predicted quantity on N [19,33,34],

$$y(N) = \sum_{k=0}^d a_k N^k, \quad (19)$$

where a_k are the regression coefficients and d denotes the polynomial degree. However, when the size of the training dataset is limited, polynomial regression models may suffer from overfitting, leading to unstable predictions and poor generalization capability [35,36]. To address this issue and improve the robustness of the model, regularized regression techniques are introduced. In Ridge regression [18,37,38], an L_2 regularization term is added to the loss function [39], defined as the sum of the squared regression coefficients ($\|a\|_2^2 = \sum_k a_k^2$). This penalty discourages excessively large coefficient values, thereby stabilizing the regression model and reducing the sensitivity to noise in the dataset. In contrast, the LASSO-LARS method incorporates an L_1 regularization term, defined as the sum of the absolute values of the coefficients ($\|a\|_1 = \sum_k |a_k|$) [38,40]. The L_1 penalty promotes sparsity in the solution by forcing some regression coefficients to become exactly zero, which effectively performs automatic feature selection and retains only the most relevant polynomial contributions. Elastic Net regression combines the advantages of both L_1 and L_2 regularization by simultaneously applying these penalties in a unified framework. This hybrid approach allows the model to benefit from both coefficient shrinkage and variable selection, which is particularly useful when the predictor variables are correlated or when the number of features is relatively large compared to the size of the dataset. The regression coefficients are obtained by minimizing the following cost function [40–42]:

$$\min_a \|y - Xa\|^2 + \alpha \left[(1 - \lambda) \|a\|_2^2 + \lambda \|a\|_1 \right],$$

where α controls the overall strength of the regularization and λ determines the relative contribution of the L_2 (Ridge) and L_1 (LASSO) penalties. When $\lambda = 0$, the formulation reduces to Ridge regression, while $\lambda = 1$ corresponds to LASSO regression. Intermediate values $0 < \lambda < 1$ define the Elastic Net model. These regularized regression techniques are particularly suitable for small datasets and allow reliable extrapolation of electronic and nonlinear optical properties to larger quantum dot systems containing several coupled dots.

3.3.2. Model Validation and Performance Metrics

To evaluate the predictive performance of the proposed models, four standard statistical metrics are employed: the Mean Absolute Error (MAE), Mean Squared Error (MSE), Root Mean Squared Error (RMSE), and the coefficient of determination (R^2). These metrics are computed on the test dataset to quantify the deviation between predicted and reference (physical) values [19,38,43,44].

The Mean Absolute Error (MAE) is defined as:

$$\text{MAE} = \frac{1}{N} \sum_{i=1}^N \left| y_{\text{th}}^{(i)} - y_{\text{pred}}^{(i)} \right| \quad (20)$$

The Mean Squared Error (MSE) is given by:

$$\text{MSE} = \frac{1}{N} \sum_{i=1}^N \left(y_{\text{th}}^{(i)} - y_{\text{pred}}^{(i)} \right)^2 \quad (21)$$

The Root Mean Squared Error (RMSE), which represents the standard deviation of the residuals, is expressed as:

$$\text{RMSE} = \sqrt{\frac{1}{N} \sum_{i=1}^N \left(y_{\text{th}}^{(i)} - y_{\text{pred}}^{(i)} \right)^2} \quad (22)$$

Finally, the coefficient of determination (R^2), which measures the proportion of variance explained by the model, is defined as:

$$R^2 = 1 - \frac{\sum_{i=1}^N \left(y_{\text{th}}^{(i)} - y_{\text{pred}}^{(i)} \right)^2}{\sum_{i=1}^N \left(y_{\text{th}}^{(i)} - \bar{y}_{\text{th}} \right)^2} \quad (23)$$

where $y_{\text{th}}^{(i)}$ and $y_{\text{pred}}^{(i)}$ denote the calculated and predicted values, respectively, and $\bar{y}_{\text{th}}$ represents the mean of the reference data.

3.4. Model Validation and Performance Analysis

Tables 3 and 4 present the validation results of the machine learning models for predicting the ground state (E_1) and the excited state (E_2) energies for $N = 4$.

Table 3. Validation results for E_1 ($N = 4$).

Model	MSE	RMSE	MAE	R^2
Polynomial	2.0×10^{-5}	4.49×10^{-3}	3.87×10^{-3}	0.858
Ridge	1.8×10^{-5}	4.23×10^{-3}	3.68×10^{-3}	0.874
LASSO_LARS	3.8×10^{-5}	6.15×10^{-3}	5.26×10^{-3}	0.734
ElasticNet	2.7×10^{-5}	5.18×10^{-3}	4.32×10^{-3}	0.811

Table 4. Validation results for E_2 ($N = 4$).

Model	MSE	RMSE	MAE	R^2
Polynomial	1.7×10^{-5}	4.08×10^{-3}	3.92×10^{-3}	0.901
Ridge	1.4×10^{-5}	3.71×10^{-3}	3.50×10^{-3}	0.918
LASSO_LARS	8.0×10^{-6}	2.90×10^{-3}	2.74×10^{-3}	0.950
ElasticNet	1.1×10^{-5}	3.24×10^{-3}	2.32×10^{-3}	0.938

For the ground state energy E_1 , Ridge regression achieves the best overall performance, with the highest coefficient of determination ($R^2 = 0.874$) and the lowest prediction errors among the tested models. This indicates that Ridge provides a good balance between bias and variance, ensuring stable and reliable predictions. In contrast, LASSO_LARS exhibits the lowest performance ($R^2 = 0.734$), suggesting that excessive sparsity may lead to underfitting. Polynomial regression shows competitive accuracy but remains less robust due to the absence of regularization.

For the excited state energy E_2 , the performance of all models improves significantly, with R^2 values exceeding 0.90. LASSO_LARS achieves the highest R^2 value (0.950), while Elastic Net provides the lowest Mean Absolute Error ($\text{MAE} = 2.32 \times 10^{-3}$) and a very high

R^2 (0.938), indicating excellent predictive accuracy. Ridge regression also maintains strong performance and stability.

Overall, the results demonstrate that regularized models outperform polynomial regression by improving generalization and reducing overfitting. The higher accuracy observed for E_2 compared to E_1 suggests that excited states exhibit smoother and more predictable trends, making them easier to learn by machine learning models.

These findings confirm that machine learning approaches, particularly Ridge and Elastic Net, are effective tools for accurately predicting electronic energy levels in coupled quantum dot systems.

3.5. Comparison Between Machine Learning Predictions and Physical Results

Figure 10 compares the energy levels predicted by different machine learning models with the physical results for $N = 4$.

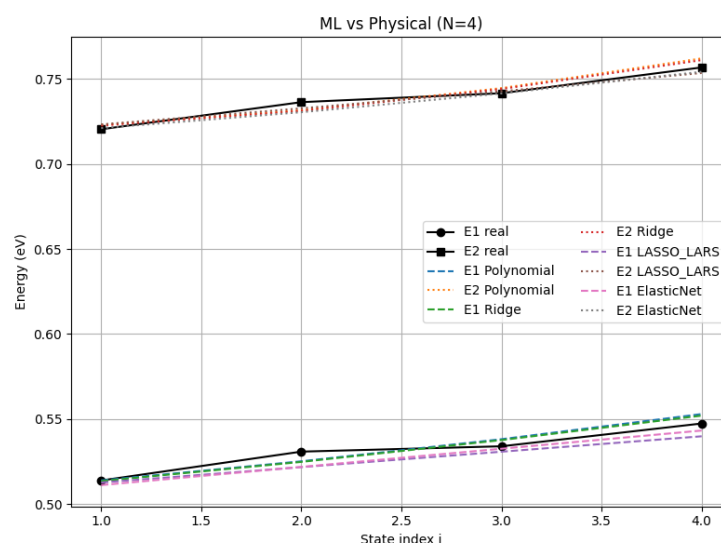


Figure 10. Comparison of machine learning predictions with physical results for $N = 4$.

All models correctly reproduce the monotonic increase of the energy levels with the state index i , indicating that the underlying physical behavior, related to miniband formation due to inter-dot coupling, is well captured.

For the ground state energy E_1 , Ridge regression shows the best agreement with the physical results, providing smooth and stable predictions across all states. Polynomial regression slightly overestimates the energies, while LASSO-LARS and Elastic Net tend to underestimate them.

For the excited state energy E_2 , all models achieve high accuracy with very small deviations. However, Ridge regression remains the most consistent, offering a smooth and physically coherent trend.

Overall, Ridge regression provides the best compromise between accuracy and stability, making it the most suitable model for reliable prediction and extrapolation.

Figure 11 presents the parity plot comparing the predicted energy values with the corresponding physical results for $N = 4$. The parity plot shows that all predictions lie close to the diagonal, confirming strong agreement with physical values. Ridge regression exhibits the most consistent alignment with minimal dispersion, while other models show slight deviations, particularly for E_1 .

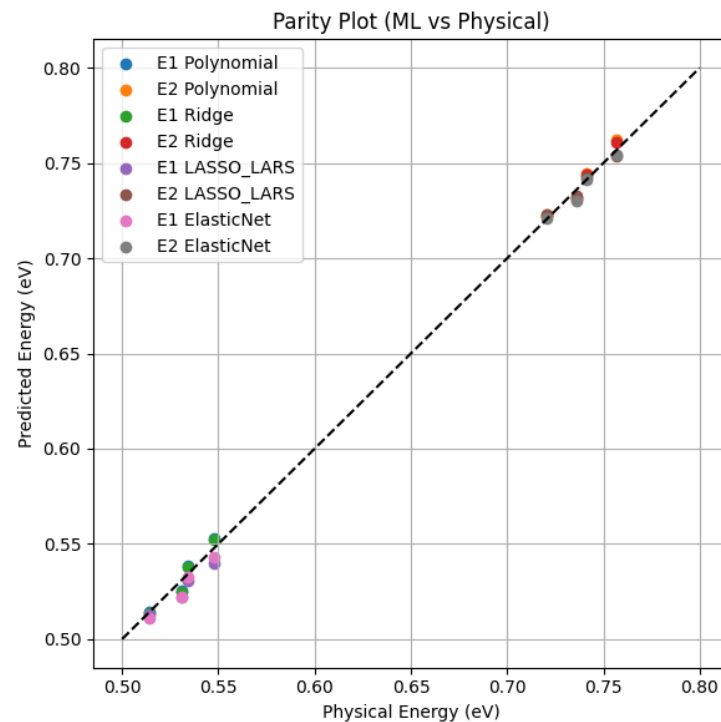


Figure 11. Parity plot showing strong agreement between predicted and physical energy values for $N = 4$.

The selection of $N = 1$ –4 quantum dots in the ML dataset was made to balance physical significance and computational expense. This range enables us to describe the transition from a single quantum dot to horizontally auto assembled quantum dot and to capture the main effects of lateral coupling on the electronic energy levels. Larger values of N would significantly increase the cost of the numerical simulations based on the combination of coordinate transformation and the finite difference method. Thus, $N = 1$ –4 offers an appropriate and manageable dataset for training the ML models, which were subsequently employed to predict larger arrays with $N = 5$ –10.

Ridge regression is selected for predicting larger systems ($N = 5$ –10) due to its stability and ability to preserve physical trends.

Figure 12 illustrates the energy spectra predicted by Ridge regression for larger systems ($N = 5$ –10) for both E_1 and E_2 . The results show a smooth and monotonic increase of the energy levels with the state index, confirming the preservation of the physical behavior. As N increases, the number of energy states becomes larger and more densely distributed, indicating miniband formation due to enhanced inter-dot coupling. The absence of oscillations highlights the stability and reliability of the Ridge model for extrapolation.

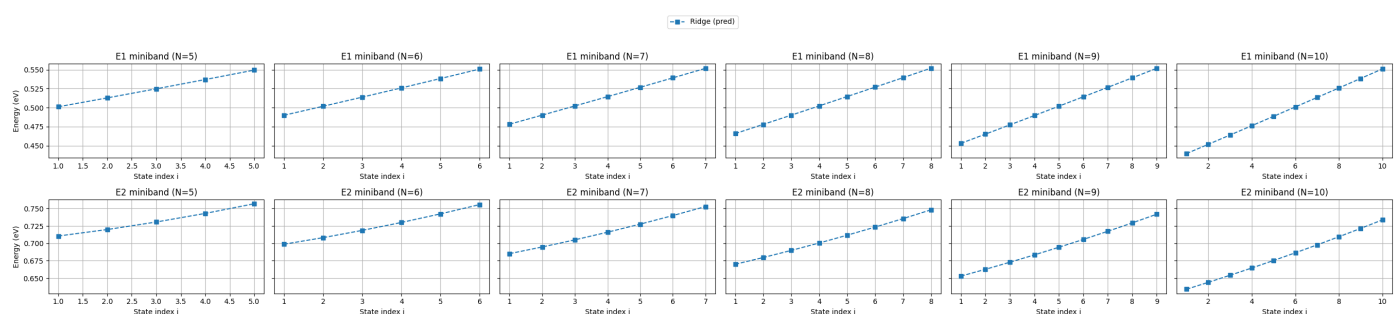


Figure 12. Ridge regression predictions of the miniband energy spectra E_1 and E_2 for coupled GaN/AlN quantum dots with $N = 5$ –10.

Figure 13 illustrates the evolution of the nonlinear optical rectification coefficient $\chi^{(2)}$ as a function of the photon energy $\hbar\omega$ for GaN/AlN quantum dots. The solid curves correspond to the physically calculated spectra for systems containing $N = 1-4$ quantum dots, while the dashed curves represent the spectra predicted by the Ridge regression-based machine learning model for larger arrays ($N = 5-10$).

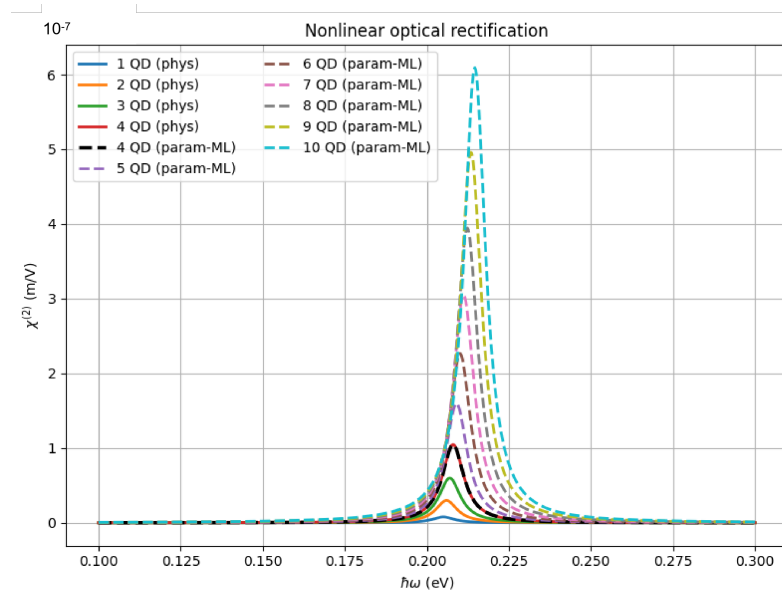


Figure 13. Nonlinear optical rectification (NOR) coefficient as a function of photon energy $\hbar\omega$ for different numbers of coupled quantum dots ($N = 1-10$).

As the number of coupled quantum dots increases, the amplitude of the nonlinear optical rectification coefficient increases significantly. In contrast, the magnitude of the rectification peak grows progressively with the number of coupled quantum dots, revealing the strengthening of the oscillator strength and the collective electronic interaction within the coupled quantum-dot structure. Overall, the excellent agreement between the physically calculated spectra and the machine-learning-based predictions demonstrates the capability of the proposed Ridge regression model to reliably describe the evolution of nonlinear optical rectification in larger quantum-dot assemblies.

The parity plot shown in Figure 14 compares the nonlinear optical rectification coefficients predicted by the machine learning model with the corresponding physically calculated values for $N = 1-4$ quantum dots. The data points are closely distributed along the diagonal line representing the ideal relation $y = x$, indicating an excellent agreement between the machine learning predictions and the physical calculations. This result demonstrates the high accuracy and reliability of the proposed Ridge regression model in reproducing the nonlinear optical rectification spectra. The near-perfect overlap confirms that the model successfully captures the underlying physical dependence of the rectification coefficient on the system parameters.

The permutation feature importance analysis highlights the relative contribution of the input variables to the machine learning model. As shown in Figure 15, the photon energy $\hbar\omega$ has the highest importance (0.130), indicating that the nonlinear optical rectification spectrum is mainly governed by the resonance condition between the photon energy and the electronic transitions. In contrast, the number of coupled quantum dots N exhibits a lower importance (0.092), suggesting that it primarily affects the amplitude of the nonlinear response rather than the spectral position of the resonance.

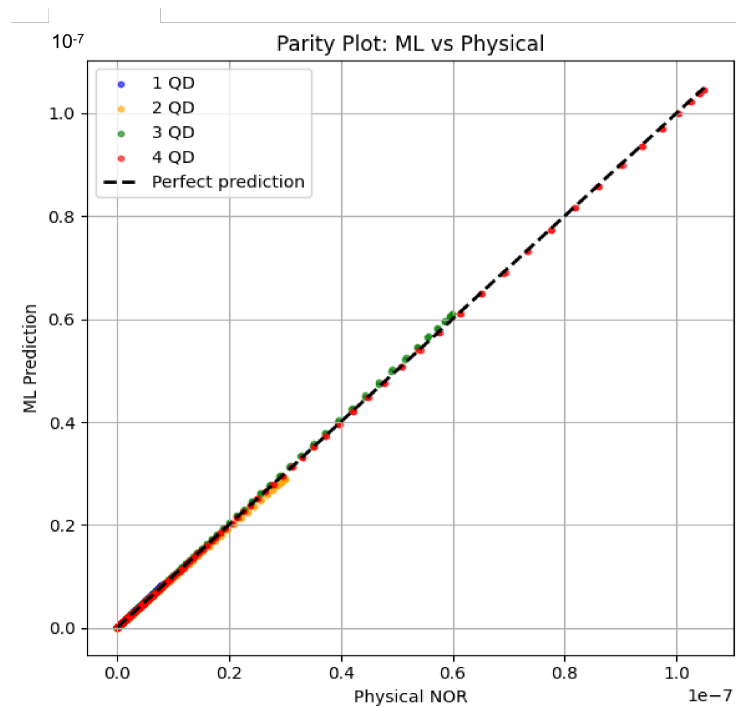


Figure 14. Parity plot comparing machine-learning predictions with physically calculated nonlinear optical rectification (NOR) values for 1–4 coupled quantum dots.

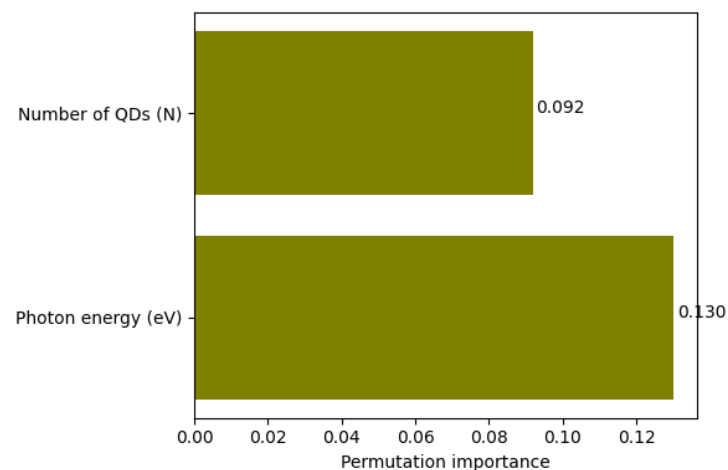


Figure 15. Permutation feature importance showing that the photon energy $\hbar\omega$ is the dominant parameter controlling the nonlinear optical rectification, while the number of quantum dots N mainly influences the amplitude of the response.

4. Conclusions

In this work, we investigated the electronic structure and nonlinear optical properties of self-assembled GaN/AlN quantum dots by integrating numerical modeling with machine learning (ML) techniques. The energy levels were initially computed using a finite difference method based on coordinate transformation, providing a rigorous physical dataset for coupled quantum dot systems.

To overcome the computational limitations associated with simulating large-scale arrays, several ML models were evaluated. Among these, Ridge regression demonstrated the superior compromise between predictive accuracy, statistical stability, and generalization capability. Consequently, it was selected as the reference model for extrapolating the electronic structure to extended quantum dot arrays.

The predicted energy spectra for larger systems ($N = 5\text{--}10$) exhibited smooth and monotonic behavior, consistent with miniband formation induced by inter-dot coupling. This alignment confirms that the ML model successfully preserves the essential physical features of the system, even when extrapolating beyond the training data range.

Furthermore, the nonlinear optical rectification (NOR) coefficient was analyzed as a function of photon energy. The results revealed a significant enhancement of the peak amplitude with an increasing number of quantum dots, while the resonance position remained nearly invariant. This behavior highlights the strengthening of collective electronic interactions and oscillator strength in larger systems.

Overall, the excellent agreement between physically computed results and machine learning predictions demonstrates the capability of the proposed framework to accurately and efficiently model complex nanostructures. This integration of ML with numerical methods provides a powerful tool for studying systems beyond the limits of conventional simulations. Future work may focus on extending this approach to include external effects, such as electric and magnetic fields, as well as exploring deep learning architectures for further enhanced predictive performance.

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