

Beyond DFT: Quantum Chaos and Neural Networks for 2D Material Device Design

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Beyond DFT: Quantum Chaos and Neural Networks for 2D Material Device Design

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Abstract

Accurate prediction of quantum stability in Selenium-doped MoS₂ field-effect transistors (FETs) remains challenging due to the computational cost of ab initio methods. Here, we combine quantum chaos theory with a multilayer perceptron (MLP) neural network to predict the Brody parameter (β) and current-voltage characteristics without relying on density functional theory. Our MLP model achieves $R^2 > 0.93$ on test data, accurately capturing the dependence of quantum chaos on bias voltage, impurity concentration, and lattice size. We demonstrate that quantum stability is tunable, not intrinsic, and uncover a universal scaling law where system size governs the transition from integrable to chaotic behavior. This framework bridges atomistic theory and device engineering, enabling rapid design of stable MoS₂-based electronic devices.

Keywords: *MoS₂ FET, Machine learning, Multilayer perceptron, Quantum chaos, Negative differential resistance*

1. Introduction

Field-effect transistors (FETs) underpin nearly every aspect of modern integrated circuitry—from logic gates and memory arrays to analog signal processors. Their function relies on precise modulation of channel conductivity through an applied electric field, enabling efficient signal amplification and switching. As a cornerstone of Moore’s Law, FETs continue to evolve with aggressive scaling, driving gains in speed, density, and energy efficiency [1].

In particular, 2D FETs stand out as promising candidates for emerging technologies such as neuromorphic computing and flexible electronics. The strong light–matter interactions exhibited by many two-dimensional materials make them ideal for phototransistors and optically responsive logic architectures [2]. Their intrinsic sensitivity also opens up nuanced investigations into phonon scattering mechanisms, impurity dynamics, and the thresholds of quantum chaos [3].

The theoretical analysis of two-dimensional (2D) materials, such as graphene-like materials [4] (hBN, BCN, Fluorographene, Graphene-Oxide), 2D chalcogenide [5] (*MoS₂*, *WSe₂*, *MoSe₂*, *WS₂*, SnSe), and 2D oxid (micas) [6], presents several significant hurdles. Foremost among these is the accurate modeling of inter-

layer interactions, the formation of Moiré patterns, and the impact of strain effects within heterostructures. Furthermore, capturing intricate quantum phenomena like excitonic effects, electron-phonon coupling, and various many-body interactions necessitates using advanced computational methods that go beyond the capabilities of standard density functional theory (DFT) [7, 8]. Finally, incorporating real-world complexities such as the presence of defects, edge states, and environmental influences is crucial, as these factors profoundly affect material behavior but are inherently challenging to simulate comprehensively.

Quantum chaos theory offers valuable insights into thermalization, charge transport, and optical behavior within complex, heterogeneous quantum systems. This is because it provides a robust framework for investigating nonlinear, non-equilibrium, and strongly interacting regimes—conditions that are fundamental to understanding transport and optical phenomena in diverse heterogeneous 2D and layered materials [9, 10]. Machine learning (ML) is revolutionizing the theoretical analysis of 2D materials like graphene [11, 12, 13, 14]. It can quickly predict properties such as band gaps, phonon spectra, and exciton binding energies, bypassing the high computational cost of traditional *ab initio* methods. ML also excels at identifying and classifying defects, stacking orders, and interfacial phenomena in complex heterostructures, tasks often beyond the scope of analytical models. Furthermore, deep learning enables the inverse design of materials. While machine learning encompasses algorithms that learn from data to make predictions or decisions, deep learning is a powerful subset of this field. It specifically leverages layer neural networks to model highly intricate patterns within data. Crucially, ML doesn't replace existing theoretical frameworks; instead, it enhances them by uncovering complex patterns, accelerating simulations, and guiding experimental design. However, two key challenges remain: data scarcity and limited interpretability. Integrating machine learning with quantum chaos theory offers a promising pathway to address both issues. The study of transport and optical phenomena in heterogeneous 2D and layered materials benefits from the complementary strengths of quantum chaos and machine learning. Quantum chaos furnishes a robust theoretical framework for investigating nonlinear, non-equilibrium, and strongly correlated dynamics. Concurrently, machine learning enables the efficient prediction of macroscopic properties, such as current stability, circumventing the prohibitive cost of *ab initio* methods.

This study investigates the performance and stability of MoS_2 FET by utilizing quantum chaos theory to generate a representative dataset for deep learning applications. The trained neural network's predictions are validated against existing experimental data to assess model reliability.

The paper is structured as follows: Section 2 presents the theoretical framework in detail; Section 3 discusses the results; and Section 4 concludes with a summary and supporting appendices.

2. Theoretical framework

The transistor structure centers around a MoS_2 lattice positioned between two leads, enabling charge exchange by functioning alternately as a donor and acceptor. In this study, we introduce a third gate conceptualized as a photon with an energy of 1.8 eV, directly interacting with the MoS_2 lattice [15]. The

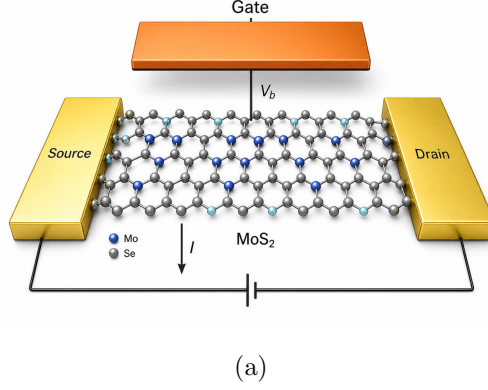


Figure 1: a) A MoS_2 -based FET features a MoS_2 channel between the Drain and Source, ideal for high-speed switching. The applied voltage (V_{ds}) drives drain current (I_{dr}), modulated by gate voltage via a SiO_2 insulating layer. Photon interaction with the MoS_2 lattice alters carrier density, enabling optical control of conductivity. This structure supports back-gated operation and integrates both electrical and photoresponsive behavior.

surrounding environment is modeled as a phonon bath, linearly coupled to the electron operator, thereby capturing dissipative effects inherent to transistor operation (Figure 1a). Different theoretical models were developed to study such heterostructures. To analyze electron transfer in the van der Waals heterostructure, we employ the tight-binding formalism under the nearest-neighbor approximation. The total Hamiltonian, expressed within the framework of second quantization, is given by:

$$H = H_{FET} + H_{Bath} + H_{Int} \quad (1)$$

where H_{FET} is derived by accounting for electron and phonon transport, along with their mutual interactions, as characterized by the following formalism:

$$H_{FET} = H_{MoS_2/Lead} + H_{Photon}$$

$$H_{MoS_2/Lead} = \sum_i \varepsilon c_i^\dagger c_i + \sum_{\langle i,j \rangle} (t_{ij} c_i^\dagger c_j + H.c.) + \omega a^\dagger a - \sum_{i,j=1}^N \gamma c_{ij}^\dagger c_{ij} (a^\dagger + a) \quad (2)$$

The tight-binding model employs a basis of Mo $4d$ ($d_{z^2}, d_{xy}, d_{x^2-y^2}, d_{xz}, d_{yz}$) and S $3p$ (p_x, p_y, p_z) orbitals. On-site energies ϵ_{Mo} and ϵ_S and nearest-neighbor hopping parameters t_{ij} are determined via the Slater-Koster formalism under D_{3h} symmetry. This captures the Mo-S hybridization governing the low-energy spectrum, accurately reproducing spin-orbit splitting and the direct band gap at K . The d -orbital basis is essential for modeling electron-phonon coupling and responses to electric fields and impurities. Where $c_i^\dagger$ and c_i create or destroy an excitation at the site, respectively. The operators $a^\dagger(a)$ and a represent phonon creation and annihilation, respectively. Given that the electron-phonon interaction coefficient γ is sensitive to factors such as the material system and environmental conditions, the applied voltage has been varied across the range of 0 to 2 volts to account for these dependencies. The application of a bias voltage V_b shifts

the on-site energies in the source and drain regions by $\pm eV_b/2$.

Electron-phonon interactions alter electron dynamics by effectively increasing the electron mass near the Fermi level. In this work, we account for the phonon-induced modifications by introducing a correction to the electron's hopping energy, as described below [16]:

$$\tilde{t}_{CC} = t_{CC} \times e^{\frac{-\gamma^2}{\omega^2}}$$

Furthermore, by accounting for three-phonon interactions, the frequency associated with anharmonic decay can be expressed as follows [17, 18]:

$$\omega = \omega_0 + \zeta \left(1 + \frac{2}{e^{\frac{\hbar\omega_0}{K_B T}} - 1} \right)$$

In this study, the phonon frequency is considered to be $w_{ph} = 46.2205 \text{ THz}$ [19]. The Boltzmann constant, denoted by K_B , and temperature T , play fundamental roles in phonon-related analyses. The accurate parameterization of the model is informed by a comprehensive review of existing experimental and theoretical literature, wherein phonon frequencies are commonly observed across a 0–100 THz range [20, 21]. Consistent with this body of work, the present study employs a phonon frequency of 46.2202 THz . Finally

$$\tilde{\tilde{t}}_{CC} = \tilde{t}_{CC} \times e^{-\eta(\frac{\Delta a}{a_0} - 1)}$$

Where $\Delta a = \alpha a_0 \Delta T$ [22, 23]. In this equation, α denotes the thermal expansion coefficient, and a_0 is the MoS_2 lattice constant.

When considering incident photon, its effect on the MoS_2 lattice can be attributed to the electric field component ($B = E/c$, where c is the velocity of light) [24]. This electric field is crucial for controlling MoS_2 's conductivity, effectively acting as a means to tune its electrical properties. The applied external electric field introduces a potential term, denoted as $H_{photon} = -eE \sum_{i=1}^N y_i c_i^\dagger c_i$. To incorporate the influence of incident photons on the system, the electric field effect was introduced into the Hamiltonian via a correction to the local electrical permittivity, following the approach in Ref. [25]. The modified permittivity is expressed as $\tilde{\epsilon}i = \epsilon i - eE y_i$ where E is the electric field amplitude and y_i denotes the position coordinate. Finally

$$H_{FET} = \sum_{i=1} \tilde{\epsilon}_i c_i^\dagger c_i - \sum_{\langle i,j \rangle} (\tilde{t}_{ij} c_i^\dagger c_j + H.c.) \quad (3)$$

The numerical values of hopping parameters are presented in Table 1. We analyze the effect of the impurity and external voltage in conductivity of MoS_2 lattice by obtaining the matrix form of the hamiltonian. The diagonal and non-diagonal elements of the matrix are determined using the Fock space (see Appendix A). One can obtain the set of eigenvalues and eigenvectors with a suitable numerical diagonalization procedure.

3. Method

3.1. Quantum chaos

Random Matrix Theory (RMT) is a fundamental tool for analyzing complex quantum systems. According to the Bohigas–Giannoni–Schmit conjecture, the statistical behavior of level spacings in quantum systems

Symbol	Parameter	Value	Unit
$\epsilon_{Mo}, \epsilon_S, \epsilon_{Au}$	On-site energy [26]	267.475, -5.629, 0.9004	(eV)
γ	Electron-phonon interaction coefficient [16]	1	
t_{MoS}, t_{AuAu}	Hopping [26]	0.015, -0.5155	(eV)
t_{AuMo}, t_{AuS}	Hopping [26]	$0.35 \times t_{AuAu}, 0.45 \times t_{AuAu}$	(eV)
α	Thermal expansion coefficient [27]	-6×10^{-6}	
ζ	Constant parameters [17]	-2.96	
η	Constant parameters [22]	3.37	

Table 1: Physical constant parameters for the MoS_2 FET.

can be described using RMT when the underlying classical dynamics are chaotic. Wigner’s surmise offers a practical approximation for the nearest-neighbor spacing (NNS) distribution in chaotic systems, enabling a clear distinction between chaotic and integrable regimes. Today, RMT serves as a key diagnostic for identifying the emergence of chaos in quantum spectra. The initial step in spectral analysis involves constructing and diagonalizing the system’s Hamiltonian matrix. A hallmark of quantum chaos is the repulsion between energy levels, typically captured by the NNS distribution. For localized states, the level spacing often follows a Brody distribution, reflecting intermediate statistics between Poisson (integrable) and Wigner-Dyson (chaotic) behavior [28, 29].

$$P_\beta(s) = As^\beta \exp(-\alpha s^{\beta+1}) \quad (4)$$

where

$$A = (1 + \beta)\alpha \quad \text{and} \quad \alpha = \left[\Gamma\left(\frac{\beta + 2}{\beta + 1}\right) \right]^{\beta+1} \quad (5)$$

with $\Gamma()$ the Gamma function. $\beta = 0$ corresponds to the Poisson statistics, whilst $\beta = 1$ to the Wigner surmise.

3.2. Machine Learning

Machine learning (ML) is significantly transforming materials science. Choosing the right ML model for research in areas like graphene or general material science depends on several key factors: the data’s nature, the problem’s complexity, the need for model interpretability, and computational limitations. For tasks such as predicting material properties or speeding up new material discovery, Multilayer Perceptrons (MLPs) are often a strong option [30]. MLPs are fundamental neural network architectures used in deep learning, excelling at classification, regression, and function approximation, especially with structured data. They consist of an input layer, one or more hidden layers, and an output layer, with each layer fully connected and employing nonlinear activation functions to identify complex data patterns. While versatile, MLPs can suffer from overfitting on small datasets, limited scalability for high-dimensional inputs, and interpretability challenges. To use MLPs effectively for analyzing material physical properties, input features should encode

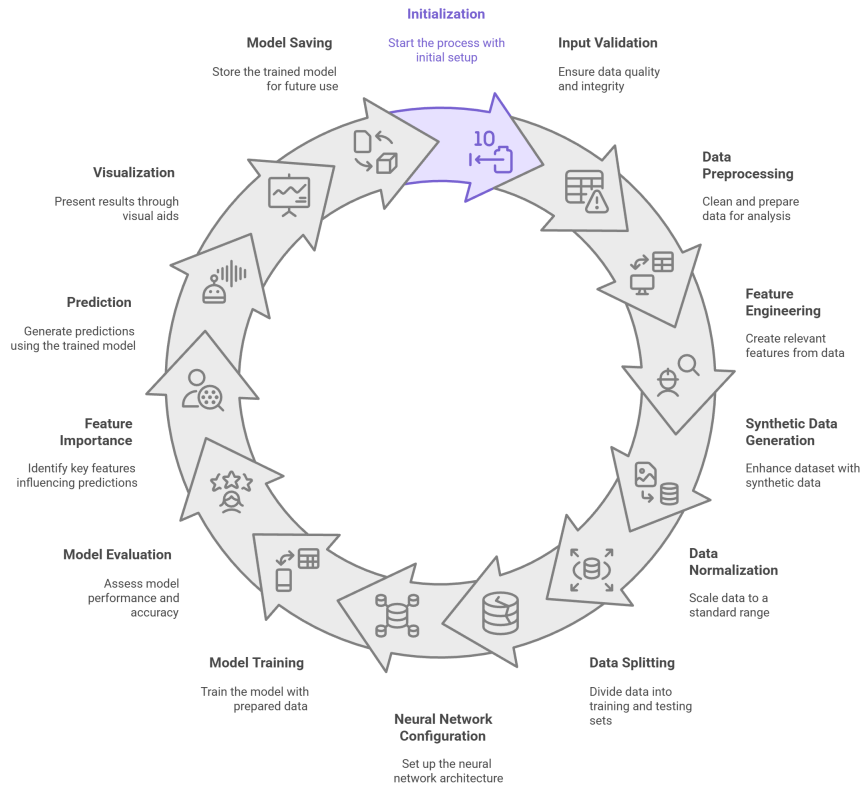


Figure 2: This flowchart presents a systematic machine learning pipeline aimed at predicting the properties of MoS_2 through an Artificial Neural Network, specifically a Multilayer Perceptron (MLP). The workflow is organized into three distinct phases: Data Preparation, Model Development and Training, and Evaluation and Deployment.

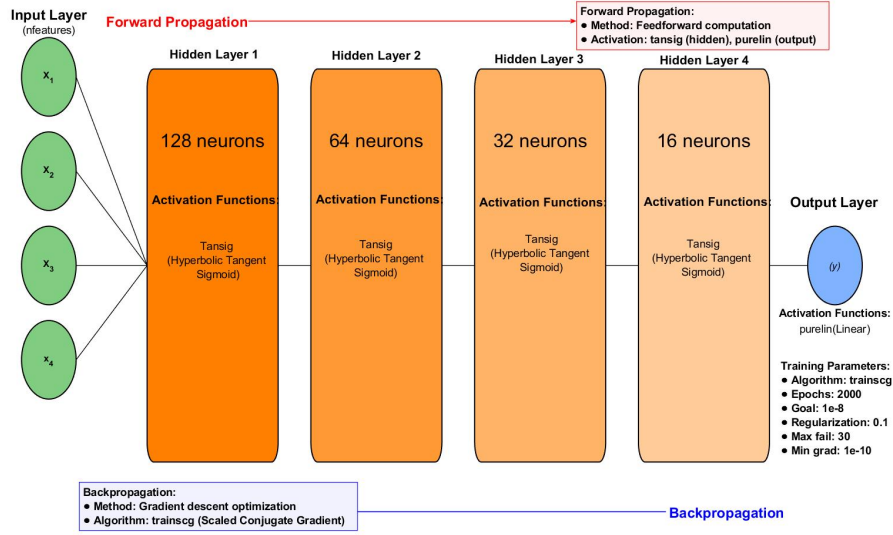


Figure 3: The architecture begins with four input neurons that capture key parameters: device dimensions, applied voltage, ambient temperature, and impurity concentration. These inputs propagate through a four-layered hidden structure comprising 32, 16, 8, and 4 neurons, respectively. The final output neuron synthesizes this information to predict the transistor’s operational behavior.

Hamiltonian matrix elements, lattice descriptors, on-site energies, hopping parameters, and environmental factors like temperature and external fields (Figure 2, and Figure 3).

MLP Architecture:

1. Input Layer (Lattice size, Bias voltage, Impurity percentage, and environment temperature)
2. Hidden Layer 1 ($32 \times$ input size, with ReLU or GELU activation function). Where the activation function defined as

$$ReLU(x) = \max(0, x)$$

$$GELU(x) = x\Phi(x)$$

where $\Phi(x)$ is the cumulative distribution function of the standard normal distribution.

3. Hidden Layer 2 ($16 \times$ input size)
4. Hidden Layer 3 ($8 \times$ input size)
5. Hidden Layer 4 ($4 \times$ input size, with ReLU or tanh)
6. Regularization with Batch Normalization or Dropout: Batch Normalization stabilizes training and speeds up convergence by normalizing layer inputs based on batch-wise statistics, while still allowing the network to learn by applying trainable scaling and shifting. Dropout, on the other hand, improves generalization by randomly turning off a portion of neurons during training, which forces the model to rely on diverse and redundant pathways rather than overfitting to specific patterns.

7. Output Layer (Brody paramter)

Training Configuration: The MLP is trained using supervised learning to minimize the prediction error. For our regression tasks—predicting the continuous Brody parameter β and electrical current—we employ the Mean Squared Error (MSE) as the loss function:

$$MSE = \frac{1}{N} \sum_{i=1}^N (y_i - \hat{y}_i)^2 \quad (6)$$

where y_i is the true target value (either β or current intensity) and $\hat{y}_i$ is the model's predicted value. MSE is chosen because it penalizes larger errors more severely and provides a smooth gradient for optimization [30].

3.3. *I-V Characteristic*

As the principal diagnostic method for FETs, current-voltage (I-V) analysis is indispensable. Its critical importance stems from its role in performance characterization, operating region identification, and the detection of defects and variability. This analysis supplies the foundational parameters required to evaluate device performance, reliability, and fitness for diverse applications, from ultra-low-power electronics to high-speed communication systems. Electrical conductivity in the MoS_2 lattice can be analyzed by examining local current dynamics. To this end, we employ the density operator defined as $n_i = c_i^\dagger c_i$. Within the Heisenberg picture, the time-dependent density operator is expressed as $(n_i(t) = e^{iHt} n_i e^{-iHt})$. Variations in the density operator over time reflect changes in the local current at each site. Consequently, the current operator is given by [31]:

$$I = \frac{d(en_i(t))}{dt} = \frac{-ie}{\hbar} [c_i^\dagger c_i, H]$$

The corresponding expression for the steady-state total electrical current operator is obtained as follows:

$$I(t) = \sum_i I_i(t) \quad (6)$$

The switching performance of MoS_2 FET is governed by the flow of electrical current, a complex process influenced by temperature, external voltage, and scattering from impurities.

4. Results

Theoretical control over the quality of a MoS_2 -based transistor relies on precisely tuning the intrinsic properties of MoS_2 and its respective surroundings to enhance electrical performance (Figure 1a). This process is grounded in a deep understanding of how these factors influence charge carrier transport and overall device behavior.

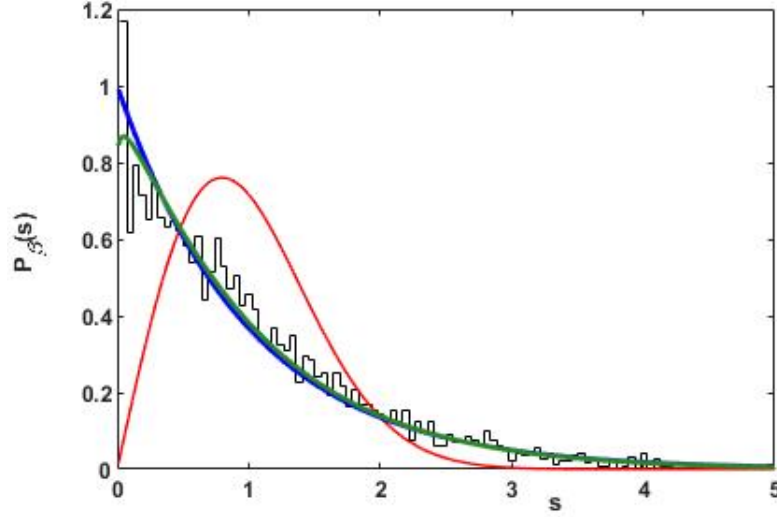


Figure 4: Nearest-neighbor energy spacing (NNS) distribution for the MoS_2 heterostructure obtained from random matrix theory (RMT) analysis. The lattice size is 120×100 , $V_b = 0.5$ V, and $T = 300$ K. The fitted Brody distribution (green line) yields a level repulsion parameter $\beta = 0.07$, indicating near-Poissonian (integrable) behavior. The red and blue lines represent the Wigner (chaotic) and Poisson (integrable) limiting distributions, respectively, while the black line shows the numerical simulation data.

4.1. Quantum stability

MoS_2 is a two-dimensional semiconductor with distinct electrical characteristics that respond to changes in environmental conditions (Figure 1b). It typically exhibits n-type behavior due to sulfur vacancies and possesses a bandgap of approximately 1.2 eV [32]. Its conductivity increases with temperature and can be further modulated through doping, mechanical strain, or engineering of the underlying substrate. With moderate charge carrier mobility, MoS_2 remains a highly tunable material suitable for diverse electronic applications. Figure 4 represents the Brody distribution by considering the lattice size as 120×100 , with an applied voltage is $V_b = 0.5$ V, at room temperature $T = 300$ K. In this figure, the dashed black line and green line represent Wigner and Poisson distributions, respectively. The red line is the numerical simulation. The quantum system remains largely ordered throughout the depicted range, but it undergoes a smooth transition toward more chaotic behavior as the control parameter increases. The very low final value of $\beta = 0.07$ confirms the system is still far from a fully chaotic state.

Voltage-Induced Effects: The applied bias voltage plays a pivotal role in tuning the electronic behavior of a MoS_2 FET. Within a specific range of V_b , the Fermi level resides inside the band gap, resulting in a depletion of free carriers and minimal current flow—this defines the transistor’s “off” state. As V_b surpasses the threshold voltage, it induces band bending that shifts the Fermi level toward the conduction band. This electrostatic effect accumulates electrons in the channel, forming a conductive path. Consequently, the

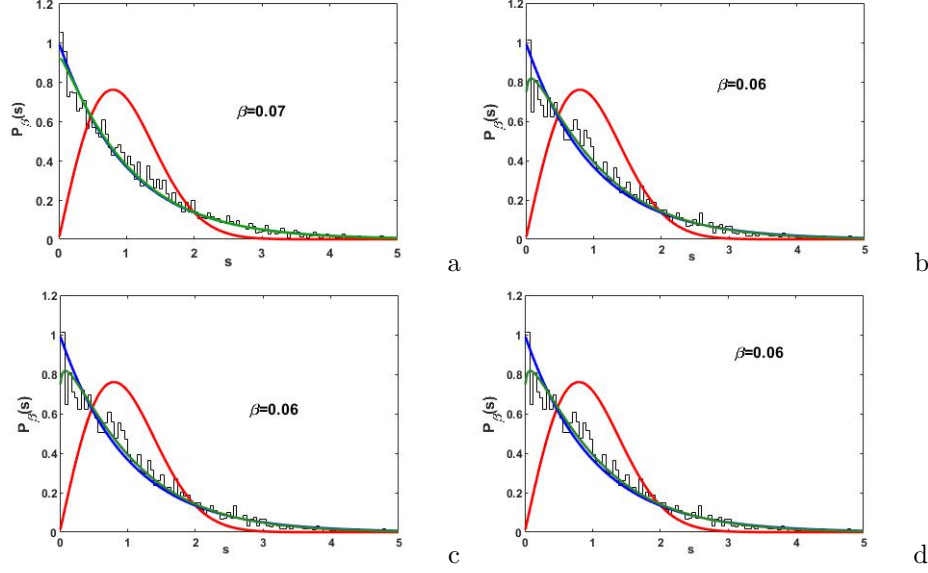


Figure 5: The electronic dispersion and density of states for a MoS_2 FET with lattice dimensions 120×100 are analyzed at room temperature. Gate voltages V_b of 0.2, 0.4, 1.4, and 2 V yield distinct repulsion parameters β of 0.07, 0.06, 0.06, and 0.06, respectively. In the visualization, red and blue lines correspond to Wigner and Poisson distributions; the black line shows numerical data, and the green line indicates a fitted Brody distribution. These results highlight voltage-dependent spectral statistics, revealing transitions in level repulsion behavior under varying electrostatic conditions.

current rises sharply—initially exponentially, then transitioning to a linear increase. The applied voltage critically influences the quantum stability, charge transport, and defect dynamics of a Se-doped MoS_2 FET [33, 34].

1. Low Voltage Regime (< 0.3 V): While gate voltage regulates channel conductivity, selenium (Se) defects act as carrier traps, leading to degradation in subthreshold swing. The introduction of Se induces a shift in the Fermi level toward the conduction band, characteristic of n-type doping. Notably, Se impurities remain structurally stable, exerting minimal impact on lattice integrity. However, the stochastic nature of Se distribution contributes to increased variability in the threshold voltage V_T .
2. Moderate Voltage Regime (0.3–1 V): In this region, the phonon scattering dominates, reducing mobility, and High-energy electrons interact with Se defects.
3. High Voltage Regime ($V > 1$ V): A strong vertical electric field can disrupt the MoS_2/SiO_2 interface, leading to lattice instability and ultimately causing irreversible degradation of the transistor.

In the configuration of $N = 120 \times 100$ atoms at $T = 300$ K, the device behaves like a quantum dot with predominantly localized electronic states. These states are spatially confined and weakly interacting, leading to near-Poissonian level spacing statistics. While gate voltage shifts the Fermi level and populates these states with additional carriers, it does not significantly alter their localized nature. As a result, charge transport proceeds via inefficient hopping mechanisms, yielding low mobility and limited performance. The

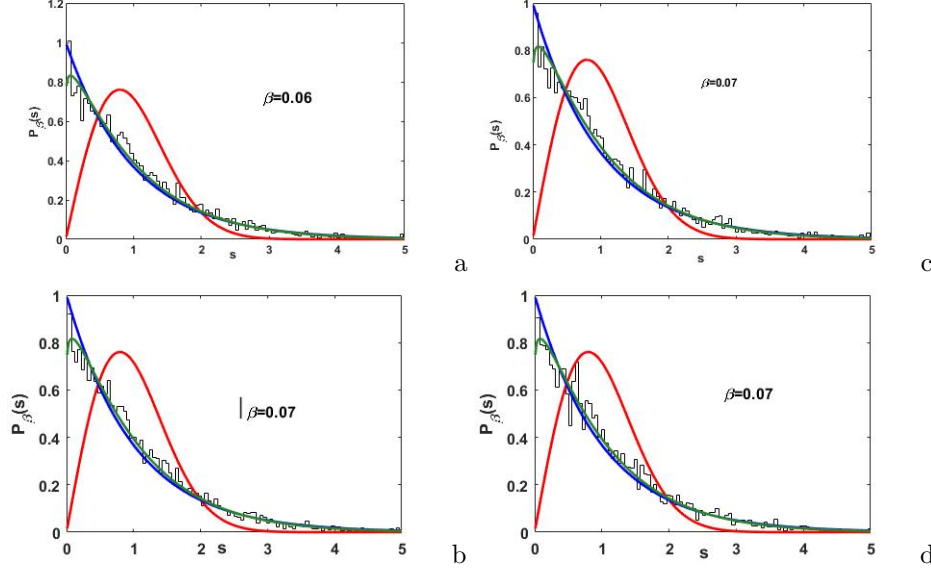


Figure 6: At room temperature, the nearest-neighbor energy spacing (NNS) distributions in a MoS_2 FET are examined using selenium (Se) atom impurities as the tunable parameter. Simulations are conducted for a 120×100 lattice under the gate bias $V_b = 0.5$ V. Impurity concentrations of 0.05%, 0.5%, 1%, and 2% yield corresponding level repulsion parameters β of 0.06, 0.07, 0.7, and 0.7..

consistently low Brody parameter values ($\beta \approx 0.06 - 0.07$) indicate that bias voltage alone does not induce strong quantum chaos, but rather tunes the system within a narrow integrable regime. This supports the notion that quantum stability in MoS_2 FETs remains robust under room-temperature conditions, especially in moderately sized lattices. The minimal variation in β across gate voltages from 0.2 V to 2.0 V confirms that electrostatic gating in this range is insufficient to trigger significant delocalization of electronic states (Figure 5). These findings demonstrate the utility of random matrix theory (RMT) as a diagnostic tool for probing the quantum nature of nanoscale devices, offering insight into the interplay between geometry, electrostatics, and spectral behavior.

At moderate bias levels (~ 0.5 V), Se-induced trap states may localize carriers and reduce mobility, yet overall lattice integrity is preserved. However, exceeding optimal voltage thresholds increases the risk of instability, especially given the complexity introduced by Se doping. Accurate prediction of these transitional regimes requires that the MLP network be sensitively trained with respect to voltage resolution and impurity configuration.

Impurity engineering: Doping is a versatile approach for optimizing MoS_2 FET performance by regulating carrier concentration, threshold voltage, and mobility. Substitutional dopants such as Nb and P induce p -type behavior, while Re and Cl promote n -type conduction [35, 36, 37]. Threshold voltage (V_{th}) shifts negatively with n -type and positively with p -type dopants. [38] Low dopant concentrations ($\sim 0.1\%$ – 2%) enable fine band alignment with minimal mobility impact, while higher levels ($> 4\%$) introduce defect-driven scattering. At low impurity concentrations (0.05%–0.5%), β remains low (~ 0.06 – 0.07), resembling pristine

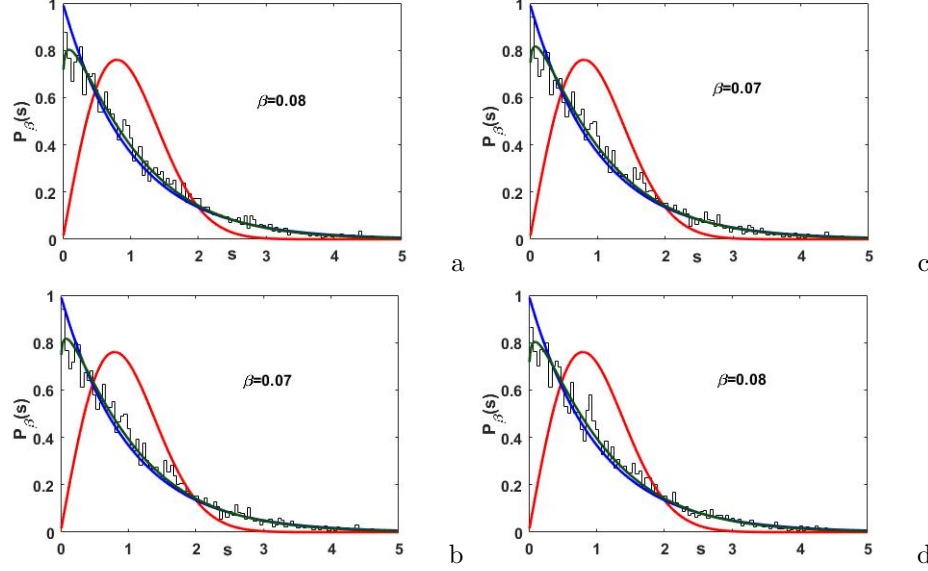


Figure 7: The Nearest-neighbor energy spacing (NNS) distributions of states of the MoS_2 FET are analyzed for a 120×100 lattice under a bias voltage of $V_b = 0.5$ V. Temperature variations yield distinct level repulsion parameters: $\beta = 0.08$ at $T = 320$ K, $\beta = 0.07$ at $T = 340$ K, $\beta = 0.07$ at $T = 360$ K, and $\beta = 0.08$ at $T = 380$ K. In the plot, red and blue lines represent Wigner and Poisson distributions, respectively; the black curve denotes numerical results, while the green line indicates a fitted Brody distribution. These outcomes reflect temperature-dependent spectral transitions, offering insight into thermal effects on electronic structure.

MoS_2 . At 1%–2%, β sharply increases to 0.7, signaling a percolation threshold where Se impurities form interconnected paths, enhancing level repulsion and promoting metallic conduction. Selenium atoms are relatively inert at low concentrations, preserving localization. Beyond a critical density, they enable carrier hopping, resulting in extended states and chaotic spectral statistics. The rise in β correlates with improved conductivity, marking a transition from insulating to metallic-like behavior. Pristine MoS_2 maintains localized states and low conductivity (Figure ??). In contrast, Se doping introduces disorder and additional states that form conductive networks (Figure 6), enhancing electron transport. Thus, impurity doping proves more effective than gate modulation alone in boosting conductivity. At very low impurity concentrations (0.05% – 0.5%), the Brody parameter β remains low (~ 0.06 – 0.07), closely resembling the behavior of pure MoS_2 . However, at 1% and 2% concentrations, β sharply increases to 0.7, signaling a pronounced transition toward chaotic spectral behavior and delocalized electronic states. This shift suggests a percolation threshold between 0.5% and 1%, where impurities begin forming interconnected paths or induce sufficient disorder to disrupt localization, enhancing level repulsion and promoting metallic conduction.

Silicon atoms, acting as dopants or scattering centers, are relatively inert at low concentrations, preserving the localized nature of the electronic states. Beyond a critical density, they enable carrier hopping or band formation, resulting in extended states and more chaotic spectral statistics. The rise in β correlates with improved conductivity, marking a transition from insulating (localized, low β) to metallic-like behavior (de-

localized, high β).

Pure MoS_2 , even under varying gate voltages, maintains highly localized states and low conductivity due to its intrinsic semiconducting nature and limited carrier density (Figure 5). In contrast, doping with impurities such as Si introduces disorder and additional states that, at sufficient concentration, form conductive networks (Figure 6). This leads to enhanced electron transport and a shift toward metallic conduction. Thus, impurity doping proves more effective than gate modulation alone in boosting conductivity in MoS_2 FETs.

Impact of temperature: Elevated temperatures enhance phonon scattering, leading to reduced carrier mobility, diminished current drive, and slower switching response. Thermal fluctuations also shift the threshold voltage, influencing the formation of conductive channels under applied bias. As temperature increases, stronger electron-phonon coupling and lattice expansion narrow the bandgap and alter the Fermi level, thereby modifying band alignment and affecting carrier injection, contingent on the contact material and doping configuration [39, 40]. Temperature further impacts the Schottky barrier height at metal- MoS_2 interfaces. At the same time, moderate heating may lower the barrier through thermionic emission and improve contact quality; excessive heat can induce degradation via oxidation or defect formation [41]. Additionally, elevated temperatures promote the mobility of sulfur vacancies and other defects, which can destabilize conductivity. Beyond certain thresholds, rapid diffusion of these defects may hinder their detectability and impair device reliability [42, 43]. Temperature significantly influences MoS_2 's response to applied voltage (≤ 2 V), modulating phase transitions, doping efficiency, oxidation rates, and defect dynamics.

The outcomes of the stability analysis of the MoS_2 lattice—considering variations in structural parameters such as network dimensions, impurity concentration and type, as well as environmental conditions like applied voltage and temperature are incorporated into the training dataset for the Multilayer Perceptron (MLP) learning process.

4.2. Learning Quantum Stability

The gap between theoretical predictions and experimental results for MoS_2 exists because models are too simple. They often ignore real-world complexities and environmental factors. Models like Density Functional Theory (DFT) are powerful but assume perfect crystal structures and struggle to simulate device-scale systems [44, 45, 46]. This “scale mismatch” means small simulations can’t capture crucial effects, such as dielectric screening from a substrate, leading to inaccurate predictions. To overcome these limitations, we are utilizing machine learning to develop models that more accurately reflect the complex behavior of real-world MoS_2 devices.

Drawing on insights from quantum chaos theory, we examined how MoS_2 lattice dimensions, impurity percentages used to modulate the energy gap, and environmental temperature variations influencing output current stability affect device performance. These parameters were incorporated as feature vectors in the input layer of a multilayer perceptron (MLP) network. The network architecture consists of four hidden layers with 128, 64, 32, and 16 neurons, respectively (Figure 2, and 3).

Utilizing the proposed MLP architecture, we investigated the quantum stability of a MoS_2 lattice measuring

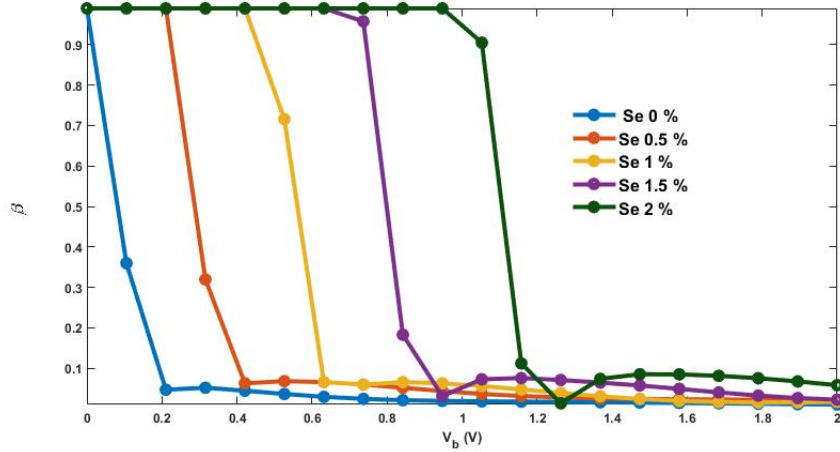


Figure 8: The electronic dispersion (β) of the MoS_2 FET are analyzed for a $N_x \times N_y = 9000 \times 7665 (\approx 4.73 \mu m^2)$ lattice at the environment temperature $T = 300 K$ concerning the variation of bias voltage V_b . The influence of impurity concentration is characterized by distinct level repulsion parameters, corresponding to different doping scenarios: pristine (no impurities, blue line), 0.5 % (brown line), 1 % (mustard line), 1.5 % (purple line), and 2 % (green line). These results reveal impurity-driven spectral transitions, providing valuable insight into how bias voltage and dopant concentration modulate the electronic structure of the device.

$1.88 \times 2.21 \mu m^2$ to design a transistor operating at room temperature ($T=300 K$). Selenium atoms were substituted at a concentration of 0.4% to adjust the Fermi level, and the lattice was exposed to an external bias voltage of ($V_b = 0.5 V$).

The dataset from the MoS_2 FET stability analysis was partitioned into training (60%), validation (20%), and test (20%) sets. The training set was used to optimize the model's weights via backpropagation and gradient descent. The validation set guided hyperparameter tuning and monitored for overfitting during training. Finally, the held-out test set provided an unbiased final assessment of the model's generalization performance after all development was complete.

Figure 8 clearly demonstrates that the repulsion parameter (β) is dependent on both the percentage of Selenium (Se) impurities and the applied voltage. The curves corresponding to higher Se concentrations are consistently positioned above those with lower concentrations, indicating that the introduction of structural disorder through Se substitution drives the system's electronic energy levels toward a more chaotic state characterized by stronger level repulsion.

For every concentration of Se, the repulsion parameter decreases with the applied voltage. This indicates that the applied electric field serves as a powerful external tuning mechanism, modulating the electronic environment and driving the system from a more chaotic one (higher β) to a more ordered state (low β). This ability to tune the system from integrable to chaotic behavior using the gate voltage is highly significant for controlling quantum transport properties [47].

The sensitivity of β to voltage changes with the doping level. At low doping (0% Se), voltage has a strong

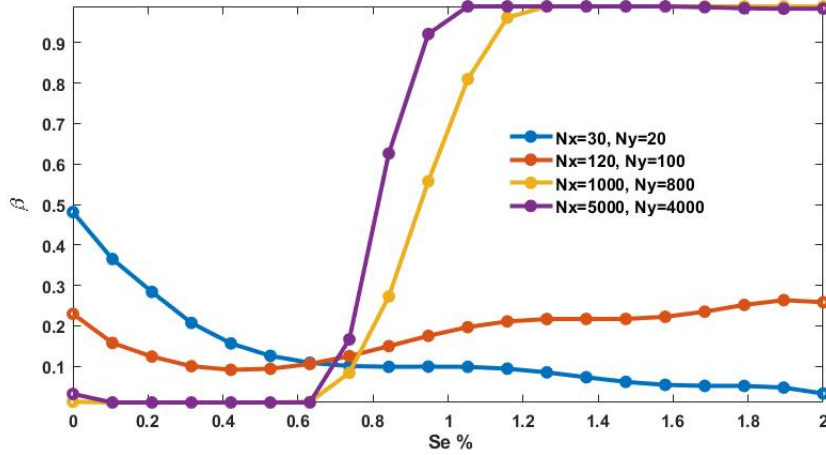


Figure 9: The electronic dispersion (β) of the MoS_2 FET is analyzed under a bias voltage of $V_b = 0.5$ V at the environment temperature $T = 300$ K with respect to the variation of Selenium (Se) atoms introduced as impurities. The impact of lattice size on the electronic structure is captured through distinct level repulsion parameters, corresponding to different configurations: blue line ($N_x \times N_y = 30 \times 20 \cong 3.5 \times 10^{-4} \mu m^2$), brown line ($N_x \times N_y = 120 \times 100 \cong 6 \times 10^{-4} \mu m^2$), mustard line ($N_x \times N_y = 1000 \times 800 \cong 0.047 \mu m^2$), and purple line ($N_x \times N_y = 5000 \times 4000 \cong 1.19 \mu m^2$). These findings highlight impurity-induced spectral transitions and underscore the role of both lattice dimensionality and dopant concentration in shaping the electronic properties of the device.

effect on β , while at high doping (2% Se), the curve flattens, indicating that disorder dominates and diminishes the efficacy of voltage control. This suggests that an optimal doping level may exist for maximizing voltage tunability [48].

Finally, the figure reveals a synergistic relationship between internal disorder (doping) and external control (voltage). The impurity concentration sets a baseline level of chaos, and the applied voltage then allows for its dynamic modulation. This dual-tuning capability provides a valuable method for manipulating the device's quantum properties, indicating that MoS_2 FETs can be engineered for specific applications—such as quantum dots or chaotic sensors—by controlling both impurity concentrations and gate voltages [49].

The most significant finding is that the Brody parameter is not an intrinsic material property but is heavily dependent on the system's size. For all impurity levels, β dramatically increases with larger lattice dimensions. This suggests that quantum confinement in smaller devices can suppress chaotic behavior, pushing the system toward a more ordered or "integrable" state. Increasing the Selenium (Se) impurity concentration has a nuanced effect. For a fixed, smaller lattice, even a minor amount of disorder seems to be enough to maintain a low β value. However, for a larger system, increasing the disorder (up to 2% Se) still increases the Brody parameter. This implies that beyond a certain point ($\sim 1\%$ Se), the extensive system size mitigates the impact of additional disorder, and the system retains its highly chaotic nature. The graph serves as a critical warning about finite-size effects. The quantum transport properties of a nanoscale transistor (small size) will be entirely different from those of a larger, more bulk-like sample. Consequently, any conclusions

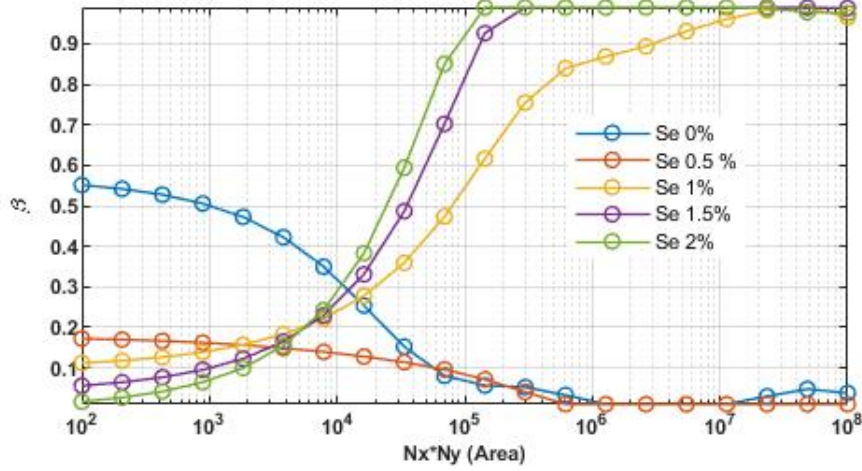


Figure 10: The electronic dispersion (β) of the MoS_2 FET is analyzed at the environment temperature $T = 300\text{ K}$ concerning the variation of dimensions of the MoS_2 lattice size. The impact of lattice size on the electronic structure is captured through distinct level repulsion parameters, corresponding to different configurations: blue line (0% Se), brown line (0.5% Se), mustard line (1% Se), and green line (2% Se). These findings highlight impurity-induced spectral transitions and underscore the role of both lattice dimensionality and dopant concentration in shaping the electronic properties of the device.

about the intrinsic chaotic nature of the MoS_2 material must account for the device's dimensions [50]. The instability in the MoS_2 FET is a result of a complex interplay between impurity-induced disorder and the physical size of the system. Larger devices exhibit stronger signatures of quantum chaos and are more resilient to the localizing effects of impurities (Figure 9).

Figure 10 illustrates the Brody parameter (β) as a function of MoS_2 lattice area on a logarithmic scale, revealing a key insight: all data points, across varying selenium (Se) concentrations from 0% to 2%, collapse onto a single universal sigmoidal curve. This indicates that the transition from integrable (low β , localized states) to chaotic (high β , extended states) behavior depends primarily on system size, with disorder (Se%) merely shifting the curve rightward—requiring larger areas to reach the same β as impurity levels increase, effectively mapping the mobility edge in a disorder-driven quantum phase transition. In contrast to Figures 8 and 9, which provide fixed-size slices showing β dependence on voltage and doping, Figure 10 uncovers a fundamental scaling law where size and disorder interplay to govern the device's quantum phase (localized vs. delocalized, integrable vs. chaotic), offering a more comprehensive view not apparent in linear-scale plots.

The collective data from Figures 9, 10, and 11 highlight that quantum chaos in MoS_2 FETs is governed by three interdependent factors: the applied electric field (voltage), internal disorder (Selenium doping), and lattice area (system size). Their intricate interaction drives the shift from integrable to chaotic quantum states. The Brody parameter (β) decreases with increasing gate voltage (V_b) across fixed Se concentrations, establishing voltage as a key tuning parameter. At 0% Se, β decreases sharply from chaotic (high β) to ordered (low β) states with voltage, but the effect saturates at 2% Se, indicating an optimal doping range

where voltage control is most effective. Higher Se levels elevate the baseline β at zero voltage, reflecting disorder-induced symmetry breaking and level repulsion. The critical role of system size, with β increasing markedly with lattice dimensions is appears. Small lattices remain near-integrable ($\beta \approx 0.1 - 0.3$) despite disorder, due to quantum confinement, while large lattices exhibit strong chaos ($\beta > 0.8$) even without impurities. In larger systems, disorder initially localizes states (lowering β) but eventually saturates, sustaining chaos at high Se%. Plotting β against lattice area on a log scale reveals a universal sigmoidal curve where all data collapse, confirming that the transition to chaos depends fundamentally on size. Disorder (Se%) shifts this curve rightward, requiring larger areas to achieve the same β in more disordered systems, thus mapping the mobility edge of a disorder-driven quantum phase transition. It synthesizes Voltage slices (Figure 8) and size slices (Figure 9) into a comprehensive scaling law. In essence, these results demonstrate that size and disorder are interconnected drivers of quantum phase behavior, with voltage acting as a tunable control, offering a unified framework for understanding and optimizing MoS_2 FET performance.

FIG. 11 validates the MLP’s ability to model Se-doped MoS_2 under bias, critical for designing stable FETs. Our study established actual values for the electronic dispersion and density of states in the MoS_2 lattice (Figures 5-7). These values were derived from investigating how external voltage (V_b), impurity types and concentrations, environmental temperature, and lattice size influence these properties. Predicted values were then generated using an MLP model, which was trained on comprehensive quantum stability data. When comparing predicted to true values, clustering along the diagonal indicates high model accuracy, whereas deviations highlight potential errors, particularly in regions with Se defects or at lattice edges. Model performance was quantified using Mean Squared Error (MSE) and the R^2 score.

The scatter plots in Figure 12 (top row) visually compare the actual (true) target values against the model’s predicted outputs across various datasets: Training, Validation, Test, and an aggregation of all data. The R^2 values confirm the model’s strong performance:

- Training: $R^2 = 0.9989$, indicating an excellent fit where the model explains 99.89% of the variance.
- Validation: $R^2 = 0.94037$, showing a very good fit, explaining 94.037% of the variance.
- Test: $R^2 = 0.9322$, representing a good fit with 93.22% of the variance explained.
- All: $R^2 = 0.97516$, demonstrating a strong overall fit by explaining 97.516% of the variance.

The points’ close alignment to the $y=x$ line (representing perfect prediction) across these plots suggests the model generalizes effectively. Minor deviations indicate robust performance under the specified conditions (300 K, 0.4% Se impurity, 0.5 V_b). The true vs. predicted plots (bottom row) illustrate the actual (blue dots) and predicted (red dashed line) current stability over samples for the Training and Test datasets. The Training plot (90 samples) shows the model closely tracks the true values, capturing the underlying quantum effects despite some fluctuations. Similarly, the Test plot (20 samples) reveals the model effectively captures the general pattern, though minor deviations suggest limitations when predicting rapid changes or

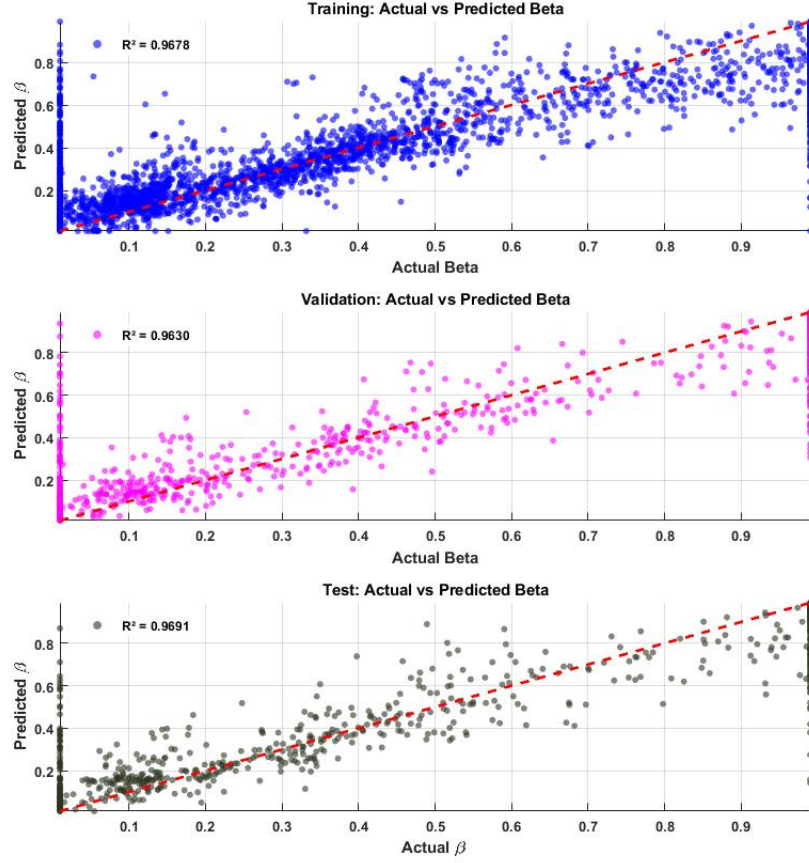


Figure 11: The electronic dispersion and density of states in the MoS_2 FET are analyzed for a lattice size of $9000 \times 7665 \approx 4.73 \mu m^2$. Selenium atoms are introduced as impurities at a concentration of 0.5 %, and the bias voltage is maintained at $V_b = 0.5 V$. At room temperature ($T = 300 K$), the blue line represents the actual value of the repulsion parameter, while the red dashed line indicates its predicted counterpart.

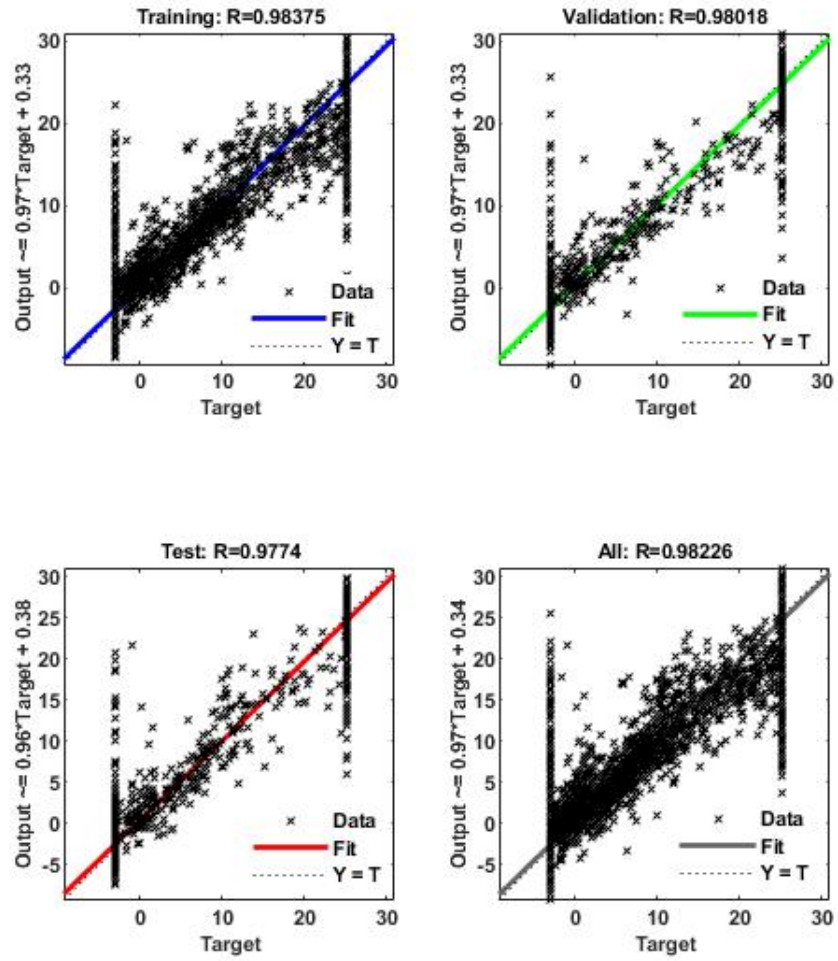


Figure 12: The regression diagram of the presented results is shown in Figure 8.

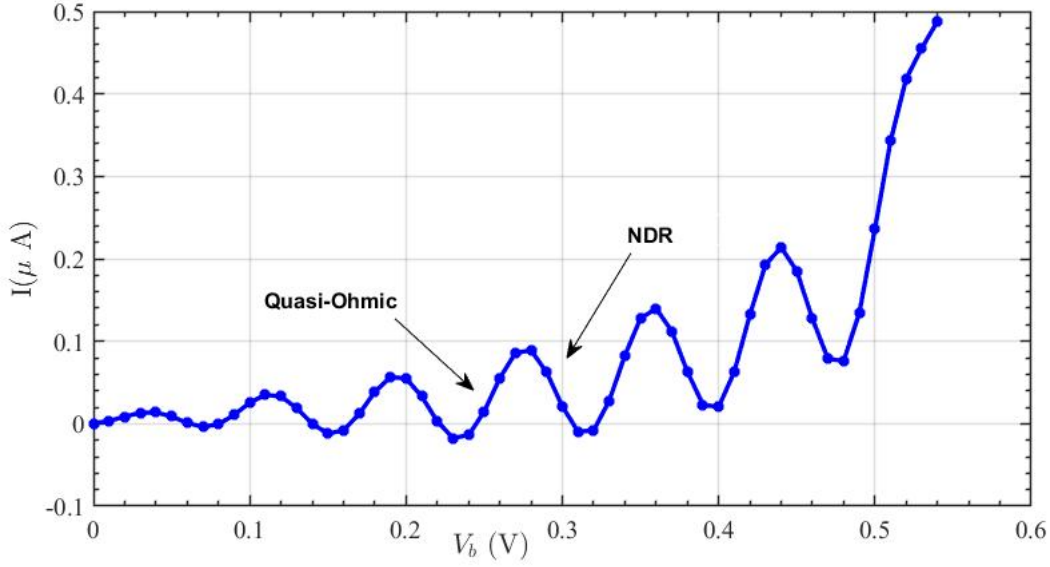


Figure 13: The electric current intensity Variation in the MoS_2 FET with increasing applied voltage in MoS_2 FET. Where selenium atoms are introduced as impurities at a concentration of 0.5 % and at room temperature ($T = 300\text{ K}$) for a lattice size of $N_T = 100 \times 80\text{ atoms}$. The q-ohmic and NDR regions are shown in the figure.

noise in the test data. The consistency between true and predicted values underscores the MLP’s ability to model the influence of lattice dimensions, impurity levels, and temperature on current stability. The high R^2 values across all datasets demonstrate that the MLP’s architecture (32-16-8-4 neurons) successfully captures both quantum stability and transistor performance under the given parameters. While a slight drop in R^2 from Training to Test/Validation suggests some minor overfitting, the model remains highly reliable for practical applications at 300 K with 0.4% Se substitution and a 0.5 V_b . These results affirm the feasibility of using this MLP for designing stable MoS_2 FETs, accurately predicting current stability despite environmental and material variations. The MLP demonstrated successful prediction of quantum stability under both Se doping and applied bias. Our findings reveal that Se doping leads to bandgap narrowing or charge localization near the dopant sites. Additionally, applied voltages (e.g., 0.5 V) appear to shift the predicted Fermi-level alignment.

5. Current-Voltage

- **Nano Scale:** We studied a specific device with a lattice size of 100×80 doped with 1% Selenium (Se) atoms at room temperature (Figure 13). By applying a bias voltage (V_b) across the metal leads, we observed a direct effect on the electrical current flowing through the MoS_2 lattice. As the voltage was increased in the range of $[0, 0.6]$ V/nm, the current first rose rapidly in a quasi-ohmic manner, indicating that the current-voltage relationship was nearly linear, with the slope of the curve representing the ohmic resistance. After reaching its peak, the current-voltage curve’s slope became negative ($dI/dV <$

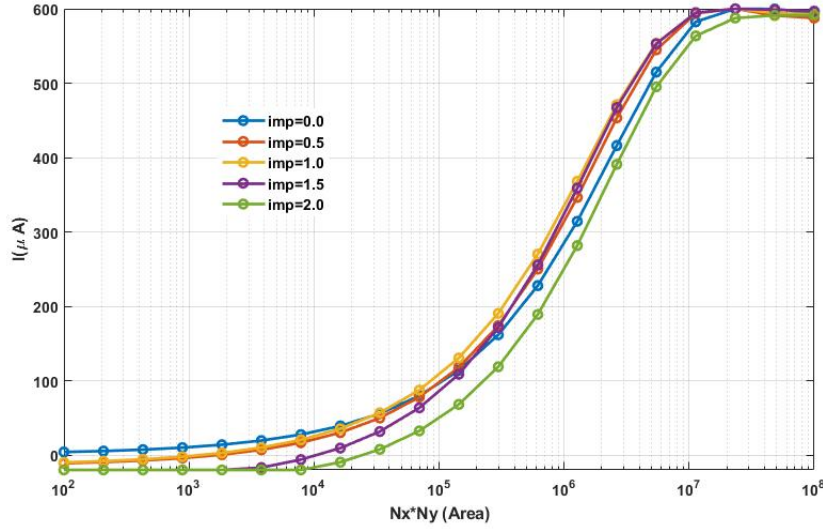


Figure 14: The variation in electric current intensity (I , in μA) within the MoS_2 FET is examined with respect to lattice size as a controlling factor, conducted at an environmental temperature of $T = 300 K$ and an applied bias voltage of $V_b = 0.2 V$. The effect of impurity concentration is assessed through distinct level repulsion parameters, represented by different doping levels: pristine (no impurities, blue line), 0.5% (brown line), 1% (mustard line), 1.5% (purple line), and 2% (green line). These findings highlight impurity-induced spectral shifts, offering significant insights into how the interplay of bias voltage and dopant concentration influences the electronic current in the device.

0). This region is known as negative differential resistance (NDR). The NDR peak is a significant electrical characteristic that can be harnessed for applications in oscillators and switching devices due to its unique nonlinear behavior [51, 52]. Charge transport in MoS_2 FET is complex and highly tunable, influenced by factors like applied voltage and impurity concentration.

- **Macro Scale:** Figures 14 - 16 illustrate the output of a Multilayer Perceptron (MLP) model trained on data derived from a MoS_2 -FET transistor. The model predicts electric current intensity (I) based on several key input parameters: lattice size (defined by $N_x \times N_y$), Selenium doping concentration (impurity percentage), bias voltage (V_B), and temperature (held constant at $300 K$). This configuration reflects realistic device conditions, where impurity doping introduces structural disorder, the applied electric field governs carrier transport, and system dimensions influence quantum phenomena such as localization and chaos. Through training, the MLP has captured the complex, nonlinear relationships between the transistor's physical characteristics, operating conditions, and resulting electrical behavior.

For any given doping level, the current increases with device area, as a larger channel provides more paths for charge carriers, reducing resistance [53]. At a fixed area (e.g., vertical slice at 10^5), the current decreases as Selenium doping increases. While Se doping in MoS_2 typically induces n-type behavior, the observed trend suggests that higher doping introduces excessive scattering centers, im-

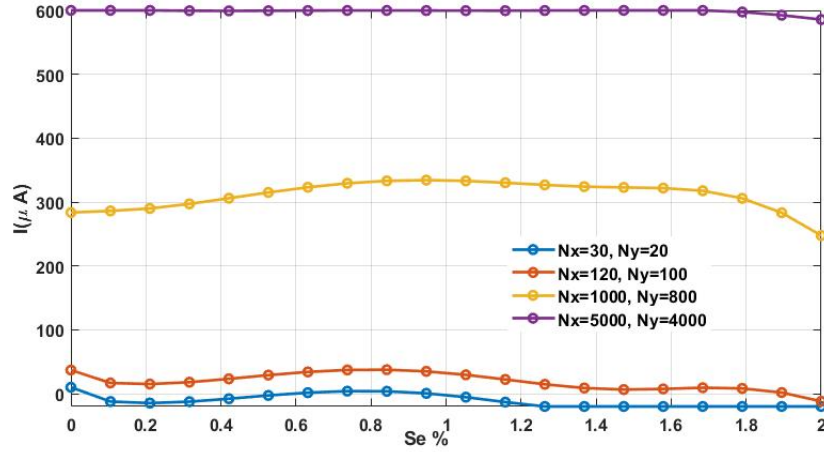


Figure 15: The variation in electric current intensity (I , in μA) within the MoS_2 FET is examined at an environmental temperature of $T = 300 K$, and an applied bias voltage of $V_b = 0.2 V$ with a focus on the effects of varying Selenium (Se) impurity concentrations. The influence of lattice size on the electronic structure is evaluated using distinct level repulsion parameters, represented by different lattice configurations: blue line ($N_x \times N_y = 30 \times 20$), brown line ($N_x \times N_y = 120 \times 100$), mustard line ($N_x \times N_y = 1000 \times 800$), and purple line ($N_x \times N_y = 5000 \times 4000$). These results highlight spectral transitions driven by impurities and emphasize the critical roles of both lattice dimensionality and dopant concentration in shaping the device’s electronic properties.

peding electron flow and reducing mobility. Alternatively, it may reflect a shift in threshold voltage. In very small devices, current remains low due to quantum confinement. As size increases, current rises sharply before saturating, indicating bulk-like behavior beyond a certain scale. The curves show that higher impurity concentrations (yellow, purple, green) require larger areas to match the current of a pristine device (blue), confirming that impurities hinder transport until the system size compensates (Figure 14). Figure 15 presents the predicted current as a function of Selenium (Se) doping percentage across various fixed lattice sizes. For smaller devices (blue and orange lines), the current initially rises at low doping levels—likely due to added charge carriers—before declining as impurity concentration increases. This drop suggests that excessive doping introduces scattering centers, which hinder carrier mobility [54].

In contrast, larger devices (yellow and purple lines) maintain a nearly constant, high current across most doping levels, with noticeable decline only at very high concentrations. This indicates that bulkier systems are less affected by individual impurities. The purple line, representing the largest device, shows the highest current overall, aligning with the saturation behavior observed in Figure 14. All curves reflect typical semiconductor channel behavior: low current at low gate voltages (“off” state), followed by a sharp increase as gate voltage rises (“on” state), eventually reaching saturation. While the absolute current scales with lattice area, the curve shapes—such as threshold voltage and subthreshold slope—remain consistent. This implies the MLP model has effectively separated geomet-

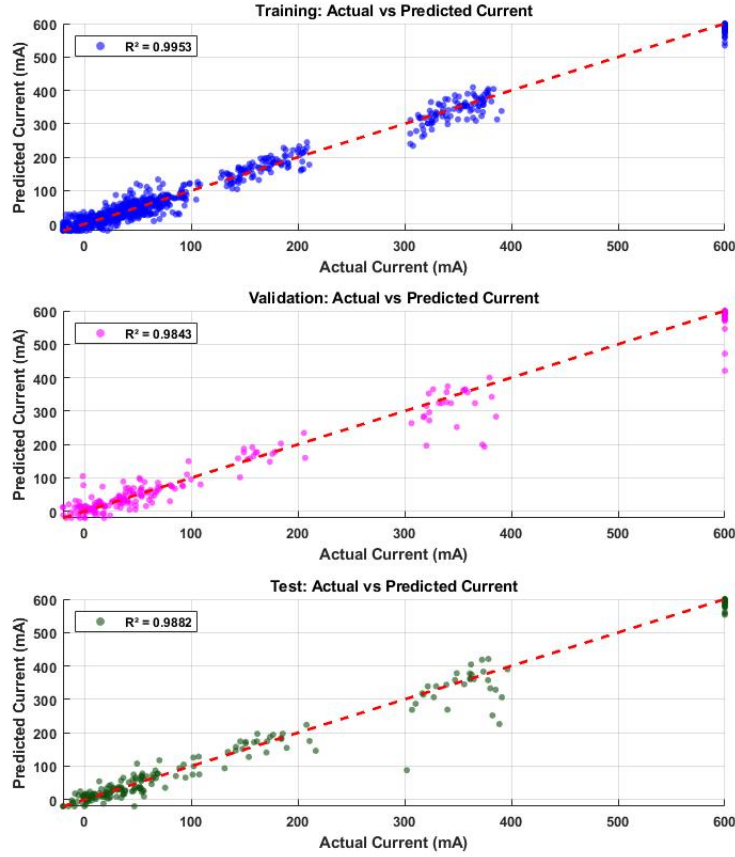


Figure 16: The variation in electric current intensity within the MoS_2 FET is examined for a lattice size of $7665 \times 9000 \text{ nm}^2$, with Selenium atoms introduced as impurities at a concentration of 0.02%. The bias voltage is held constant at $V_b = 0.2 \text{ V}$, and the analysis is conducted at room temperature ($T = 300 \text{ K}$). In this context, the blue line depicts the measured value of the repulsion parameter, while the red dashed line represents its predicted counterpart.

ric scaling from the intrinsic electronic response to gate modulation. Figure 16 presents scatter plots comparing actual current values—either measured or simulated from the physical model—with those predicted by the MLP. Across the Training, Validation, and Test sets, the predicted points closely follow the ideal prediction line (red dashed), demonstrating strong agreement. This is further supported by high R^2 values near 1, indicating that the MLP has effectively captured the underlying relationship between input parameters (such as device size and doping level) and the resulting current.

The MLP deep learning model (Figure 3) has effectively captured the underlying physics of Se-doped MoS_2 FETs. Its predictions (Figures 14 and 15) closely mirror the expected behavior of real semiconductor devices, where current scales with device area and responds to variations in doping concentration and gate voltage. Performance metrics in Figure 15 show near-perfect alignment with true data, reflected in R^2 values exceeding 0.98. The model demonstrates strong robustness and generalizability: its high accuracy on validation and test sets—data not seen during training—indicates reliable performance for predicting new combinations of input parameters, such as novel device sizes or doping levels within the trained domain.

6. Conclusion

This study integrates theoretical modeling and machine learning to analyze quantum stability and electronic performance in Se-doped MoS_2 FETs, considering bias voltage, impurity concentration, temperature, and lattice size to capture realistic device behavior. Quantum stability is quantified via the Brody parameter β , which distinguishes localized ($\beta \rightarrow 0$) from delocalized ($\beta \rightarrow 1$) states and directly links to charge transport. Bias voltage emerges as a powerful control knob, consistently reducing β and pushing the system toward ordered electronic states, an effect most pronounced in pristine or lightly doped lattices. Selenium doping shifts the universal β response, mapping a disorder-driven mobility edge, yet its influence is strongly size-dependent: confinement dominates in small lattices, while in larger systems doping initially increases β before saturation or reversal signals a transition from symmetry-breaking chaos to defect-induced localization. The most dominant factor is system scale, with β following a universal sigmoidal scaling law with logarithmic area, indicating that nanoscale devices remain integrable whereas larger systems become chaotic. An MLP model predicts these trends with $R^2 > 0.93$, successfully bridging ab initio simulations to device-level behavior. The macroscopic implications are captured in I - V characteristics, where a distinct negative differential resistance region emerges, pointing to applications in high-frequency oscillators and ultrafast switches. Future work should extend the MLP to time-dependent phenomena, incorporate DFT data for material-specific accuracy, and consider non-uniform disorder such as clustering. Applying the framework to other 2D materials like WSe_2 or heterostructures would test generalizability, while experimental validation of the predicted NDR and scaling laws remains essential. Finally, developing interpretable surrogate models via symbolic regression could deepen the physical understanding of quantum chaos in 2D devices, completing the pathway from fundamental theory to practical design.

7. Declarations

- Conflict of interest: The authors have no relevant financial or non-financial interests to disclose.
- Funding: No funding was received to assist with the preparation of this manuscript.
- Availability of data and materials: All data generated or analysed during this study are included in this published article.

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