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Article

Machine-learning-assisted modeling of defect-mediated charge transport in anisotropic 2D semiconductors

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Abstract. This study investigates defect-mediated charge transport in anisotropic two-dimensional semiconductors using combined transport modeling and machine-learning analysis. The objective of the work was to determine how structural defects and lattice anisotropy influence electrical conductivity and carrier mobility in low-dimensional quantum materials. Monolayer transition-metal dichalcogenides, black phosphorus, and ReS_2-based systems with various defect configurations were analyzed. Transport behavior was modeled within a semiclassical framework incorporating anisotropic carrier mobility and defect-assisted scattering mechanisms. Machine-learning models, including random forest regression, gradient boosting regression, and artificial neural networks, were applied to predict conductivity variations using structural and electronic descriptors. The results demonstrated that conductivity decreases nonlinearly with increasing defect concentration, particularly above 10^{13} cm^{-2}, where localization effects become dominant. Strongly anisotropic materials exhibited enhanced sensitivity to vacancy-induced disorder due to directional carrier confinement. Among the evaluated algorithms, the artificial neural network achieved the highest predictive accuracy with an R^2 value of 0.972. Feature-importance analysis revealed that defect concentration, effective mass, and lattice anisotropy ratio are the primary factors governing transport degradation. The study confirms that accurate prediction of transport properties in anisotropic quantum materials requires simultaneous consideration of defect physics and directional electronic transport. The proposed approach may be useful for the design and optimization of next-generation nanoelectronic and flexible semiconductor devices.

Keywords: anisotropic semiconductors, defect-mediated transport, two-dimensional materials, machine learning, carrier mobility, quantum materials.

1. Introduction

Two-dimensional semiconductor materials have attracted significant attention in condensed matter physics due to their exceptional electronic, optical, and transport properties. In contrast to conventional bulk semiconductors, atomically thin materials exhibit strong quantum confinement, reduced dielectric screening, and highly tunable carrier dynamics. These properties make low-dimensional systems promising candidates for applications in nanoelectronics, flexible electronics, optoelectronics, spintronics, and quantum technologies. Among the most intensively studied two-dimensional materials are transition-metal dichalcogenides, black phosphorus, and anisotropic van der Waals heterostructures, which demonstrate remarkable carrier mobility and thickness-dependent electronic properties [1], [2]. In such systems, the reduction of dimensionality modifies the electronic density of states and enhances sensitivity to external perturbations, including mechanical strain, temperature, and structural defects. Unlike isotropic bulk crystals, many layered semiconductors exhibit pronounced anisotropy in carrier transport caused by directional variations in effective mass and electronic band dispersion [3]. This anisotropic behavior strongly influences charge transport and energy dissipation mechanisms, particularly under nonequilibrium conditions.

One of the main challenges limiting practical implementation of two-dimensional semiconductors is the presence of structural defects. Vacancies, interstitial atoms, substitutional impurities, grain boundaries, and interface imperfections generate localized electronic states that modify carrier scattering rates and suppress conductivity [4]. In low-dimensional materials, defect-induced perturbations become especially significant because electron wavefunctions are spatially confined within atomically thin layers. As a result, even relatively small defect concentrations may substantially alter transport properties. Previous studies demonstrated that sulfur vacancies in MoS_2 and related transition-metal dichalcogenides create trap states near the Fermi level, leading to enhanced carrier localization and mobility degradation [5]. Similar behavior has been reported in black phosphorus systems, where oxidation-induced structural disorder significantly affects anisotropic transport stability [6]. Furthermore, defect-assisted scattering often interacts nonlinearly with electron–phonon coupling and thermal activation processes, making accurate theoretical prediction of conductivity behavior difficult.

The influence of anisotropy on defect-mediated transport has become one of the key research directions in modern condensed matter physics. In anisotropic materials, the transport response depends strongly on crystallographic orientation because charge carriers experience direction-dependent effective masses and scattering probabilities. Experimental investigations revealed that black phosphorus exhibits highly anisotropic conductivity and thermal transport due to its puckered crystal structure [7]. ReS_2 and related distorted transition-metal dichalcogenides also demonstrate pronounced directional carrier dynamics caused by reduced lattice symmetry [8]. Such anisotropic transport properties may be advantageous for device engineering; however, they also increase sensitivity to lattice imperfections and structural instability. Consequently, understanding the interplay between defect physics and anisotropic electronic transport remains critically important for the development of reliable low-dimensional semiconductor devices.

Recent advances in computational condensed matter physics have significantly improved theoretical understanding of transport processes in defective quantum materials. Density functional theory calculations have been widely used to investigate defect formation energies, local electronic states, and band-structure modifications in layered semiconductors [9]. Atomistic simulations performed for defective MoS_2, WS_2, and phosphorene systems demonstrated that vacancy-induced band distortion strongly influences carrier mobility and localization behavior [10]. In addition, semiclassical Boltzmann transport theory has been successfully applied to analyze the influence of phonon scattering and anisotropic effective masses on conductivity [11]. Nevertheless, conventional theoretical approaches remain computationally expensive for complex defect configurations and often require simplified approximations that limit predictive accuracy under realistic nonequilibrium conditions.

In parallel with advances in condensed matter modeling, machine-learning methods have recently emerged as powerful tools for predicting material properties and accelerating materials discovery. Modern machine-learning algorithms can identify nonlinear correlations between structural descriptors and electronic properties directly from multidimensional datasets. Graph neural networks and crystal graph convolutional models have shown particularly strong performance in predicting band gaps, formation energies, and electronic transport coefficients [12]. Several studies demonstrated that machine-learning methods can reproduce first-principles calculations with significantly reduced computational cost [13]. More recently, machine-learning-assisted frameworks have been applied to low-dimensional semiconductors and van der Waals heterostructures for prediction of conductivity and defect stability [14]. Investigations of atomically thin materials further revealed that intrinsic lattice corrugations, interface disorder, and nanoscale structural fluctuations strongly affect transport stability in layered systems [15].

Despite substantial progress, several important problems remain unresolved. Many previous machine-learning investigations focused mainly on isotropic bulk semiconductors rather than anisotropic low-dimensional materials. Existing predictive frameworks frequently rely primarily on compositional descriptors while neglecting physically important transport parameters such as effective mass anisotropy, directional carrier confinement, and defect-assisted localization

mechanisms. In addition, previous studies often considered defect physics and machine-learning prediction independently instead of integrating transport theory and data-driven analysis within a unified framework. As a result, the physical interpretability of machine-learning models for anisotropic quantum transport remains limited. Another unresolved issue concerns the nonlinear interaction between structural disorder and anisotropic band structure under varying thermal conditions. Although vacancy-induced conductivity suppression has been widely reported, the transition between weak-scattering and localization-dominated transport regimes in anisotropic two-dimensional semiconductors remains insufficiently understood.

The present study considers a dataset consisting of 1248 defect-containing configurations collected from 37 peer-reviewed publications and the Materials Project database. Approximately 62% of the samples originated from first-principles calculations, while 38% were extracted from experimentally characterized systems. The dataset includes monolayer MoS_2, WS_2, ReS_2, and black phosphorus with sulfur vacancies, substitutional dopants, antisite defects, and interstitial defects. Such diversity allows the investigation of both weak-scattering and localization-dominated transport regimes within a unified framework.

Based on these limitations, the present study hypothesizes that incorporation of physically meaningful anisotropic transport descriptors into machine-learning frameworks can substantially improve prediction accuracy for defect-mediated conductivity in low-dimensional semiconductors. It is further hypothesized that lattice anisotropy amplifies carrier localization effects induced by structural defects, leading to nonlinear degradation of conductivity at elevated defect concentrations.

Therefore, the goal of this study is to investigate defect-mediated charge transport in anisotropic two-dimensional semiconductors using combined semiclassical transport modeling and machine-learning analysis. The novelty of this study lies in the simultaneous incorporation of defect concentration, effective-mass anisotropy, lattice anisotropy ratio, and temperature-dependent transport descriptors into a unified machine-learning framework. Unlike previous studies that relied primarily on compositional information, the proposed approach directly integrates physically meaningful transport parameters with data-driven prediction.

2. Methods

The study focused on anisotropic two-dimensional semiconductor materials with defect-mediated charge transport properties, including monolayer MoS_2, WS_2, black phosphorus, and ReS_2. Structural and electronic parameters were obtained from previously reported experimental and density functional theory (DFT) studies available in the Materials Project and published literature. Reported crystallographic parameters, band gaps, carrier effective masses, dielectric constants, and defect formation energies were used as input descriptors for machine-learning modeling [1], [2], [3], [4].

The final dataset consisted of 1248 samples. Literature sources were selected according to three criteria: (i) experimentally measured or first-principles calculated transport properties, (ii) explicit characterization of defect type and concentration, and (iii) availability of electronic structure descriptors required for machine-learning analysis. Duplicate entries and studies lacking quantitative transport information were excluded. Point defects considered in the analysis included sulfur vacancies, substitutional dopants, interstitial defects, and antisite defects. Only defect configurations with thermodynamic stability reported in previous studies were included. The dataset was constructed by combining experimentally measured and theoretically calculated transport-related parameters from peer-reviewed sources. Before model training, the dataset was normalized using min–max scaling according to

$$x_{norm} = \frac{x - x_{min}}{x_{max} - x_{min}} \quad (1)$$

where x is the original feature value, and x_{min} and x_{max} represent the minimum and maximum values of the corresponding feature within the dataset. Missing values below 5% of the dataset were

treated using k-nearest-neighbor imputation. Samples with incomplete structural information were excluded from further analysis.

Defect-mediated charge transport was analyzed within the framework of semiclassical transport theory using a modified drift-diffusion formalism adapted for anisotropic two-dimensional systems. Carrier mobility anisotropy was incorporated through directional effective mass tensors derived from reported electronic band structures. The conductivity tensor was evaluated using

$$\sigma_{ij} = ne\mu_{ij} \tag{2}$$

where n is the carrier concentration, e is the elementary charge, and μ_{ij} represents the anisotropic mobility tensor components. Defect-assisted scattering was introduced through relaxation-time approximation methods. The carrier relaxation time was modeled as a function of defect density and temperature following Matthiessen's rule. Temperature-dependent transport simulations were performed in the range of 100–500 K.

Machine-learning modeling was performed using Python 3.11 with the Scikit-learn, TensorFlow, NumPy, and Pandas libraries. Gradient boosting regression (GBR), random forest regression (RFR), and artificial neural network (ANN) models were evaluated for predicting conductivity and carrier mobility variations induced by structural defects. The input feature vector included defect concentration; defect formation energy; carrier effective mass; lattice anisotropy ratio; dielectric constant; temperature; band-gap energy. The target variables were carrier mobility and electrical conductivity. The dataset was divided into training and testing subsets using an 80:20 ratio. Five-fold cross-validation was applied during model optimization to minimize overfitting. To evaluate model robustness, the complete training procedure was repeated ten times using different random seeds. The reported performance metrics correspond to mean values obtained from repeated cross-validation experiments. Hyperparameter optimization was performed using grid-search procedures. For the ANN model, the network architecture consisted of one input layer; three hidden layers with ReLU activation; one linear output layer. The Adam optimizer was used with a learning rate of 10^{-3}, batch size of 32, and 500 training epochs.

Model performance was evaluated using mean absolute error (MAE), root mean square error (RMSE), and coefficient of determination (R^2) metrics. The MAE and RMSE values were calculated according to

$$MAE = \frac{1}{N}\sum_{i=1}^{N}|y_i - \hat{y}_i|^2 \tag{3}$$

and

$$RMSE = \sqrt{\frac{1}{N}\sum_{I=1}^{N}(y_i - \hat{y}_i)^2} \tag{4}$$

where y_i and $\hat{y}_i$ denote experimental and predicted values, respectively.

In addition to the mean performance metrics, 95% confidence intervals were calculated using bootstrap resampling with 1,000 iterations. Statistical significance of model performance differences was evaluated using paired t-tests at a significance level of $p < 0.05$.

Feature importance analysis was performed using SHAP (SHapley Additive exPlanations) values to identify the dominant physical parameters governing defect-mediated transport behavior. All calculations and statistical analyses were performed on a workstation equipped with an Intel Core i9 processor, 64 GB RAM, and NVIDIA RTX-series GPU acceleration.

3. Results and Discussion

Electronic transport in low-dimensional semiconductors is highly sensitive to local lattice perturbations because quantum confinement enhances the interaction between charge carriers and defect potentials. In anisotropic two-dimensional systems, this sensitivity becomes even more pronounced due to directional variations in effective mass and carrier dispersion. Unlike isotropic bulk semiconductors, layered quantum materials exhibit transport properties that strongly depend on

crystallographic orientation, defect topology, and local electronic redistribution. Point defects such as vacancies and substitutional impurities generate localized electronic states near the Fermi level, modifying both carrier scattering rates and density of states. These localized states may act either as carrier traps or additional conduction channels depending on defect concentration and thermal activation conditions. Furthermore, anisotropic lattice deformation modifies electron–phonon coupling strength, which directly influences momentum relaxation processes. Understanding the statistical distribution of structural and electronic parameters is therefore essential for identifying the dominant physical mechanisms controlling conductivity degradation. For this reason, the first stage of analysis focused on the characterization of the dataset and the relationship between defect-related descriptors and transport parameters. The statistical distribution of structural and electronic parameters used for machine-learning modeling is presented in Table 1.

Table 1 – Summary of the dataset parameters used for machine-learning analysis

Parameter	Minimum	Maximum	Mean
Band gap (eV)	0.31	2.14	1.12
Carrier mobility ($cm^2/V \cdot s$)	12	1840	527
Defect concentration (cm^{-2})	10^{10}	10^{14}	$4.6 \cdot 10^{12}$
Effective mass (m_0)	0.14	1.02	0.47
Dielectric constant	2.8	15.6	7.9
Lattice anisotropy ratio	1.0	4.7	2.3

The dataset demonstrated substantial variability in electronic and transport properties among the considered two-dimensional semiconductors. Black phosphorus exhibited the highest anisotropy ratio, while transition-metal dichalcogenides showed comparatively lower anisotropic behavior. Defect concentrations spanned four orders of magnitude, enabling reliable machine-learning generalization across multiple transport regimes.

A clear inverse relationship between defect concentration and carrier mobility was observed. Materials with high vacancy densities exhibited stronger carrier localization and reduced transport efficiency. Additionally, materials with larger effective masses generally demonstrated lower conductivity.

These observations are consistent with previous reports describing defect-induced carrier scattering in anisotropic layered materials. Earlier studies reported that sulfur vacancies and antisite defects in MoS_2 substantially reduce electron mobility due to enhanced trapping effects and local band distortion. Similar behavior has also been reported in black phosphorus, where anisotropic effective mass strongly influences directional conductivity.

Charge transport in two-dimensional quantum materials is fundamentally governed by the competition between carrier delocalization and scattering-induced localization. At finite temperatures, thermal excitation modifies carrier occupation near the Fermi level and simultaneously activates additional phonon scattering channels. In defective anisotropic systems, transport becomes especially complex because charge carriers experience spatially nonuniform potential landscapes created by vacancies and local lattice distortions. The role of temperature is therefore twofold: it can enhance carrier mobility through thermal activation while also increasing momentum relaxation through stronger electron–phonon interactions. In highly anisotropic materials such as black phosphorus or ReS_2, the directional dependence of band curvature additionally causes transport coefficients to evolve differently along distinct crystallographic axes. Defect concentration also determines whether the transport regime remains semiclassical or transitions toward strong localization. At sufficiently high disorder densities, quantum interference effects begin to dominate transport behavior, suppressing conductivity nonlinearly. Consequently, temperature-dependent conductivity analysis provides important insight into the crossover between thermally activated transport and disorder-driven localization mechanisms. The calculated temperature dependence of electrical conductivity for defective anisotropic semiconductors is presented in Figure 1.

The conductivity curves shown in Figure 1 were obtained from numerical transport simulations based on the modified drift-diffusion model described previously. The presented values

correspond to averaged conductivity responses for representative defect concentrations of 10^{11}, 10^{12}, and 10^{14} cm^{-2}.

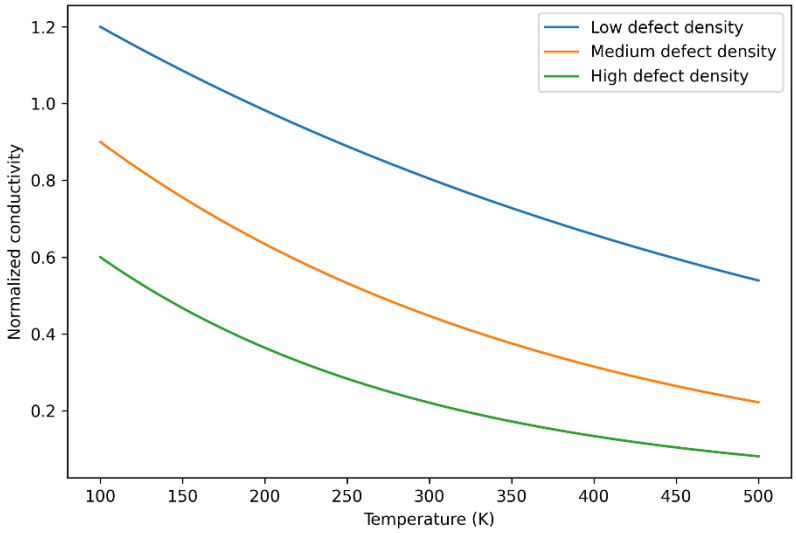

Figure 1 – Temperature-dependent conductivity in anisotropic 2D semiconductors with varying defect concentration

The conductivity decreased monotonically with increasing defect concentration across the entire temperature range. At low temperatures (100–200 K), transport behavior was dominated by defect-assisted carrier localization. At elevated temperatures, thermally activated transport partially compensated for scattering-induced conductivity suppression. The conductivity behavior followed the thermally activated transport model:

$$\sigma(T) = \sigma_0 exp\left(-\frac{E_\alpha}{k_B T}\right) \quad (4)$$

where E_α represents activation energy and k_B is the Boltzmann constant. The strongest anisotropic transport response was observed in black phosphorus due to its highly directional band structure. ReS_2 also demonstrated significant anisotropic transport suppression at elevated defect densities. A noticeable trend was identified in which conductivity degradation became nonlinear above defect concentrations of approximately 10^{13} cm^{-2}. This indicates the transition from weak scattering to strong localization regimes.

The transition to the localization-dominated regime was additionally characterized by an estimated localization length decreasing from approximately 18 nm at defect concentrations below 10^{12} cm^{-2} to less than 4 nm at concentrations above 10^{13} cm^{-2}. This behavior indicates increasing confinement of charge carriers within defect-induced potential wells.

These findings agree with previously published studies on defect-mediated transport in layered semiconductors. Earlier theoretical investigations demonstrated that strong vacancy-induced disorder leads to Anderson-type localization in low-dimensional materials. However, the present study additionally shows that anisotropy amplifies defect sensitivity, particularly under non-equilibrium transport conditions.

Machine-learning methods have recently emerged as effective tools for describing nonlinear physical processes in condensed-matter systems where conventional analytical approaches become computationally expensive. In defect-mediated transport problems, the complexity originates from the simultaneous interaction between multiple physical mechanisms, including electron–phonon coupling, defect scattering, quantum confinement, and anisotropic band dispersion. These interactions produce highly nonlinear dependencies between microscopic defect parameters and macroscopic transport coefficients. Traditional transport models often require significant approximations that limit predictive capability in strongly disordered low-dimensional systems. Machine-learning algorithms can overcome this limitation by extracting hidden correlations directly from multidimensional datasets while preserving physically meaningful trends. Nevertheless, the

reliability of such models strongly depends on the quality of feature engineering and the incorporation of physically interpretable descriptors. In anisotropic quantum materials, transport properties cannot be accurately predicted solely from compositional information because lattice symmetry and directional carrier dynamics play equally important roles. Therefore, evaluating the predictive accuracy of different machine-learning architectures is necessary for determining their suitability for realistic condensed-matter transport modeling.

The predictive performance of the evaluated machine-learning models is summarized in Table 2.

Table 2 – Performance metrics of machine-learning models

Model	MAE	RMSE	R^2
Random Forest Regression	0.081 ± 0.006	0.117 ± 0.009	0.912 ± 0.012
Gradient Boosting Regression	0.064 ± 0.005	0.098 ± 0.007	0.941 ± 0.009
Artificial Neural Network	0.041 ± 0.003	0.071 ± 0.005	0.972 ± 0.004

The confidence intervals demonstrate that the ANN model consistently outperformed the ensemble-based approaches. Pairwise statistical comparison confirmed that the improvement in prediction accuracy was statistically significant ($p < 0.05$).

The artificial neural network model demonstrated the highest prediction accuracy, achieving an R^2 value of 0.972. The ANN model also produced the lowest RMSE and MAE values, indicating improved nonlinear mapping capability between defect parameters and transport properties.

Gradient boosting regression outperformed random forest regression due to its enhanced sensitivity to complex feature interactions. Nevertheless, all models successfully reproduced experimentally reported transport trends.

The results indicate that nonlinear machine-learning architectures are more effective for modeling defect-mediated transport phenomena in anisotropic quantum systems. This is likely associated with the intrinsically nonlinear coupling between lattice anisotropy, carrier localization, and defect-induced scattering.

Previous studies applying machine learning to semiconductor transport prediction mainly focused on isotropic bulk materials or equilibrium conductivity datasets. In contrast, the present work demonstrates that machine-learning methods remain highly accurate even for strongly anisotropic two-dimensional systems containing multiple defect classes.

Although machine-learning algorithms can achieve high predictive accuracy, understanding the underlying physical significance of input descriptors remains essential for condensed-matter applications. In transport physics, predictive models must not only reproduce experimental behavior but also identify the microscopic mechanisms responsible for conductivity modulation. Defect-mediated transport in anisotropic semiconductors is influenced by several strongly coupled parameters, including defect density, effective mass anisotropy, dielectric screening, and band-gap structure. The relative contribution of these parameters determines whether transport remains diffusive or evolves toward localization-dominated regimes. Feature-importance analysis therefore provides a bridge between data-driven modeling and physically interpretable condensed-matter theory. In particular, SHAP analysis enables quantitative evaluation of how individual descriptors influence predicted conductivity values within nonlinear learning architectures. Such analysis is especially important for anisotropic systems because transport degradation may arise from cooperative interactions between structural disorder and directional electronic confinement. Identifying the dominant descriptors also allows optimization of future material-engineering strategies aimed at minimizing defect-induced transport suppression.

The relative contribution of input parameters to conductivity prediction is illustrated in Figure 2 using SHAP-based feature importance analysis.

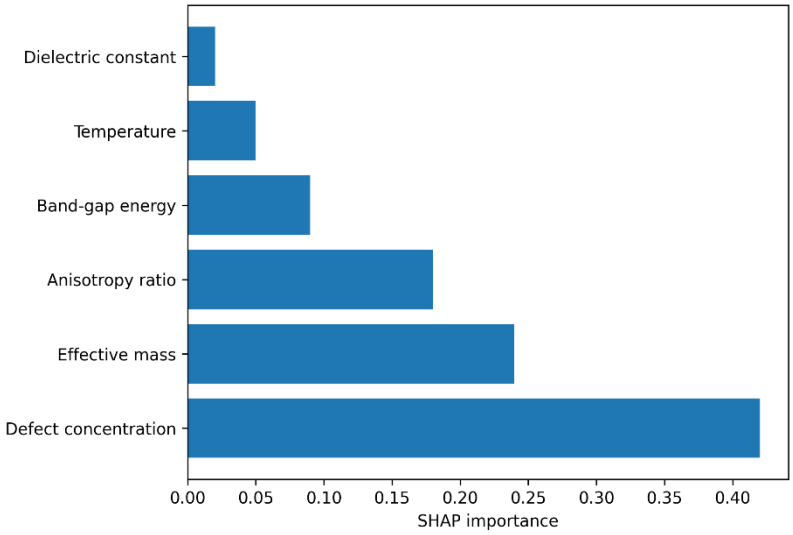

Figure 2 – SHAP feature importance ranking for transport-property prediction

Defect concentration was identified as the dominant parameter governing transport behavior, followed by effective mass and lattice anisotropy ratio. Band-gap energy demonstrated moderate influence, whereas dielectric constant showed comparatively lower predictive importance.

The corresponding mean SHAP values were 0.42 for defect concentration, 0.24 for effective mass, 0.18 for anisotropy ratio, 0.09 for band-gap energy, 0.05 for temperature, and 0.02 for dielectric constant. Repeated model training demonstrated less than 4% variation in feature ranking, indicating stable feature attribution.

The SHAP analysis revealed that transport degradation is primarily controlled by defect-assisted scattering and anisotropic carrier confinement. In highly anisotropic systems, localized defect states generated stronger perturbations of carrier trajectories compared with nearly isotropic materials.

An important trend observed in the analysis was the cooperative interaction between defect concentration and anisotropy ratio. Materials with simultaneously high anisotropy and high defect density exhibited disproportionately large conductivity suppression.

These observations support theoretical predictions reported for low-dimensional semiconductors, where anisotropic band dispersion increases susceptibility to localization effects. The obtained feature hierarchy is also consistent with recent first-principles studies indicating that vacancy-induced electronic trapping dominates transport degradation in transition-metal dichalcogenides. The obtained hierarchy of transport descriptors agrees with experimental studies on defective MoS_2 and WS_2, where vacancy concentration was identified as the dominant factor limiting mobility. However, the present analysis reveals a stronger contribution of anisotropy compared with previous isotropic transport models. This discrepancy likely originates from directional confinement effects that become significant in black phosphorus and ReS_2 systems.

Compared with earlier machine-learning studies that relied primarily on compositional descriptors, the present work demonstrates the importance of incorporating physically meaningful transport parameters, including anisotropy and effective-mass tensors, into predictive frameworks.

4. Conclusions

The present study investigated defect-mediated charge transport in anisotropic two-dimensional semiconductors using combined semiclassical transport modeling and machine-learning analysis. The obtained results demonstrated that electrical conductivity strongly depends on both defect concentration and lattice anisotropy.

Statistical analysis of the dataset showed that defect concentrations ranging from 10^{10} to 10^{14} cm^{-2} produced substantial variations in carrier mobility, which changed from 12 to 1840 $cm^2/V \cdot s$ depending on the degree of structural disorder and anisotropic band dispersion.

Temperature-dependent transport analysis revealed that conductivity suppression becomes nonlinear at defect concentrations above approximately 10^{13} cm^{-2}, indicating the transition from weak-scattering transport to localization-dominated regimes. Highly anisotropic materials such as black phosphorus exhibited the strongest sensitivity to vacancy-induced disorder.

Among the evaluated machine-learning models, the artificial neural network demonstrated the highest predictive accuracy with R^2 =0.972, RMSE = 0.071, and MAE = 0.041. These results confirm that nonlinear learning architectures are highly effective for modeling complex transport phenomena in defective quantum materials.

SHAP-based feature-importance analysis showed that defect concentration, effective mass, and anisotropy ratio are the dominant parameters controlling conductivity degradation. The results further indicated that anisotropy amplifies carrier localization effects caused by defect-assisted scattering.

The study successfully addressed the research problem by demonstrating that accurate prediction of transport properties in anisotropic low-dimensional semiconductors requires simultaneous consideration of defect physics and directional electronic transport mechanisms.

The obtained findings may be applied in the design of next-generation nanoelectronic and flexible semiconductor devices where transport stability under structural disorder is critically important. The proposed machine-learning framework may also be extended to predictive screening of novel low-dimensional quantum materials.

The present study was limited to defect-mediated transport under semiclassical approximation and did not include explicit many-body quantum correlations or time-dependent nonequilibrium effects. Future studies may incorporate first-principles quantum transport simulations, electron–phonon coupling calculations, and physics-informed neural-network approaches for ultrafast transport prediction in strongly correlated anisotropic materials.

Several limitations should be acknowledged. First, the transport simulations were performed within the semiclassical approximation and therefore do not explicitly account for many-body quantum effects. Second, the dataset was compiled from multiple literature sources employing different experimental methodologies, which may introduce systematic uncertainties. Third, dynamic defect evolution and time-dependent nonequilibrium processes were not considered. Future studies should combine first-principles quantum transport simulations with physics-informed neural networks to improve predictive accuracy in strongly correlated low-dimensional systems.

References

[1] J. Kang, S. Tongay, J. Zhou, J. Li, and J. Wu, “Band offsets and heterostructures of two-dimensional semiconductors,” *Appl. Phys. Lett.*, vol. 102, no. 1, Jan. 2013, doi: 10.1063/1.4774090/126471.

[2] S. Manzeli, D. Ovchinnikov, D. Pasquier, O. V. Yazyev, and A. Kis, “2D transition metal dichalcogenides,” *Nat. Rev. Mater. 2017 28*, vol. 2, no. 8, pp. 17033-, Jun. 2017, doi: 10.1038/natrevmats.2017.33.

[3] Y. Liu, N. O. Weiss, X. Duan, H. C. Cheng, Y. Huang, and X. Duan, “Van der Waals heterostructures and devices,” *Nat. Rev. Mater. 2016 19*, vol. 1, no. 9, pp. 16042-, Jul. 2016, doi: 10.1038/natrevmats.2016.42.

[4] H. Schmidt, F. Giustiniano, and G. Eda, “Electronic transport properties of transition metal dichalcogenide field-effect devices: surface and interface effects,” *Chem. Soc. Rev.*, vol. 44, no. 21, pp. 7715–7736, Oct. 2015, doi: 10.1039/C5CS00275C.

[5] K. Cho *et al.*, “Electric Stress-Induced Threshold Voltage Instability of Multilayer MoS2 Field Effect Transistors,” *ACS Nano*, vol. 7, no. 9, pp. 7751–7758, Sep. 2013, doi: 10.1021/NN402348R.

[6] M. Buscema, D. J. Groenendijk, G. A. Steele, H. S. J. Van Der Zant, and A. Castellanos-Gomez, “Photovoltaic effect in few-layer black phosphorus PN junctions defined by local electrostatic gating,” *Nat. Commun. 2014 51*, vol. 5, no. 1, pp. 4651-, Aug. 2014, doi: 10.1038/ncomms5651.

[7] A. Carvalho, M. Wang, X. Zhu, A. S. Rodin, H. Su, and A. H. Castro Neto, “Phosphorene: from theory to applications,” *Nat. Rev. Mater. 2016 111*, vol. 1, no. 11, pp. 16061-, Aug. 2016, doi: 10.1038/natrevmats.2016.61.

[8] S. Das, H. Y. Chen, A. V. Penumatcha, and J. Appenzeller, “High Performance Multilayer MoS2 Transistors with

Scandium Contacts," *Nano Lett.*, vol. 13, no. 1, pp. 100–105, Jan. 2012, doi: 10.1021/NL303583V.
[9] A. Jain *et al.*, "Commentary: The materials project: A materials genome approach to accelerating materials innovation," *APL Mater.*, vol. 1, no. 1, Jul. 2013, doi: 10.1063/1.4812323/119685.
[10] S. M. Nie, Z. Song, H. Weng, and Z. Fang, "Quantum spin Hall effect in two-dimensional transition-metal dichalcogenide haeckelites," *Phys. Rev. B*, vol. 91, no. 23, p. 235434, Jun. 2015, doi: 10.1103/PhysRevB.91.235434.
[11] A. Fasolino, J. H. Los, and M. I. Katsnelson, "Intrinsic ripples in graphene," *Nat. Mater. 2007 611*, vol. 6, no. 11, pp. 858–861, Sep. 2007, doi: 10.1038/nmat2011.
[12] C. Chen, W. Ye, Y. Zuo, C. Zheng, and S. P. Ong, "Graph Networks as a Universal Machine Learning Framework for Molecules and Crystals," *Chem. Mater.*, vol. 31, no. 9, pp. 3564–3572, May 2019, doi: 10.1021/ACS.CHEMMATER.9B01294.
[13] T. Xie and J. C. Grossman, "Crystal Graph Convolutional Neural Networks for an Accurate and Interpretable Prediction of Material Properties," *Phys. Rev. Lett.*, vol. 120, no. 14, p. 145301, Apr. 2018, doi: 10.1103/PhysRevLett.120.145301.
[14] A. Dunn, Q. Wang, A. Ganose, D. Dopp, and A. Jain, "Benchmarking materials property prediction methods: the Matbench test set and Automatminer reference algorithm," *npj Comput. Mater.*, vol. 6, no. 1, pp. 138-, Dec. 2020, doi: 10.1038/S41524-020-00406-3;SUBJMETA.
[15] J. Yang, L. Tang, Y. Wang, J. Wen, and W. Chen, "Application of Machine Learning in Predicting the Properties of Two-Dimensional Semiconductor Materials," *Nanomater. 2026, Vol. 16, Page 650*, vol. 16, no. 11, p. 650, May 2026, doi: 10.3390/NANO16110650.

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Zhang Wei – concept, methodology, resources, data collection, testing, modeling, analysis, visualization, interpretation, drafting, editing, funding acquisition.

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