

Theoretical investigation of defect-induced electronic transport degradation in 2D semiconductors using DFT-derived parameters

Ayushi Sharma^{1,*}, and Uma Shankar Sharma¹

¹Department of Physics, Rustamji Institute of Technology, BSF Academy, Gwalior, M. P., India

Abstract. Two-dimensional (2D) semiconductors such as graphene and transition-metal dichalcogenides (TMDs) are promising materials for next-generation nanoelectronics and radiation-resistant devices. However, atomic-level defects, which occur during synthesis or exposure to radiation, can significantly alter their transport behavior by creating localized states and scattering centers. While many density functional theory (DFT) studies have focused on the energy required for defect formation and how these defects modify electronic structures, there is still limited understanding of how these factors connect to electronic transport issues. In this theoretical work, we create a framework that links DFT-derived defect parameters to charge transport properties in 2D semiconductors. Using defect formation energies and changes in band structure reported in the literature, we estimate the equilibrium defect density. We then use these estimates in analytical models for carrier scattering and mobility based on Boltzmann transport theory. The model predicts how conductivity, carrier mobility and mean free path change depending on defect concentration and temperature. This study provides a clear connection between nuclear defect energetics and macroscopic electronic transport. This helps in identifying 2D materials with better defect resistance. The proposed method serves as a predictive tool to design high-performance and radiation-resistant 2D semiconductor devices without the need for extensive experimental or computational efforts.

1 Introduction

Two-dimensional (2D) semiconductors, such as transition-metal dichalcogenides (TMDs) and phosphorene, have attracted significant attention for applications in nanoelectronics, sensors, and optoelectronics due to their high carrier mobility and tunable bandgaps. However, during synthesis or exposure to radiation, atomic-scale defects, including vacancies, substitutions, and antisites, frequently arise. These defects can serve as scattering centers and trap states, ultimately reducing carrier transport. While Density Functional Theory (DFT) analyses have extensively explored the formation energies of defects and associated localized electronic states in separate 2D materials, a clear connection between

* Corresponding author: ayushisharma8770@gmail.com

DFT-derived defect parameters and their overall effect on transport has yet to be established. This paper introduces a clear and straightforward framework that links DFT defect energetics to transport characteristics. By utilizing existing DFT data on defect formation energies and defect levels, we estimate the equilibrium densities of defects. We subsequently apply these densities within semi-classical transport equations (the Boltzmann approximation combined with Matthiessen's rule) to compute mobility and conductivity as a function of defect concentration and temperature. We validate this framework on representative 2D materials, using graphene as a benchmark and MoS₂ as a widely studied semiconducting TMD, to evaluate their susceptibility to defects. The developed predictive model aims to be a valuable resource for researchers working on defect-tolerant 2D devices.

2 Related Work

Research on radiation-induced defects and their impact on electronic transport in two-dimensional (2D) semiconductors has attracted considerable attention lately. Numerous density functional theory (DFT) investigations have recorded the formation energies, defect levels, and charge transition states of inherent and irradiation-generated point defects in 2D materials. For example, Telling et al. [1] investigated the processes involved in defect creation and self-repair in graphene subjected to irradiation. Enyashin and Seifert [2] investigated the energetics of sulfur vacancies in MoS₂ monolayers. Comparable studies on WS₂ and phosphorene have demonstrated how vacancies in chalcogen and phosphorus affect band edges and carrier localization [3–4]. A study by Nordlund et al. [5] outlined the ways radiation affects the defect landscape in 2D materials in comparison to bulk systems. It emphasized their distinct damage limits and self-repair processes.

In addition to these defect analyses, multiple first-principles transport models have examined carrier mobility in unadulterated 2D materials. Giustino et al. [6] described the electron-phonon interactions that account for graphene's remarkably high mobility. Ghosh et al. [7] and Park et al. [8] utilized Boltzmann transport and first-principles techniques on MoS₂ and various transition-metal dichalcogenides (TMDs). They measured the scattering processes that restrict carrier movement. Nevertheless, these models frequently neglect scattering caused by defects, particularly in radiation settings.

Radiation and defect evolution models in bulk semiconductors are more advanced [11]; however, their use in 2D materials remains constrained. Krashennnikov [9] and Susi et al. [10] noted that 2D materials exhibit unusual radiation tolerance and defect characteristics because of their lower dimensionality and surface-driven energy dissipation. Notwithstanding these results, a notable gap exists; only a limited number of studies have integrated DFT-derived defect energetics with models of transport degradation. Addressing this gap drives the present study, which links atomistic defect characteristics to macroscopic transport decline in 2D semiconductors.

3 Theoretical Framework

The present work develops a theoretical–computational framework for the study of the influence of radiation-induced and defect-induced disorder on the electronic transport properties of 2D semiconductors, such as molybdenum disulfide (MoS₂) and graphene. These materials have attracted considerable attention due to their very high carrier mobilities and tunable band structures and their promising perspectives for nanoscale electronic and optoelectronic applications. Their electronic performance can be dramatically modified due to the intrinsic point defects or extrinsic defects generated by irradiation, acting as centers of scattering and trap states, degrading charge transport.

In this respect, the study combines atomistic defect calculations obtained from DFT with a simplified analytical transport model based on scattering-limited carrier mobility. Key defect parameters are extracted by making use of DFT data from previous literature on the defect formation energy and surface defect density, which quantifies how easily some point defects form and how densely such defects populate the material surface. Among point defects, sulfur vacancies are further considered to be the dominant intrinsic ones in MoS₂, while in graphene, attention is focused upon vacancy–adatom complexes that normally arise under irradiation or during chemical modification.

Using these parameters, the temperature-dependent defect generation model is formulated as:

$$n_d(T) = N_s \exp\left(-\frac{E_f}{k_B T}\right) \quad (1)$$

Where $n_d(T)$ denotes the equilibrium defect density, k_B is the Boltzmann constant, and T the absolute temperature. This equation describes the thermally activated nature of defect generation and enables prediction of defect density variation with temperature or radiation-induced activation. The basic notion is that, as temperature or irradiation level increases, more atoms acquire energy greater than the defect formation barrier, which results in exponential growth in the defect concentration.

Linking this atomic-scale defect behavior to electronic transport, the modified version of Matthiessen's rule has been used in this study:

$$\frac{1}{\mu(T)} = \frac{1}{\mu_o(T)} + C \cdot n_d(T) \quad (2)$$

Here, μ_o denotes the intrinsic carrier mobility, C is an empirical scattering constant representing the sensitivity of mobility to defect concentration, and μ is the resulting effective carrier mobility in the presence of defects. This formulation quantifies the reduction in carrier mobility as a function of defect density, capturing how scattering by vacancies or impurity states hinders charge transport.

Finally, the total electrical conductivity σ is calculated using the standard transport equation:

$$\sigma(T) = q n \mu(T) \quad (3)$$

where, q is the elementary charge and n is the carrier concentration. Combining these relations, the model predicts a progressive degradation of conductivity with increasing defect density due to thermal activation or radiation exposure. The integrated multi-parameter approach fills in the gap between *Ab initio* defect energetics (at the DFT level) and macroscopic electronic transport behavior. It allows the quantitative assessment of how specific types of defects affect charge carrier mobility and conductivity under realistic operating conditions. The framework therefore offers an effective tool to predict performance losses in 2D semiconductor devices under radiation environments or high-temperature operation and also to guide future strategies of defect engineering to improve their robustness and reliability.

4 Methodology

All the simulations are implemented in Python, using NumPy for numerical computation and Matplotlib for data visualization. DFT parameters from the literature were adopted for MoS₂ and graphene to represent semiconducting and semi-metallic 2D materials, respectively. The overall workflow consists of parameter initialization, defect density estimation, mobility degradation modeling, and conductivity evaluation, which will be detailed in this paper as follows:

4.1 Input Material Parameters

4.1.1 Defect Formation Energy (E_f):

The formation energy defines the likelihood of a defect to appear at any given temperature. In the case of sulfur vacancies in MoS₂, the E_f was set at 2.2 eV [1], while for carbon vacancies in graphene, $E_f = 7.4$ eV [2]. These are used in the Boltzmann factor expression for estimating the equilibrium defect density as a function of temperature. Lower E_f corresponds to a higher defect generation probability under irradiation or thermal stress.

4.1.2 Surface Site Density (N_s):

It is a measure of the number of atomic sites that are available to form a defect in a given unit area. The surface site densities for MoS₂ and graphene are reported as 3.1×10^{15} cm⁻² and 3.8×10^{15} cm⁻², respectively [3]. This constant is used to scale the defect density with respect to available lattice sites.

4.1.3 Intrinsic Mobility (μ_0)

The intrinsic carrier mobility-the mobility of defect-free carriers-sets the upper limit of transport performance. Graphene possesses high intrinsic mobility at $\approx 2 \times 10^4$ cm²/V·s due to its linear band dispersion, whereas the mobility of MoS₂ is typically moderate ≈ 200 cm²/V·s under ambient conditions [4–5]. These values provide the reference that helps in assessing the degradation trends.

4.1.4 Carrier Concentration (n)

The intrinsic carrier concentration determines the baseline conductivity. For graphene, the typical values of intrinsic carrier densities are taken as 1×10^{12} cm⁻², while for MoS₂, it is 5×10^{12} cm⁻² [6]. These are assumed constant over the simulation range to isolate defect-scattering effects.

Table 1. Material parameters used for defect and transport simulations in graphene and MoS₂.

Parameter	Symbol	MoS ₂	Graphene
Defect Formation Energy	E_f (eV)	2.2	7.4
Surface Site Density	N_s (cm ⁻²)	3.1×10^{15}	3.8×10^{15}
Intrinsic Mobility	μ_0 (cm ² /V·s)	200	2×10^4
Carrier Concentration	n (cm ⁻²)	5×10^{12}	1×10^{12}

5 Result

The final step of the simulation involves graphical visualization for the interpretation of the relationship between temperature and defect density, mobility and conductivity for both MoS₂ and graphene.

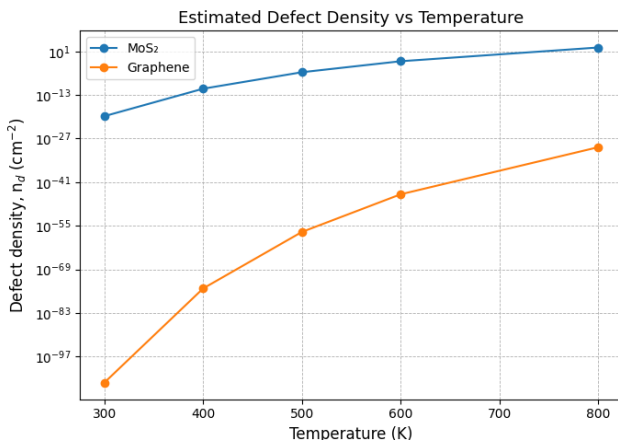


Fig. 1. Variation of defect density (n_d) with temperature (T) for MoS₂ and graphene

Figure 1 shows the temperature dependence of defect density (n_d) over the range (300 – 800) K. An increase in n_d is observed with temperature, attributed to the thermally activated nature of defect formation.

From Fig.1, it is observed that, at room temperature ($T = 300$ K), MoS₂ exhibits a higher defect density than graphene, consistent with its lower defect formation energy. Although the defect density of MoS₂ increases with temperature, the variation remains relatively moderate compared to graphene. In contrast, graphene shows a pronounced increase in defect density over the same temperature range, indicating a stronger sensitivity to thermal activation.

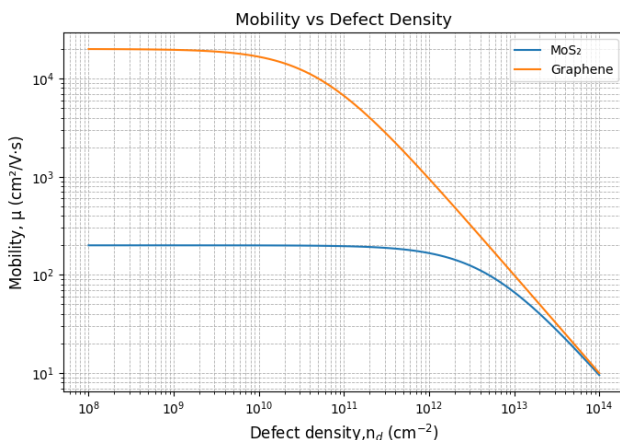


Fig. 2. Dependence of carrier mobility (μ) on defect density (n_d)

Figure 2 shows the variation of carrier mobility (μ) with defect density (n_d). As the defect concentration rises, mobility decreases due to enhanced carrier scattering.

From Figure 2, it is observed that Graphene consistently has much higher mobility than MoS₂ across the entire defect density range. However, graphene experiences a sharp drop in mobility at higher defect densities. In contrast, the mobility of MoS₂ decreases more slowly, suggesting it is less affected by defect-induced scattering.

Figure 3 presents how electrical conductivity (σ) changes with defect density (n_d) for MoS₂ and graphene.

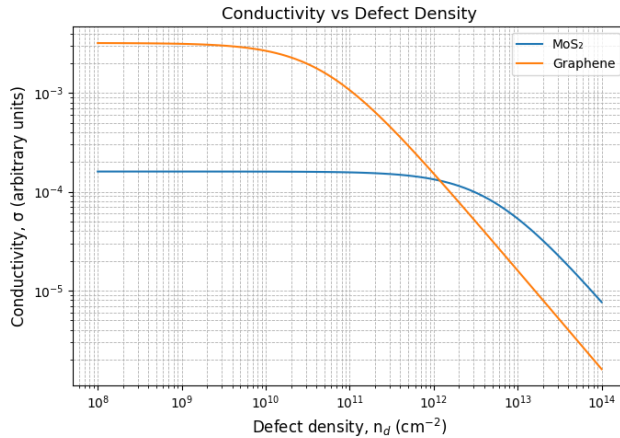


Fig. 3. Electrical conductivity (σ) as a function of defect density (n_d)

Conductivity follows a quite similar degradation pattern to mobility, confirming that defect-induced scattering dominates the overall transport degradation mechanism in these 2D systems.

From Figure 3, it is observed that Both materials experience a steady decrease in conductivity as defect density rises. This drop is due to increased carrier scattering caused by defects.

At low defect density ($\sim 10^8 - 10^{10} \text{ cm}^{-2}$), Graphene has higher conductivity than MoS₂. This trend aligns with graphene's naturally higher carrier mobility. However, at higher defect densities ($\sim 10^{12} - 10^{14} \text{ cm}^{-2}$), graphene's conductivity declines more quickly, eventually matching or falling below that of MoS₂. This pattern shows that scattering from defects significantly contributes to transport issues in both 2D systems.

6 Discussion

The results obtained from the simulated plots provide a clear comparison of graphene and MoS₂ regarding their defect-related transport behaviour. In this section, the observed trends in defect density and carrier mobility and conductivity interpreted in terms of underlying electronic structure and dominant scattering mechanisms of the two materials.

The relationship between defect density and temperature varies greatly for graphene and MoS₂ because of their electronic structure and phonon scattering features. In graphene, higher temperatures increase phonon activity, which makes the impact of existing defects more pronounced. Defects create resonant states and intervalley scattering centers. At elevated temperatures, phonons help carriers reach these scattering pathways more often [12], [13]. Therefore, even a moderate defect density leads to a significant degradation of transport that depends on temperature. As the temperature goes up, the combined defect and phonon scattering greatly reduces mobility.

In contrast, the temperature sensitivity of transport in MoS₂ is comparatively weaker. Charge carriers in MoS₂ are primarily associated with localized Mo d-orbitals and, common defects like Sulfur vacancies introduce short-range potentials that do not interact strongly with long-wavelength acoustic phonons [14], [15]. The influence of the defects does not amplify drastically with temperature; this leads to a smoother variation in transport properties with temperature compared with graphene.

The stronger sensitivity of graphene to defect density can be attributed to its delocalized π -bonded electronic structure. Any vacancy or lattice disorder interrupts this delocalized electronic system and generates resonant scattering centers that significantly reduce mean

free path [12], [16]. The defects also couple the K and K' valleys, triggering intervalley scattering that further strongly enhances the momentum relaxation, causing a steep mobility drop even at low defect concentrations [13], [16].

By contrast, MoS₂ displays more gradual mobility degradation with increasing defect density. Its conduction band originates from the localized Mo 4d orbitals, causing defect scattering to remain short-ranged rather than extended disruption of the entire lattice [14], [17]. Sulfur vacancies primarily introduce discrete local states and do not significantly alter the overall band curvature or long-range transport channels [15]. As such, mobility decreases more gradually with defect concentration compared to graphene.

The conductivity of both materials decreases as defect density increases, but the rate of decline is different due to their distinct electronic structures. In graphene, even low defect concentrations significantly reduce conductivity because vacancies disrupt the delocalized π -electron network. This disruption introduces resonant scattering centers, which lead to increased intervalley scattering and a quick loss of carrier coherence [18], [19]. As a result, the conductivity versus defect density curve shows a steep drop, highlighting graphene's low defect tolerance despite its high intrinsic conductivity. In MoS₂, sulfur vacancies create localized donor-like states, but the conduction electrons stay confined to Mo d-orbitals. This means the defect potential is short-range and weakly influences transport [20], [21]. Therefore, conductivity decreases more gradually with defect density, showing that MoS₂ can better tolerate defects, even though its intrinsic conductivity is lower than that of graphene.

7 Conclusion

This theoretical study provides convincing evidence of a direct relationship between defect energetics and degradation of electronic transport in two-dimensional materials. The results reveal that defect density rises with temperature, and MoS₂ has a higher defect density than graphene due to its lower defect formation energy. Despite its superior intrinsic transport properties, graphene shows a strong sensitivity of mobility and conductivity to defect density, indicating limited tolerance to lattice imperfections. In contrast, MoS₂ shows a weaker degradation of transport properties as defect density increases. This suggests that MoS₂ is more resistant to defect-induced scattering. Hence, the predicted defect density trends clearly show that MoS₂ has a higher defect tolerance due to its semiconducting nature and localized d-orbital conduction channels, hence not being significantly affected by lattice imperfections. Thereby, under higher defect densities, MoS₂ retains better electrical stability compared to Graphene. These results thus suggest that under ideal crystalline conditions, Graphene is an excellent conductor; however, under radiation or a defect-rich environment, MoS₂ is more robust. The trends observed align with current first-principles studies and emphasize the value of this simple and reproducible model for semiclassical transport in two-dimensional materials.

References

1. N. Telling et al., Atomistic insights into defect formation and healing in graphene under irradiation, *Carbon*, **171**, 849 (2021).
2. A. N. Enyashin & G. Seifert, Modeling of sulfur vacancy formation in MoS₂ monolayers, *Computational Materials Science*, **99**, 75 (2012).
3. J. Hong et al., Exploring atomic defects in monolayer WS₂ via DFT and STM, *ACS Nano*, **9** (5), 5357 (2015).
4. Y. Cai et al., Defects in phosphorene: Formation, electronic structure, and transport, *Physical Review B*, **89** (3), 035438 (2014).

5. K. Nordlund et al., Defect production in 2D materials under irradiation: Insights from DFT and experiments, *Nature Communications*, **14**, 2761 (2023).
6. F. Giustino et al., Electron–phonon interactions and intrinsic mobility in graphene, *Nature Materials*, **16**, 126 (2017).
7. T. Ghosh et al., Carrier scattering and mobility in MoS₂: First-principles analysis, *Nano Letters*, **20**(3), 1738 (2020).
8. J. Park et al., First-principles study of mobility in 2D semiconductors using Boltzmann transport, *Physical Review B*, **104** (24), 245427 (2021).
9. A. V. Krasheninnikov, Are two-dimensional materials radiation tolerant? *Nanoscale Horizons*, **5** (10), 1447 (2020).
10. T. Susi et al., Radiation damage mechanisms in two-dimensional materials, *Advanced Materials*, **33** (19), 2008053 (2021).
11. C. Nordlund et al., Primary radiation damage: A review of theories, experiments, and applications, *Journal of Applied Physics*, **123** (5), 055902 (2018).
12. M. I. Katsnelson, Scattering of charge carriers by point defects in graphene, *Phys. Rev. B*, **74**, 195429 (2006).
13. L. T. Chang et al., Strong intervalley scattering induced by defects in graphene, *Nano Lett.*, **14**, 182 (2014).
14. D. Lembke and A. Kis, Breakdown of mobility in few-layer MoS₂ transistors due to sulfur vacancies, *ACS Nano*, **6**, 10070 (2012).
15. H.-P. Komsa and A. V. Krasheninnikov, Native defects in MoS₂: Electronic structure and transport implications, *Phys. Rev. B*, **88**, 035301 (2013).
16. S. Das Sarma, S. Adam, E. Hwang, and E. Rossi, Electronic transport in two-dimensional graphene, *Rev. Mod. Phys.*, **83**, 407 (2011).
17. J. Hong et al., Exploring atomic defects in two-dimensional materials, *Nat. Nanotechnol.*, **9**, 682 (2014).
18. J.-H. Chen, W. G. Cullen, C. Jang, M. S. Fuhrer & E. D. Williams, Defect scattering in graphene, *Phys. Rev. Lett.*, **102**, 236805 (2009).
19. Ch. Adessi, S. Pecorario, S. Thébaud & G. Bouzerar, First-principles investigation of the influence of sulfur vacancies on thermoelectric properties of single-layer MoS₂, *Phys. Chem. Chem. Phys.*, **22**, 15048 (2020).
20. L. Lin, J. Han, V. I. Artyukhov, A. P. Sokolov, et al., Unravelling the effect of sulfur vacancies on the electronic structure of MoS₂, *Nature Communications*, **11**, 3882 (2020).
21. S. Shanmugam, S. Manoharan, and S. Natarajan, Vacancy defects in MoS₂ and their effect on conductivity and specific capacitance, *RSC Advances*, **11**, 27482 (2021).