

**SIMULATION AND ANALYSIS OF TMDC SOLAR CELLS UNDER PROTON
RADIATION USING MONTE-CARLO METHODS, SCAPS, AND MACHINE
LEARNING TECHNIQUES**



**A Thesis Submitted in partial fulfillment of the requirements for the degree of
Master of Science (MS) in the Department of Physics, Hajee Mohammad Danesh
Science and Technology University, Dinajpur-5200**

Submitted By

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Student ID: 1708105

Session: 2021-2022

DEPARTMENT OF PHYSICS

**HAJEE MOHAMMAD DANESH SCIENCE AND TECHNOLOGY UNIVERSITY,
DINAJPUR-5200**

BANGLADESH

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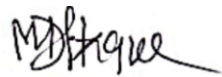
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Candidate's Declaration

This is “Naimur Rahman” declare that Master of Science (MS) thesis entitled as “**Simulation and Analysis of TMDC Solar Cells Under Proton Radiation Using Monte-Carlo Methods, SCAPS, and Machine Learning Techniques**” comprises of independent investigation carried out by me at the Laboratory of Physics, Department of Physics, Hajee Mohammad Danesh Science and Technology University, Dinajpur. The present research work is done under the joint supervision and guidance of **Dr. Md. Dulal Haque**, Professor, Department of Electronics and Communication Engineering, Hajee Mohammad Danesh Science and Technology University, Dinajpur. At the time of this writing, he is a Post-Doctoral researcher at the State Key Laboratory of Infrared Physics, Shanghai Institute of Technical Physics, Chinese Academy of Sciences, 188 Xinlai Rd, Jiading District, Shanghai 201800, China. The supervisor of this research work is **Dr. Md. Mominul Islam**, Professor and Chairman, Department of Physics, Hajee Mohammad Danesh Science and Technology University, Dinajpur-5200. This thesis contains no material that has been submitted previously, in whole or part, for the award of any other academic degree or diploma. Wherever the references have been made to the work of others has been clearly indicated with the source information under reference sections. Except where otherwise indicated, this thesis is my own work.

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List of Relevant Publications by the Author

1. N. Rahman et al., “Assessing the performance of MoTe₂ based solar cell with Cu₂O hole transport layer through device simulation,” *Discov. Mater.*, vol. 3, no. 1, p. 25, Sep. 2023, doi: 10.1007/s43939-023-00061-7.
2. S. Ahmed et al., “Performance investigation of MAPbI₃ /MASnI₃ based all-perovskite tandem solar cell using SCAPS simulation,” *Phys. Scr.*, vol. 99, no. 5, p. 055520, May 2024, doi: 10.1088/1402-4896/ad36bd.

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Author

Abstract

The space-based energy solutions are currently relying on expensive silicon-based solar cells. In recent years, perovskite materials are also participating in this area as thin-film third generation solar cells. However, these materials come with built-in drawbacks against radiation environments. To address this issue, this research explores the possibility of using transition metal dichalcogenide (TMDC) materials as absorbers in space solar cells. Proton radiation is a common and primary occurrence in space. Hence, we investigated the effect of 0.15 MeV and 3 MeV proton radiation on four different TMDC heterojunction thin-film solar cells with frequently used hole and electron transport materials. We have used SR-NIEL web application, Monte-Carlo simulation toolkit SRIM, solar cell capacitance simulation SCAPS-1D, and machine learning analysis for evaluating the energy loss, defect creation and performance analysis. For 0.15 MeV and 3 MeV proton radiation, energy loss to ionization by ions, energy loss to ionization by recoils, energy loss to phonons by ions, energy loss to phonons by recoils, energy from ions, vacancies by ions, and replacement collisions are calculated. MoS₂ and MoSe₂ had higher power conversion efficiencies (PCE) of 28.16% and 28.11%, respectively, while WSe₂ and WS₂ had high short-circuit current densities (J_{sc}) of 39.36 mA/cm² and 35.15 mA/cm², respectively, under standard operating conditions (AM 1.5G, 1000 W/m² incident photon flux). However, when exposed to 0.15 MeV proton radiation, the performance of all devices significantly decreased. MoSe₂ and WS₂ had relatively higher PCEs of 19.47% and 17.01%, respectively, compared to WSe₂ and MoS₂, indicating some resistance to radiation-induced deterioration. Machine learning predictions revealed that WS₂ and WSe₂ are more sensitive to proton radiation than MoSe₂ and MoS₂ absorbers. This implies that, despite their possibility for high J_{sc} and efficient power generation, WS₂ and WSe₂-based solar cells may be less suitable for areas with high proton radiation, as their performance can decrease rapidly under such conditions. MoSe₂ and MoS₂ absorber-based solar cells, on the other hand, appear to be more resistant to the negative effects of proton radiation, making them better candidates for use in radiation-rich areas. These findings emphasize the relevance of material robustness to radiation when building solar cells for space or radiation environments, as well as the promise of MoSe₂ and MoS₂ absorbers in such applications.

Keywords: TMDC, Solar cells, proton radiation, SCAPS, SRIM, SR-NIEL, ML, Monte-Carlo

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List of Abbreviations

2D	Two-dimensional	XGB	XGBoost
BSF	Back Surface Field		
CE	Counter Electrode		
CIGS	Copper Indium Gallium Sulfo-selenide		
CM	Center of Mass		
CZTS	$\text{Cu}_2\text{ZnSnS}_4$		
CZTSe	$\text{Cu}_2\text{ZnSnSe}_4$		
DSSC	Dye Sensitized Solar Cell		
emf	Electromotive force		
ETM	Electron Transport Material		
FF	Fill Factor		
FFP	Free-flight-path		
GCR	Hole Transport Material		
HTM	Dye Sensitized Solar Cell		
Jsc	Short-circuit Current Density		
LEO	Low Earth Orbit		
ML	Machine Learning		
NIEL	Non-Ionizing Energy Loss		
NSRDB	National Solar Radiation Data Base		
PCE	Power Conversion Efficiency		
PSC	Perovskite Solar Cell		
PV	Photovoltaic		
RF	Random Forest		
SC	Solar Cell		
SHAP	SHapley Additive exPlanations		
SPE	Solar Particle Event		
SPP	surface plasmon polariton		
SRIM	Stopping and Range of Ions in Matter		
TFSC	Thin-film Solar Cell		
TMDC	Transition Metal Dichalcogenide		
TRIM	Transport of Ions in Matter		
Voc	Open circuit voltage		

Chapter One

1 Introduction

1.1 Background

Energy consumption in the form of electricity is possible due to two primary sources: renewable and non-renewable. While non-renewable sources are abundant in terrestrial regions, renewable sources are the only practical option in space. Specifically, stellar radiations (e.g., solar radiation) are used as input power in spacecrafts, satellites, and rovers to keep them operational. Solar cells (SCs) are used to harness this power and to convert it into electricity. Researchers are rigorously working on the efficiency improvement of this device. On the other hand, such photosensitive devices are prone to radiations. Exposure to certain types of particle radiations can significantly change its characteristics in a negative way. Hence, the shielding and defect properties of the materials used in the SCs are also researched.

According to the National Solar Radiation Data Base (NSRDB) [1], the annual average Global Horizontal Irradiance (GHI) in the USA and neighboring areas vary from 5.2 kWh/m²/day to 6.7 kWh/m²/day, and the Direct Normal Irradiance (DNI) is approximately 6 kWh/m²/day. In the Low Earth Orbit (LEO), the accepted value of solar irradiance obtained by NASA in 2008 is $1360.8 \pm 0.5 \text{ W/m}^2$, which is equivalent to $\sim 32.659 \text{ kWh/m}^2/\text{day}$ [2]. Lack of atmospheric absorption and scattering is responsible for such high quantity of radiation. In-orbit solar cells undergo irradiation damage when there is presence of energetic particles. Solar particle events (SPE) can contain protons and alpha particles from ~ 0.1 to 100 MeV/nucleon energy range [3], whereas Galactic Cosmic Rays (GCR) can contain these particles from ~ 0.1 MeV to hundreds of GeV [4]. Protons are also trapped in Van Allen radiation belts surrounding the earth having the energy range of 0.1-400 MeV [5]. As long as the SCs are concerned, particles up to few hundred keV which stop inside the cell can cause the most severe damage [6].

1.2 Review of the Conventional Materials Used in Solar Cells

SCs are designed to capture the photons coming from the sun, which then excites the electrons present in the absorber layer, which gain enough electromotive force (emf) to complete the circuit. Semiconductor devices have the matching bandgap (1-2 eV) to absorb photons ranging from the UV region to the infrared region. Naturally, silicon is the first candidate when semiconductors are concerned. Single junction silicon SCs were the first ones to be used in space [7]. It is still popular and being researched for further improvement. Measured under the global AM1.5 spectrum (1000 Wm^{-2}), the latest certified efficiency of single junction crystalline silicon (c-Si) SC is $26.8 \pm 0.4\%$ whereas the amorphous Si (a-Si) SC has gained $10.2 \pm 0.3\%$ [8]. The major drawback of Si-based SCs is their weight as they range from 100 to 500 μm . The power-to-weight ratio is low compared to the newer generations of Thin-film Solar Cells (TFSCs).

Fabrication cost of c-Si materials is relatively high, a hindrance towards mass production. Only recent development of new methods has reduced the cost which used to be ~76 USD/Watt in 1977 [9]. Over time, c-Si manifests light-induced degradation (LID), a phenomenon where the efficiency of the SC decreases when exposed to sunlight [10]. There can be degradation at the interface between the cell and the contact finger, causing series resistance which continues to increase [11]. Also, the cells can have different characteristics depending on different paste and firing conditions used during manufacturing [11].

Group III elements (e.g., Al, Ga, In, Ti) and group V elements (e.g., P, As, Sb, Bi) are used in the construction of another type of light absorber materials (e.g., GaInP, GaInAs, GaAs) known as III-V materials. III-V multijunction SCs contain several advantages over c-Si SCs. Higher efficiency, suitable bandgap, and bandgap engineering, and radiation resistance are some of them [12]. For single junction, the highest power conversion efficiency (PCE) of GaAs thin film cell is $29.1 \pm 0.6\%$, whereas GaInP/GaInAsP/Si (bonded) multijunction SC has achieved $36.1 \pm 1.3\%$ [8]. However, the increased fabrication cost and complicated fabrication methods are yet to be improved [13]. Koval et. al. [5] numerically measured the electronic stopping power of protons in $\text{Ga}_{0.5}\text{In}_{0.5}\text{P}/\text{GaAs}/\text{Ge}$ triple-junction SCs and concluded that the stopping power is heavily dependent on the trajectory of the protons.

1.3 Emergence of Thin-Film Solar Cells

TFSCs are typically few nanometers to few micrometers thick. These devices are made by depositing one or more thin layers of photovoltaic (PV) materials on a substrate. Copper Indium Gallium Sulfo-selenide (CIGS) for instance, demonstrates good defect resistance due to defect-defect interactions, which in return provides long minority carrier lifetime of 10-100 ns [14]. For multijunction CIGS SCs, lattice matching is not mandatory, giving the opportunity to use different substrates [14]. For single junction, CIGS SCs have achieved $23.35 \pm 0.5\%$ PCE [8]. In conjunction with III-V compounds, GaInP/AlGaAs/CIGS multijunction device has achieved $28.1 \pm 1.2\%$ PCE [8]. Multijunction devices are getting popular and researched more for their increased charge extraction capabilities and better efficiency. However, indium is relatively rare in the Earth's crust (~0.05 ppm), making it less probable for long-term construction [15]. $\text{Cu}_2\text{ZnSnS}_4$ (CZTS) and $\text{Cu}_2\text{ZnSnSe}_4$ (CZTSe) are called kesterite chalcogenides which replace indium with more available elements. The band gaps of CZTS and CZTSe are ~1.5 and ~0.76 eV respectively [14]. Highest recorded PCE of CZTS and CZTSe SCs are $12.1 \pm 0.3\%$ and $10.0 \pm 0.2\%$ respectively [8]. It is noteworthy that their open circuit voltage (V_{oc}) are 0.5379 V and 0.7083 V respectively, which is much lower than other types of new SCs [8], [16].

Dye sensitized solar cells (DSSC) are another type of TFSC which use luminescent dyes as sensitizer to convert photon energy to electricity. Ru(II)-polypyridyl dye is an example [17]. Metal-free organic dyes like Hemicyanine, merocyanine, squarylium, and cyanine are being researched as potential alternative [17]. Some of its advantages are low cost, simple preparation methodology, low toxicity, ease of production, low-

light performance, and flexibility [18], [19]. At current stage, the only major drawback of these devices is their low efficiency. For single junction, the highest recorded PCE is only $11.9\pm0.4\%$.

One area of photovoltaic technology that has advanced quickly in recent years is perovskite solar cells (PSC). The molecular structure of perovskites is of the ABX_3 type, where A and B are the cations (e.g., organic $CH_3NH_3^+$, $CH_3(NH_2)^{2+}$ or inorganic Ag^+ , Cs^+ , Sn^+ or a combination of them) and X are the halogen anions [20]. They are renowned for being very efficient, having cheap production costs, and having a wide variety of light wavelengths that they can absorb [21]. PSCs come in two primary forms: normal n-i-p and inverted p-i-n configurations [22]. The difference is in which transport material on the perovskite's outside is exposed to light rays first. Perovskite-silicon tandem architectures and transport layer-free arrangements are examples of other types. Park et. al. [23] used fluorinated aniliniums to enhance the efficiency of single-junction PSCs to 24.09%. The recorded highest multi-junction perovskite-perovskite SC is 29.1% [24]. While PSCs have benefits, they also have certain disadvantages. When perovskite material is exposed to heat, moisture, or snow, it is known to degrade its performance [25]. In practice, Cardinaletti et. al. [26] deployed $MAPbI_3$ PSC 32 kilometers above the earth, in a near space environment. However, this experiment did not reveal the prolonged, temperature dependent effects on the PSC device. Li et. al. [27] simulated the effects of proton and electron irradiation on perovskite solar cells using Monte-Carlo simulation where they have found degradation PSC characteristics under accumulated fluence.

1.4 Two-dimensional Transition Metal Dichalcogenide Solar Cells

The class of materials known as two-dimensional (2D) materials is made up of atomically thin sheets that are spatially restricted in the z-direction and that are derived from bulk crystals with layered structures [28]. Graphene is a good example of such materials [29]. These materials are single-dimensional at the nanoscale or smaller because they are made of a single layer of atoms arranged in a lattice structure. They have exceptional carrier mobility, strong anisotropy between the in-plane and out-of-plane mechanical properties, high strength, ultralow weight, and high Young's modulus [30]. The electronic band structure and screening of 2D materials play a major role in determining their electrical properties. Materials' electronic band structure and screening primarily dictate their optical characteristics. At the nanoscale, a material's mechanical characteristics, chemical reactivity, electrical conductivity, and even its interaction with light can all vary.

Two-dimensional materials called transition metal dichalcogenides (TMDCs), have shown a lot of promise for SC applications. They possess exceptional semiconducting qualities and high optical absorption coefficients [31]. As such, they can be utilized to create semitransparent, flexible SCs that have potential uses in the fields of wearable electronics, architecture, electric vehicles, and aerospace [32]. TMDCs are generally denoted as MX_2 where M stands for transition metals e.g., Mo, W, and X stands for chalcogens e.g., S, Se, and Te. The crystal structure of MoS_2 and $MoSe_2$ is illustrated in Figure 1.1, adapted from the

CIF file provided by Persson [33], [34]. The bandgap of these materials are within 1.1-1.5 eV [35]–[38]. The bandgap can be adjusted via bandgap engineering. Modern heterojunction SCs use thin transport materials at both sides of the absorber materials to enhance the charge extraction and reduce charge recombination. This is one of the most effective ways to achieve a PCE above the Shockley-Queisser limit (~30%), the maximum theoretical PCE of a single p-n junction SC [39]. P⁺ type hole transport materials (HTMs) are generally used at the rear side of the heterojunction structure. Some conventional HTMs include spiro-OMeTAD, PTAA, Cu₂O, In₂Te₃, NiO, and CuSCN where their primary role is to transport holes and at the same time, block electrons at the interfaces [40], [41]. HTMs are also recognized as back surface fields (BSFs) [42]. Different interface passivation techniques are generally used to improve the quality of the SC [43]. n⁺ type Electron transport materials (ETMs) do the opposite of HTMs and they are placed underneath the glass substrate. Since it a front layer, it must withstand harsh environmental conditions e.g., heat, radiation, moisture, and corrosion for long-term stability [44]. TiO₂, ZnO, SnO₂, WO_x, CeO_x, In₂O₃, C₆₀ are some of the commonly used ETMs [44].

Researchers have advanced the effectiveness and usefulness of TMDC SCs through several creative experiments. By maximizing Au geometrical parameters to effectively excite surface plasmon polaritons (SPPs), Iqbal et al. [45] demonstrated increased efficiency in MoS₂-Au multilayer plasmonic-based solar cells, offering potential uses for raising the PCE of plasmonic-based solar cells. Ahmed et al.'s [46] proposal to add a Cd-free WS₂ buffer layer to Cu₂Te thin-film solar cells provided a high-efficiency substitute. This new method outperforms conventional CdS buffers with a good 24.23% efficiency, and the 'spike-like' band structure at the Cu₂Te/WS₂ interface reduces carrier recombination. For DSSCs, Althomali et al. [47] introduced a unique Pt-free counter electrode (CE) based on Ni-doped MoSe₂, exhibiting increased electrocatalytic behavior and performance. With an optimum efficiency of 6.94%, the Ni-doped MoSe₂ CE outperforms DSSCs using a costly platinum CE (6.68%), providing a more affordable option for DSSC applications. For DSSCs based on crystalline WSe₂ doped with Zn, Abbood et al. [48] developed a novel CE, showing a noteworthy 42% improvement in DSSC efficiency (from 5.78% to 8.19%) under ideal conditions. Zn dopants improve the electrochemical and electrocatalytic capabilities of the CEs, outperforming platinum-based CEs (7.66% efficiency). Ali et al. [35] concentrated on improving an In₂Te₃ BSF and a TiO₂ buffer layer to increase the efficiency of a MoS₂-based solar cell. The improved solar cell, which has a PCE of 33.32%, a V_{oc} of 1.084 V, a J_{sc} of 37.22 mA/cm², and an FF of 82.58%, exhibits superior performance metrics using SCAPS simulation software.

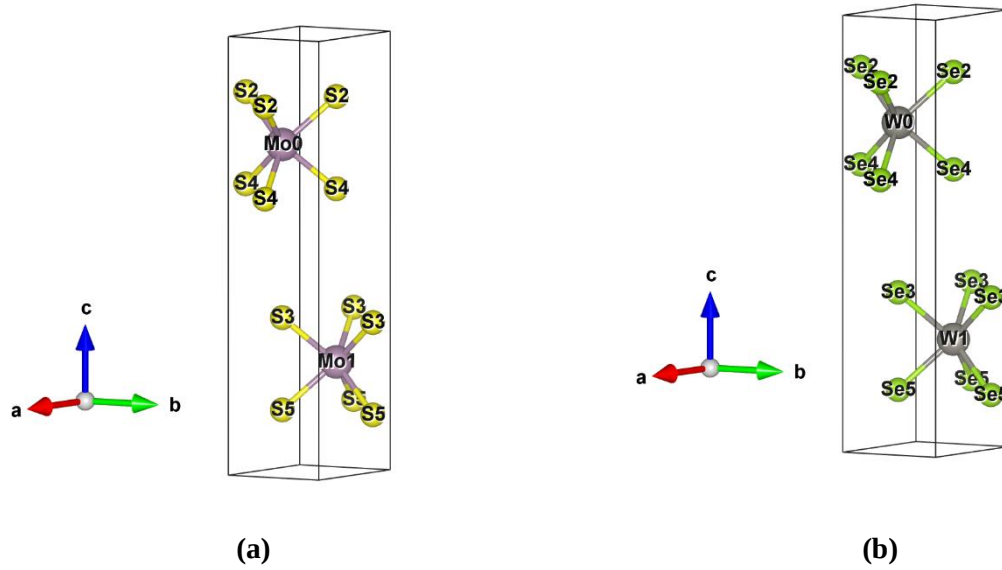


Figure 1.1 Hexagonal $P6_3/mmc$ (194) structure of (a) MoS_2 and (b) WSe_2 [33], [34]

1.5 The Research Question

Although several other materials are being tested under space environments, no reports of TMDC SCs for space environments have been found as of now. Since they are promising in terrestrial environments, it is important to investigate their ability to handle particle radiations. How effective will the features and advantages of these materials be against proton radiation? Before experimental research, a theoretical simulation approach will be very essential to gain insights and prevent costly design mistakes.

1.6 Objectives of the Research

In this research, we have investigated the effect of proton and alpha radiation of two different energies on four different TMDC based SC models. Specifically, our goals were:

- To calculate the initial performance of the four different TMDC devices.
- To calculate the Non-Ionizing Energy Loss (NIEL), absorbed energy, ionization energy, vacancies created, and phonons with respect to the depth of the devices, caused by proton radiation.
- To calculate the performance with the new defect parameters.
- To investigate the results of various collision parameters on the four different absorbers by applying Machine Learning (ML) techniques.
- To propose improvement methods for the TMDC solar cells for proton radiation environment.

1.7 Thesis Outline

- **Chapter 1:** In this chapter, we have briefly discussed the history of SCs and their applications in space. We reviewed the important categories of SCs and their current stage for space applications, with an emphasis on TMDC SCs.
- **Chapter 2:** In this chapter, we have discussed the theoretical background of particle matter interaction and the energy loss associated with them, non-Ionizing energy loss, theory of solar cells and their performance parameters, and two machine learning techniques for the analysis of the results.
- **Chapter 3:** This chapter provides the working procedures of the SR-NIEL website, TRIM calculation, SCAPS calculation. The data needed to initialize the research is also provided here.
- **Chapter 4:** This chapter analyzes and discusses the results found from different numerical analysis, including energy loss calculations, damage calculations, performance of the four solar cells calculations, and machine learning analysis results.
- **Chapter 5:** This conclusion chapter summarizes the research and provides implications of our findings.

Chapter Two

2 Theoretical Background

2.1 Particle-Matter interaction

In this research, we have used the Transport of Ions in Matter (TRIM) computation tool to perform various calculations related to radiation damage [49]. This is part of a software package called ‘Stopping and Range of Ions in Matter (SRIM). There are two main approximation methods that are used in this program. These are (a) the formula for Atom-Atom Collisions and (b) Free Flight Path (FFP) between collisions.

When a particle faces a binary nuclear collision, it is assumed to change direction and move in straight FFPs between collisions. The energy is reduced as a result of nuclear and electronic (inelastic) energy losses. The target is considered amorphous with atoms at random locations, so the directional properties of the crystal lattice are ignored. The particle’s FFP between collisions is longer at high energies and is steadily reduced in the course of slowing down. The continuous energy loss from electronic interactions is also calculated.

2.1.1 Equation of Atom-Atom Scattering

This technique was developed by J. P. Biersack et. al. [50]–[52] which provides a quick solution to the scattering problem with high accuracy. Figure 2.1 represents the scattering of incident particle M_1 with kinetic energy E by initially stationary particle M_2 in the center of mass (CM) system. This forms a scattering triangle for convenient calculation. Here:

P : impact parameter

r_0 : distance of closest approach

ρ_1, ρ_2 : radii of curvature of the trajectories at closest approach

δ_1, δ_2 : small correction terms

θ : scattering angle

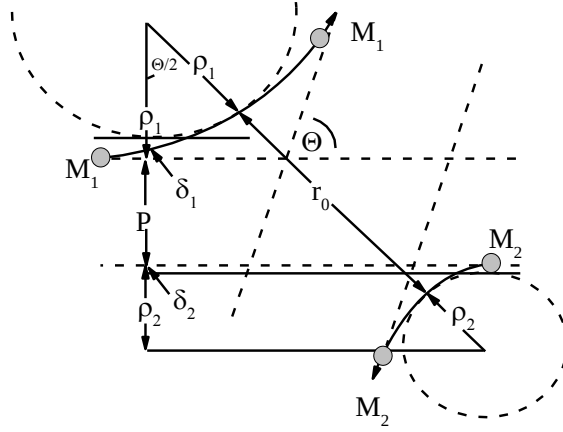


Figure 2.1: Particle trajectories in the CM system [49]

From the triangle,

$$\cos \Theta = \frac{\rho + p + \delta}{\rho + r_0} \quad [\text{where } \rho \equiv \rho_1 + \rho_2, \delta \equiv \delta_1 + \delta_2] \quad (2.1)$$

The CM energy here is expressed in terms of Thomas-Fermi screening length $\mathbf{a}$. Screening length is a parameter defining the radial spread of the electronic charge about the nucleus [53]:

$$\mathbf{a} = \frac{0.8853 a_0}{\frac{Z_1^3 + Z_2^3}{2}} \quad (2.2)$$

Where Z_1 and Z_2 are atomic numbers of the two particles. In terms of $\mathbf{a}$, the other parameters are defined as:

$$B \equiv \frac{P}{\mathbf{a}}, R_0 \equiv \frac{r_0}{\mathbf{a}}, R_C \equiv \frac{\rho}{\mathbf{a}}, \Delta \equiv \frac{\delta}{\mathbf{a}} \quad (2.3)$$

Finally, the of atom-atom collisions formula is expressed as:

$$\cos \frac{\Theta}{2} = \frac{B + R_C + \Delta}{R_0 + R_C} \quad (2.4)$$

This is the governing equation of TRIM, which performs an analytic solution to the scattering of the ion and target atom.

2.1.2 The Free Flight Path Between Collisions

Only a few collisions between high energy ions result in substantial deflections. TRIM maximizes computing efficiency by eliminating collisions that result in insignificant energy transfer and deflection angles for ions. This method greatly decreases CPU time, with over a thousand monolayers frequently skipped between each estimated collision of high-energy protons. The FFP idea is used to measure the greatest distance an ion can travel without colliding. The impact parameter is determined using probability distributions, guaranteeing that collisions occur randomly within the FFP. For high-energy ions, the FFP length is set to ensure a consistent mean angular deflection per route interval. This keeps deflections short as compared to the average distance between large-angle deflections.

Efficiency gains in TRIM are obtained by scaling collisions that result in minimal ion paths deflection and negligible energy transfer. These collisions are considered "negligible" if they have an impact on the outcome of less than 0.1%. This includes small-angle deflections of less than 0.1° . Thorough analysis is necessary for collisions close to surfaces or interfaces to precisely evaluate phenomena such as sputtering or backscattering. When appropriate, TRIM uses the FFP idea, which permits ions to hop between calculated collisions. These leaps result in distributed energy loss, whereby intermediate collisions are combined into a single, non-negligible collision. The lowest energy needed to recoil a target atom is represented by the displacement energy (E_d), which is commonly used as the predetermined energy transfer threshold, T_{min} . The usual range of values for E_d is 10–30 eV.

2.2 The Monte-Carlo Method

The Monte Carlo method is a statistical technique that allows for numerical solutions to complex problems through random sampling. Named after the famous Monte Carlo Casino in Monaco, this method relies on the law of large numbers, which states that as the number of trials increases, the experimental probability approaches the theoretical probability[54]. In the context of SRIM software, the Monte Carlo method is used to simulate the transport of ions through matter. The software generates random paths of ions based on probabilistic scattering events, and by simulating a large number of these paths, it can predict the average behavior of ions in the material. The Monte Carlo method is particularly useful in this context because it can handle the inherent randomness and complexity of ion transport, including energy loss, scattering angles, and nuclear reactions. By using a large number of simulations, the method can provide accurate predictions of ion range, energy distribution, and damage profiles in the target material.

2.3 Non-Ionizing Energy Loss (NIEL)

NIEL is a physical quantity describing the non-ionizing energy loss as the particle travels through the medium[55]. The amount of NIEL can be correlated to the amount of radiation damage and therefore to predict the lifetime of the detectors. To write the expression for NIEL, it is convenient to use the displacement damage function as:

$$D(T) = \sum_i \int_{T_{min}}^{T_{max}} Q(T)T \left(\frac{d\sigma}{dT} \right)_i dT \quad (2.5)$$

where,

T : Energy transferred to the recoil atom, T_{max} being maximum and T_{min} being minimum

$\frac{d\sigma}{dT}$: Differential partial cross section for a particle with energy T_0 to create a recoil atom with energy T in the i -th reaction

$Q(T)$: Partition factor giving the fraction of T that is going into further displacements

Now we can write the expression of NIEL as:

$$NIEL(T_0) = \frac{N_A}{A} D(T) \quad (2.6)$$

Where N_A : Avogadro number and A : atomic mass of the target atom. The unit of NIEL as $\text{MeV cm}^2 \text{g}^{-1}$ is used frequently.

2.4 Working Principle of a Solar Cell

SCs are devices that use the PV effect to capture solar energy and turn it into electrical power. When two materials are exposed to electromagnetic radiation, this phenomenon creates a potential difference at their junction. A substance that can absorb photon energy, raise an electron's energy level, and allow it to pass via external circuits is needed for the conversion process. The working principle of an SC is shown in Figure 2.2. Photons easily travel through the thin p-type layer and into the junction as light enters it, providing enough energy to form electron-hole pairs. The light disturbs the junction's thermal equilibrium, which makes it easier for free electrons to move from the depletion zone into the n-type portion of the junction. In a similar vein, depletion holes can readily reach the junction's p-type area. Nevertheless, the barrier potential of the junction prevents recently produced free electrons from passing through into the n-type region. Similar to the p-type area, newly created free holes that enter it have the same barrier potential as the p-n junction. The p-n junction functions as a little battery cell when the concentration of holes increases on the p-type region and that of electrons increases on the n-type region. The highly doped p^+ and n^+ layers act as HTL and ETL respectively. They help the extraction of the carriers and prevent recombination in the p-n junction.

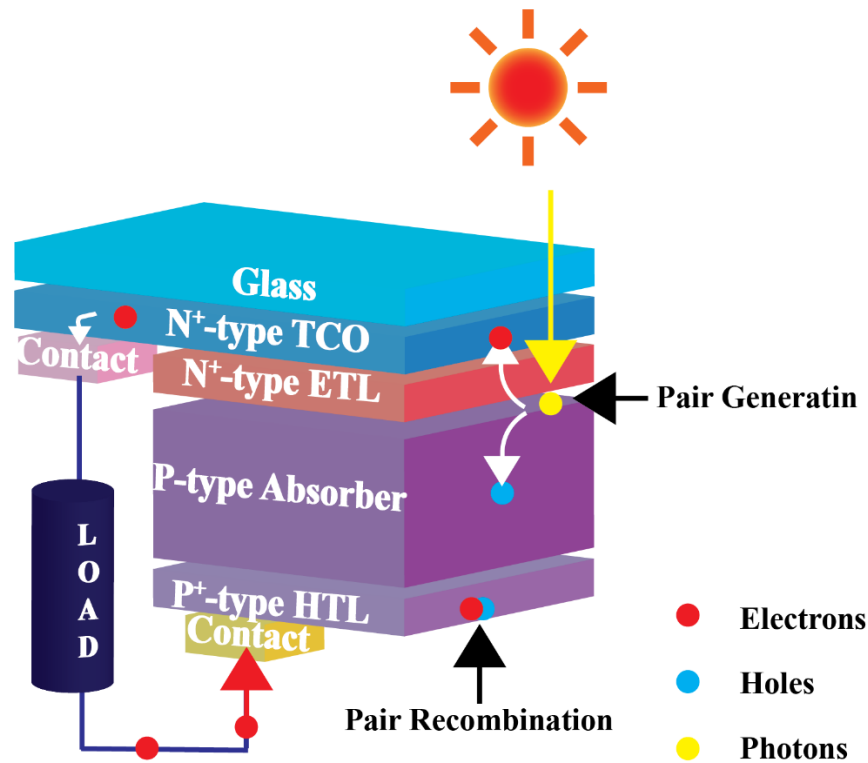


Figure 2.2: Working Principle of a p-n junction solar

2.5 Solar Cell Performance Parameters

The current density-voltage curve, or J-V curve, is a graph that shows how well a SC is working. On the y-axis, it displays the current density (J), and on the x-axis, the voltage (V). Usually, the curve is plotted in two different scenarios: one with light and the other with darkness. The voltage zero point, also known as the x-axis intercept under illumination, is known as the J_{sc} or I_{sc} . It stands for the highest amount of current that a shorted SC is capable of producing. It is precisely correlated with the intensity of the light. V_{oc} , or the y-axis intercept under illumination, is the point at which the current is zero. It shows the highest voltage that the SC is capable of producing when it is open circuited or disconnected from any load. J_{mp} is the current at which the SC produces the maximum amount of power. The voltage at which a SC produces its maximum power is known as V_{mp} . The power output of the SC is represented by the region bounded by the axes and the illuminated curve. The SC's efficiency increases with the size of this area. The SC functions like a diode in the dark, with current growing exponentially with voltage. The curve slopes downward when there is light because photocurrent is produced.

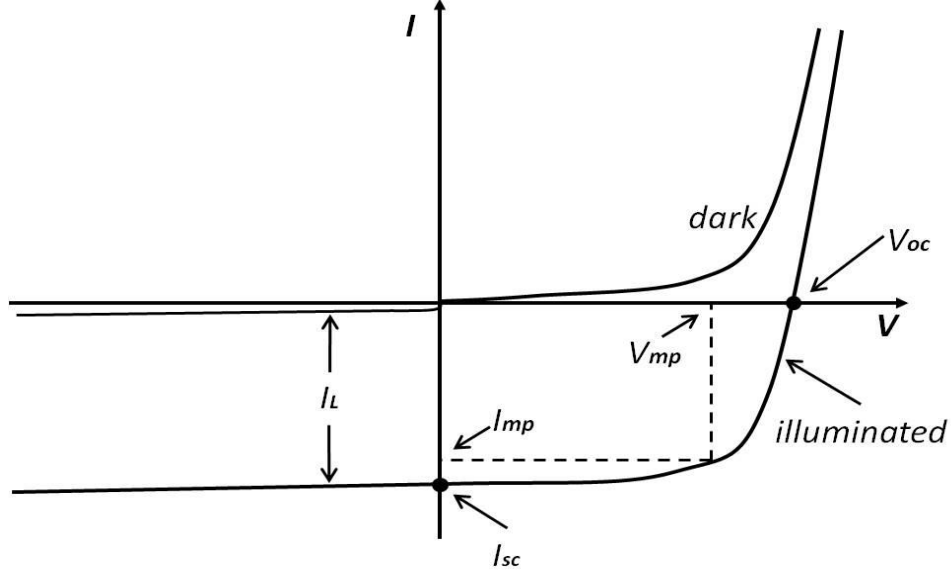


Figure 2.3: J-V characteristics curve of a solar cell

2.5.1 Open Circuit Voltage (V_{oc})

The maximum voltage that a SC is capable of producing when the current drops to zero is known as the V_{oc} . The forward bias on the SC resulting from the junctional bias of the SC with respect to the light-generated current is represented by the V_{oc} . Voltage between the terminals of the SC is used to determine V_{oc} when no load is connected to it. Temperature and manufacturing methods have an impact on this voltage, although light intensity and surface area exposure have a less significant effect. A single junction SC's typical voltage is between 0.5 and 0.6 volts. V_{oc} is a frequently used acronym for it. V_{oc} is typically determined by the photo-generated current and the saturation current of the SC. The saturation current, which can vary by orders of magnitude, is the most important factor, even if J_{ph} typically has a minimal effect. The saturation current density, or J_0 , is influenced by the SC's recombination rate. V_{oc} is therefore a measurement of the recombination rate of the apparatus. The equation of V_{oc} can be expressed as[56]:

$$V_{oc} = \frac{kT}{q} \ln \left(\frac{J_{sc}}{J_0} \right) \quad (2.7)$$

Where, K : Boltzmann constant, T : Temperature, q : Elementary charge, J_0 : Reverse saturation current.

2.5.2 Short Circuit Current Density (J_{sc})

One important factor affecting a SC's performance is its J_{sc} . When a SC is short-circuited, or when the voltage across it is zero, it can generate current density, or current per unit area. J_{sc} is the highest current density that a SC can produce when it is illuminated, to put it practically. It is directly correlated with light intensity, indicating that the short-circuit current density rises with increasing light intensity. The quantity

of photogenerated carriers that the SC gathers determines the value of J_{sc} . This in turn is dependent upon variables like the material's absorption coefficient, the absorber layer's thickness, and the carrier lifetime. The y-intercept of the curve under illumination represents J_{sc} in the J-V curve of a SC. Along with the V_{oc} and the FF, it is one of the main parameters that determines the PCE. The equation of J_{sc} can be stated as[57]:

$$J_{sc} = \int_0^{\infty} q \phi(\lambda) R(\lambda) d\lambda \quad (2.8)$$

Here, $\phi(\lambda)$: Generation rate of wavelength λ , $R(\lambda)$: Responsivity at wavelength λ , $d\lambda$: Differential wavelength element.

2.5.3 Fill Factor (FF)

The FF is a key parameter that characterizes the performance of a solar cell. The ratio of the maximum power from the SC to the product of the V_{oc} and the J_{sc} is known as the "squareness" of the J-V curve of the SC. It can be stated mathematically as follows[58]:

$$FF = \frac{V_{oc} J_{sc}}{V_{mp} J_{mp}} \times 100 \quad (2.9)$$

where V_{mp} : voltage at maximum power point, J_{mp} : Current at maximum power point, P_{in} : incident power.

One of the most important factors in assessing the SC's overall efficiency is its FF, which is always less than 1 (or less than 100%). A more "square" J-V curve, which is indicative of a higher-quality solar cell, is indicated by a greater FF.

2.5.4 Power Conversion Efficiency (PCE)

The ratio of the maximum produced power and the incident power is called conversion efficiency. Conversion efficiency is also defined as the ratio between SC energy output to input. The earth's radiation power is calculated to be about 1000 watts per square meter, so if the cell's illuminated surface area is A, the cumulative radiation energy on the cell would be 1000 watts. As a result, a SC's efficiency can be expressed as[58],

$$PCE = \frac{FF \times V_{oc} \times J_{sc}}{P_{in}} \quad (2.10)$$

Where, Pmax stands for maximum power, Pin stands for incident power.

2.5.5 External Quantum Efficiency (EQE)

The ratio between the number of carriers obtained by the SC to the number of photons of a given energy incident on the SC is known as External Quantum efficiency (EQE). The EQE of a given wavelength is unity if all lights of that wavelength are absorbed and the resulting minority carriers are captured. If the incident photons have energies below the bandgap, then the EQE is zero.

2.6 Machine Learning Methods

To analyze and interpret the outcome found from the results, two machine learning techniques were deployed in this research. These regression models are effective in analyzing the data by predicting the outcome first. A training set and a test set is randomly selected from the entire dataset to train the models first, then to predict the test dataset with a certain number of accuracy.

2.6.1 Random Forest Regression

Random Forest (RF) Regression is a supervised learning technique that uses ensemble learning [59]. It works by creating numerous decision trees and making the ultimate conclusion based on the majority of the trees. This strategy makes use of the 'wisdom of crowds'. The process starts by generating a 'forest', which is a set of decision trees. Each tree is built from a portion of the data that is randomly picked and replaced; a process known as bootstrapping. Furthermore, for each node in the tree, a random subset of features is chosen for splitting. This randomization serves to strengthen the model by lowering the correlation between the trees, which improves overall performance. Each decision tree in the forest produces an independent forecast, and the final prediction is produced by averaging all of the trees' predictions in the case of regression. This technique frequently produces greater prediction performance than a single decision tree. Figure 2.4 provides a schematic diagram of the working procedures of RF regression.

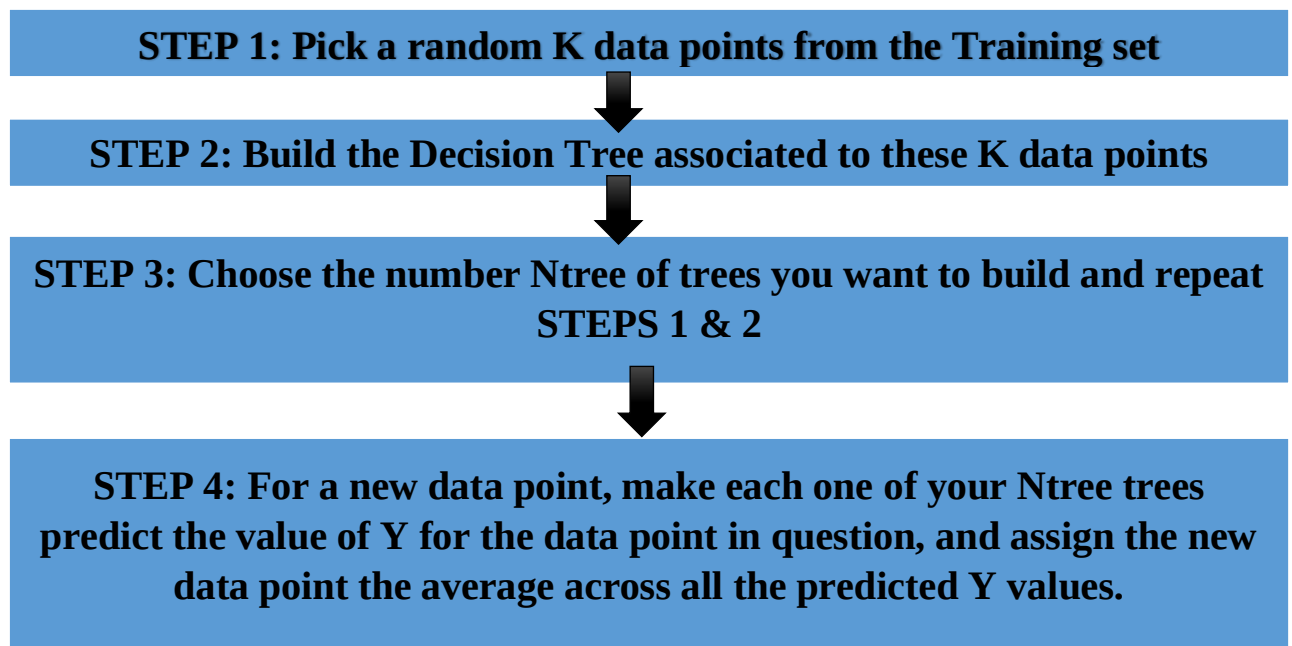


Figure 2.4: Working Procedures of RF Regression

2.6.2 XGBoost Regression

XGBoost (XGB), short for eXtreme Gradient Boosting, is an efficient and effective open-source implementation of the gradient boosting algorithm. It's known for its efficiency and effectiveness in predictive modeling, particularly on structured or tabular datasets. The XGB algorithm operates by constructing multiple decision trees and then combining their predictions[60]. Each tree is added one at a time, and each new tree helps to correct the prediction errors made by the ensemble of previously built trees. This is a type of ensemble machine learning model referred to as boosting. XGB uses any arbitrary differentiable loss function and gradient descent optimization algorithm. The most common loss functions in XGB for regression problems is `reg:linear`, and that for binary classification is `reg:logistics`. The objective function of XGB contains both a loss function and a regularization term. The loss function measures the difference between actual values and predicted values, i.e., how far the model results are from the real values. The regularization term helps to control the complexity of the model, preventing overfitting. XGB has gained popularity due to its execution speed and model performance. It often outperforms other algorithms on classification and regression predictive modeling problems. Figure 2.5 provides a schematic diagram of the working procedures of XGB regression.

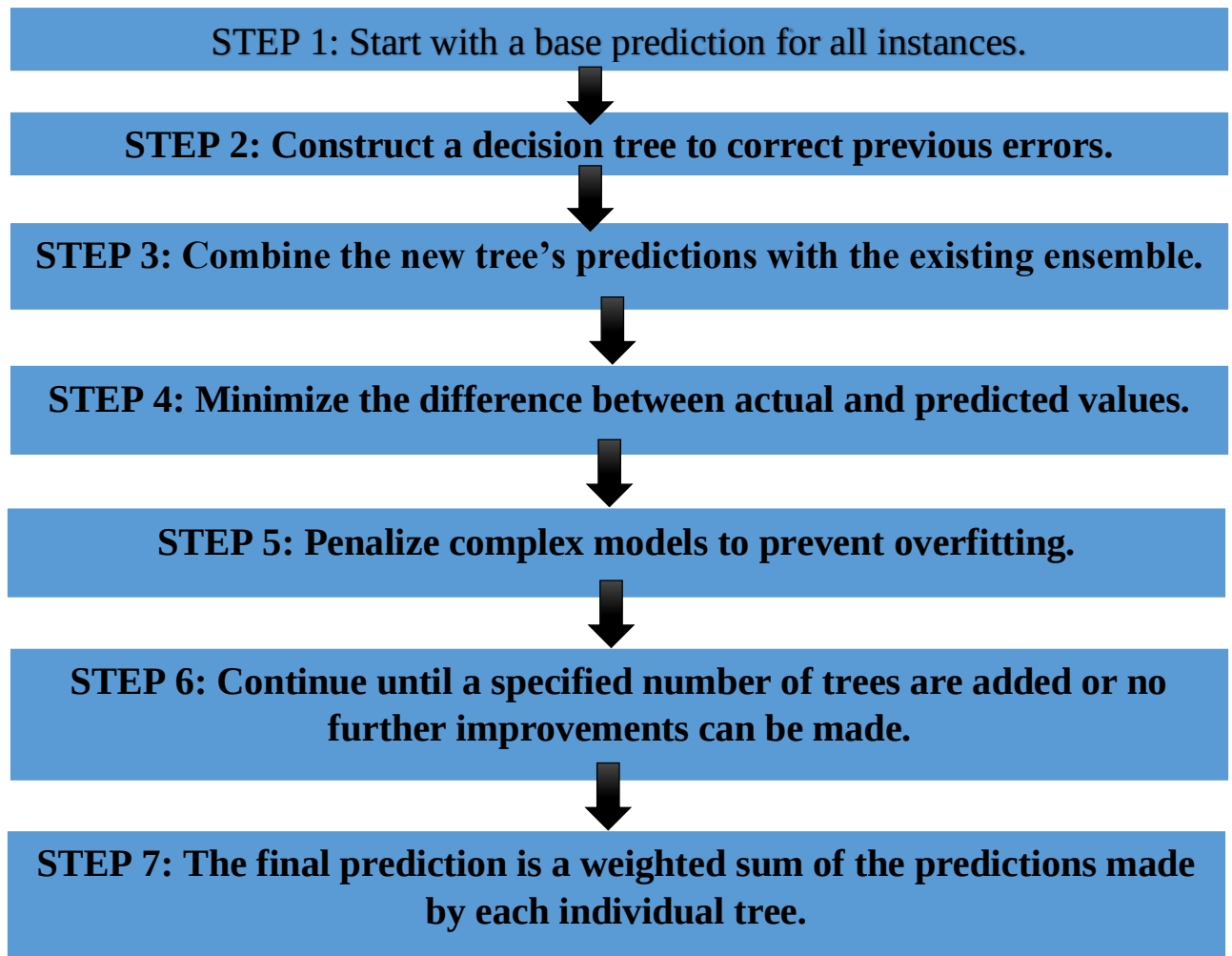


Figure 2.5: Working Procedures of XGB Regression

2.6.3 SHapley Additive exPlanations (SHAP) values

SHAP (SHapley Additive exPlanations) values are a method used in machine learning to explain the output of a model by attributing the contribution of each feature to the final prediction[61]. The concept of SHAP values is rooted in cooperative game theory, specifically the Shapley value, which calculates the contribution of each player to the overall outcome of a coalition game. In the context of machine learning, SHAP values provide a way to interpret the importance of each feature in predicting the model's output for a specific instance. They quantify the impact of each feature on the prediction by considering all possible combinations of features and their effects on the model's output.

Chapter Three

3 Methodology and Simulation Procedures

3.1 NIEL Calculation from the SR-NIEL Website

Protons & Ions NIEL Calculator

Incident Particle: 1:H		
Proton and Ion Model:	Hadron + Coulomb	
Hadronic Contribution:	No Scaling	
Target Materials		
Target Selection:	User Defined	
N° Elements:	2	
Target Material Z	Stoichiometric Index or Element Fraction	Displacement Threshold Energy [eV] *
42:Mo	1	25
34:Se	2	25
NIEL Energy ranges		
Minimum Energy:	0.0001 [MeV]	
Maximum Energy:	10000 [MeV]	
Additional Energies (optional):	[MeV]	
Dose Imparted for		
Particle Fluence:	1 [cm ⁻²]	
CALCULATE		

Figure 3.1: NIEL calculation input panel

Figure 3.1 shows a web-based tool titled “Protons & Ions NIEL Calculator” from the SR-NIEL website. To calculate the NIEL for proton radiation, we have to select H as the incident particle. The proton and ion model was set to Hadron + Coulomb for more realistic calculations. The hadronic contribution comes from interactions involving particles that are affected by the strong nuclear force, such as protons and neutrons. The displacement threshold energy (E_d) is the minimum energy required to displace an atom from its lattice site in the material. When “no scaling” is selected, the hadronic contribution to NIEL is calculated as a constant, independent of the displacement threshold energy (E_d). This behavior is consistent with the results obtained for neutron damage functions with MeV neutrons (up to 20 MeV) by means of the NJOY-2012 code [55]. In the target selection section, we select the elements that make up the TMDC compounds. We then set the range of the energy of the protons for which NIEL will be calculated. The term particle fluence refers to the number of radiant-energy particles that are incident on a surface per unit area. We kept it as default value 1.

3.2 Solar Cell Device Construction and Simulation

Numerous simulation software options are available for PV device design and evaluation. Among these options are wxAMPS, AFORS-HET, ATLAS, Sentaurus TCAD, AMPS-1D, and SCPAS-1D[62]. Out of all of them, SCPAS-1D is a very good choice for modeling and simulating different solar cell architectures versus adjustable factors such as metal contacts, operating temperature, recombination process, series and shunt resistance, and calculations for single and batch use. A modeling program called SCAPS-1D allows for the grading of nearly all pertinent parameters for up to seven semiconductor layers[63]. Mark Burgelman of the University of Gent in Belgium is the one developing it. To replicate various lighting situations, the software includes a range of conventional illumination condition presets (e.g., AM0, AM1.5D, AM1.5G, monochromatic, etc.). However, the initial configuration needs to be as accurate as possible to yield the greatest outcome.

3.2.1 Working Procedures of SCAPS-1D

SCAPS-1D (Solar Cell Capacitance Simulator in One Dimension) is a one-dimensional solar cell simulation program developed at the Department of Electronics and Information Systems (ELIS) of the University of Gent, Belgium¹. It’s designed to simulate thin-film solar cells, but recent developments have made it applicable to crystalline solar cells (Si and GaAs family) and amorphous cells (a-Si and micromorphous Si)[64]. We start by defining the structure of the solar cell you want to simulate. This includes specifying the semiconductor layers, their material properties, and any grading of parameters. Next, we set the operating conditions for the simulation. This includes the illumination conditions (spectrum and intensity), the working point for calculations (voltage, frequency, temperature), and any bias light or voltage. Once the setup of the solar cell structure and operating conditions is complete, we can run the simulation. SCAPS-1D will calculate the energy bands, concentrations, and currents at the given working point. After the

simulation is complete, SCAPS-1D provides various outputs for analysis. This includes J-V characteristics, AC characteristics (C and G as a function of V and/or f), spectral response, and more.

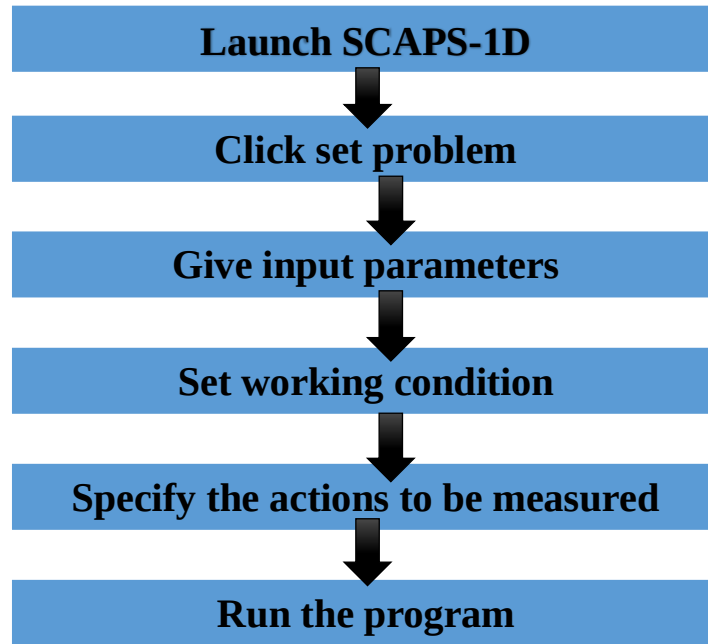


Figure 3.2: Working Procedures of SCAPS-1D

3.2.2 The Governing Equations of SCAPS-1D

In order to perform calculations, SCAPS-1D solves the differential equation of continuity (3.1), equation of Poisson (3.2), and carrier diffusion equation (3.3)[65].

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{v}) = G - R \quad (3.1)$$

$$\nabla^2 \phi = -\frac{\rho}{\varepsilon} \quad (3.2)$$

$$\frac{\partial n}{\partial t} = \nabla \cdot (D\nabla n) + G - R \quad (3.3)$$

Where, n : Carrier concentration, $\mathbf{v}$: Velocity vector, G : Generation rate of carriers, R : Recombination rate of carriers, ρ : Charge density, ε : Permittivity, D : Carrier diffusion constant. The primary performance parameters of SC devices are V_{oc} , J_{sc} , FF and PCE. We have discussed about them in chapter 2.

3.2.3 Device Structure Schematics

Before calculation, we need to construct the device and provide proper simulation environments. In this study, we focused on four different TMDC absorber materials (MoS₂, MoSe₂, WS₂, WSe₂). These materials

are the bulk of the device. We also have HTL and ETL materials (Spiro-OMeTAD, In_2Te_3 , TiO_2 , CdS) as no more than $0.2 \mu\text{m}$ thick layers at the front and back of the absorber layers. As discussed in chapter 1, to obtain a high performance, these transport layers are necessary and frequently used.

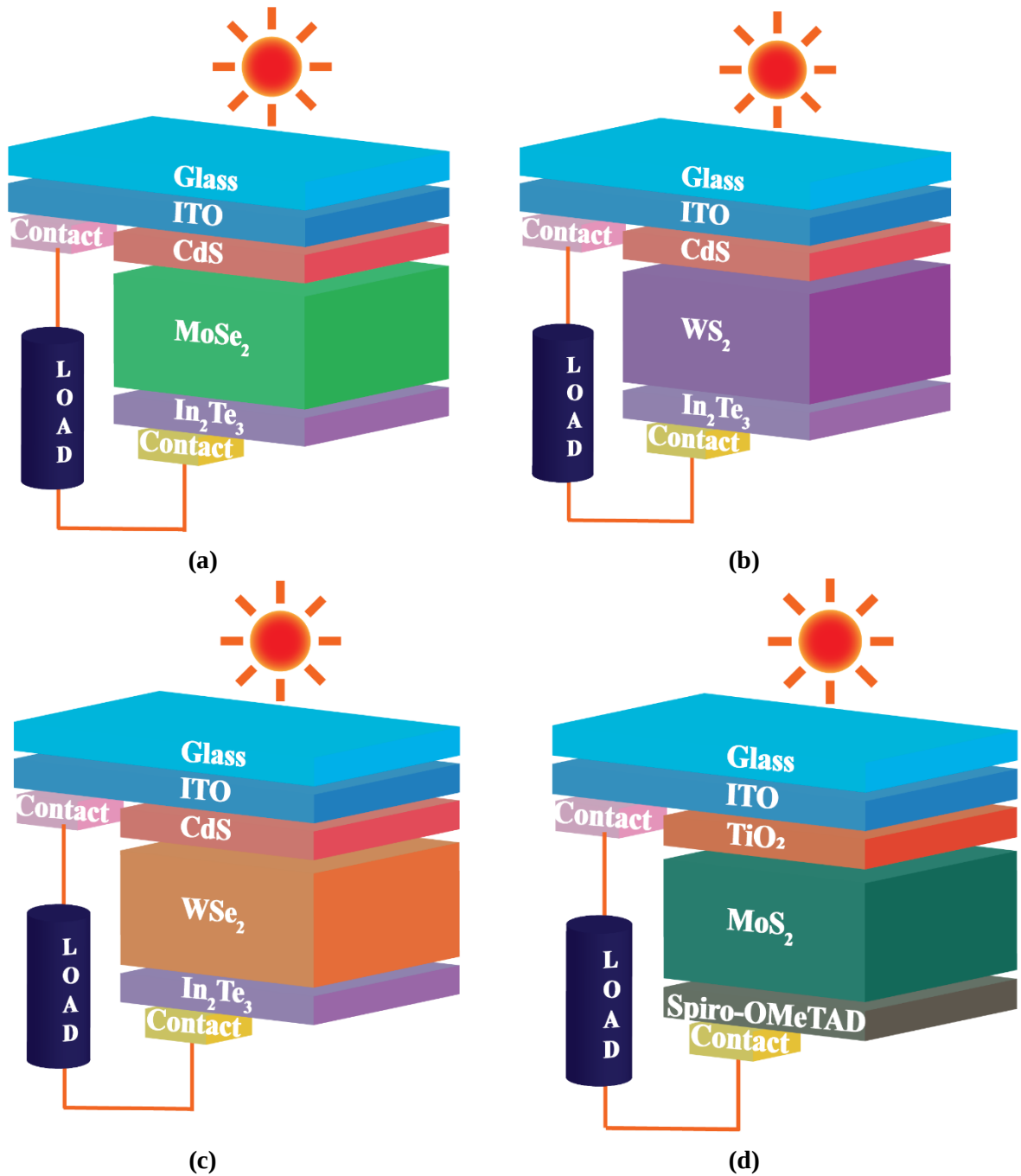


Figure 3.3: Schematic structure of the four SC devices

We call the four devices as:

Figure 3.3(a) ITO/CdS/MoSe₂/In₂Te₃,

Figure 3.3(b) ITO/CdS/WS₂/In₂Te₃,

Figure 3.3(c) ITO/CdS/WSe₂/In₂Te₃, and

Figure 3.3(d) ITO/TiO₂/MoS₂/Spiro-OMeTAD.

3.2.4 Device Input Parameters

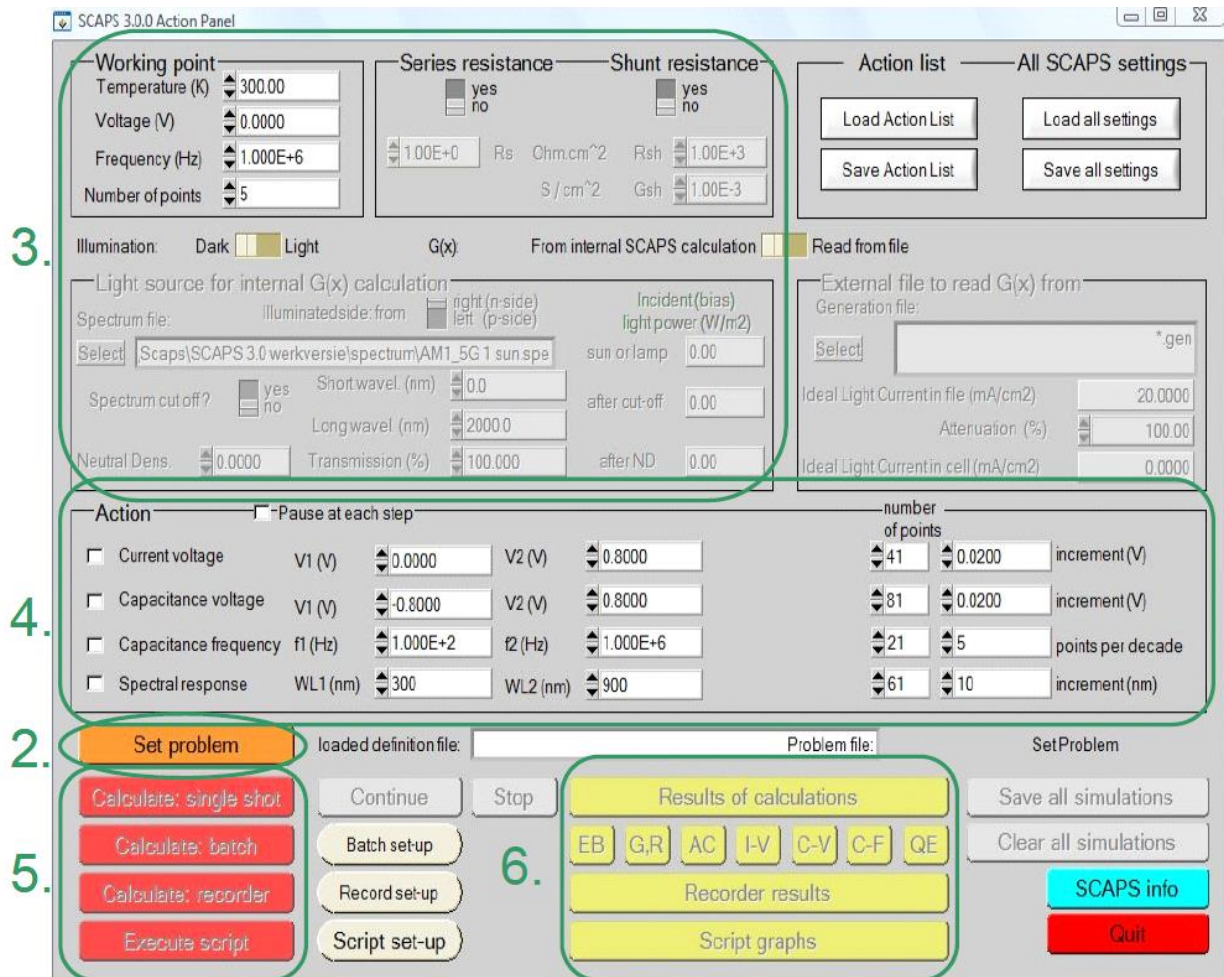


Figure 3.4: Starting panel of SCAPS (1); (2) To define the problem (geometry, materials, all properties); (3) To indicate the circumstances in which we want to do the simulation; (4) To indicate what to calculate; (5) To start the calculations; (6) To display the simulated curves[63].

The starting window of the SCAPS-1D is shown in Figure 3.4. We have used standard AM 1.5G 1sun illumination condition at 1000 W/m² incident sunlight. The temperature condition was set to 300K. Upon pressing ‘set problem’, a second panel will appear like Figure 3.5. Here we add new layers by pressing ‘add layer’.

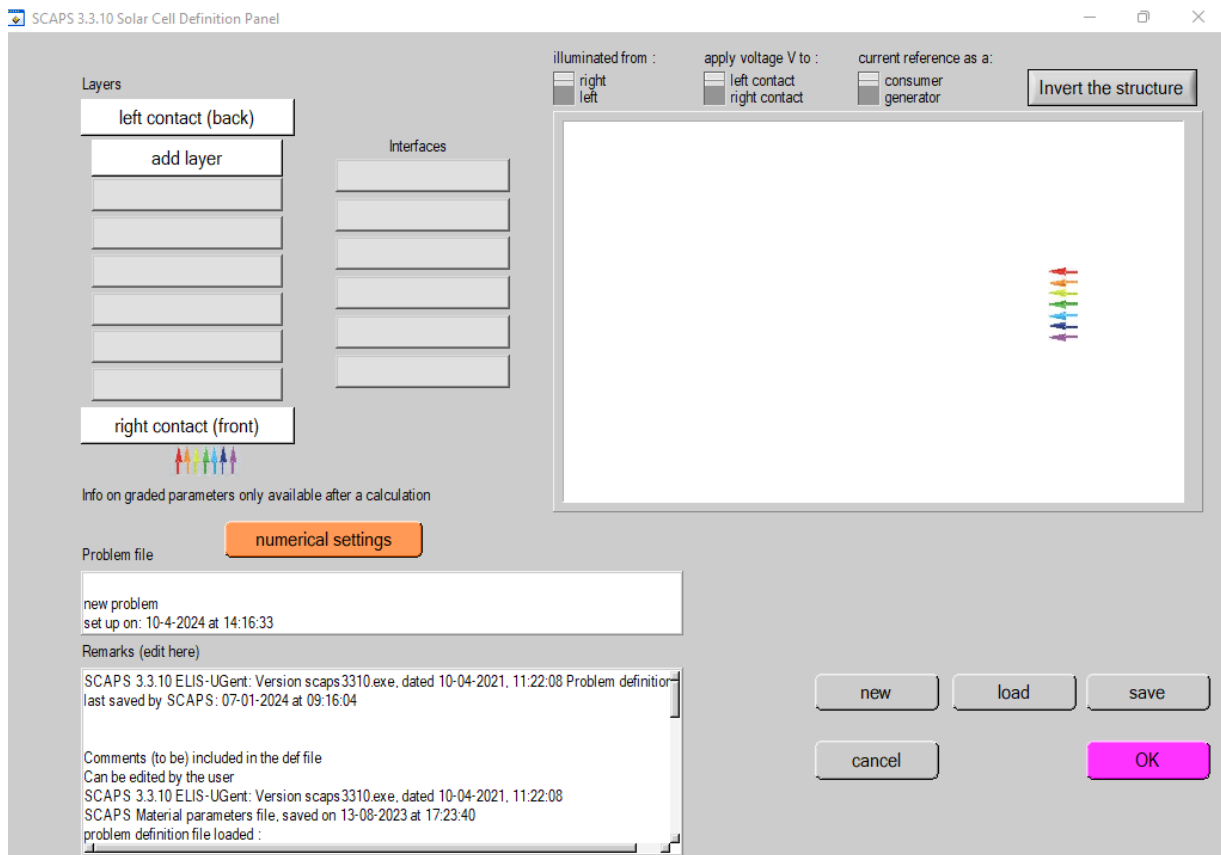


Figure 3.5: Solar Cell Definition Panel

The ‘add layer’ button leads to another panel called ‘Layer Properties Panel’, as shown in Figure 3.6. We must input accurate experimental and theoretical data of our absorber, HTL and ETL layer in this panel, one layer at a time. The layer properties are tabulated in Table 3.1 and the interface defect properties are tabulated in Table 3.2.

SCAPS 3.3.10 Layer Properties Panel

LAYER 1 layer 1

thickness (μm) 2.000

uniform pure A (y=0) 0.000

The layer is pure A: y = 0, uniform

Semiconductor Property P of the pure material pure A (y = 0)

bandgap (eV)	1.200
electron affinity (eV)	4.500
dielectric permittivity (relative)	10.000
CB effective density of states ($1/\text{cm}^3$)	$1.000\text{E}+19$
VB effective density of states ($1/\text{cm}^3$)	$1.000\text{E}+19$
electron thermal velocity (cm/s)	$1.000\text{E}+7$
hole thermal velocity (cm/s)	$1.000\text{E}+7$
electron mobility (cm^2/Vs)	$5.000\text{E}+1$
hole mobility (cm^2/Vs)	$5.000\text{E}+1$
☐ Allow Tunneling	
effective mass of electrons	$1.000\text{E}+0$
effective mass of holes	$1.000\text{E}+0$

no ND grading (uniform)

shallow uniform donor density ND ($1/\text{cm}^3$) $1.000\text{E}+15$

no NA grading (uniform)

shallow uniform acceptor density NA ($1/\text{cm}^3$) $1.000\text{E}+15$

Absorption interpolation model

alpha pure A material (y=0)

from file ☐ from model ☐

Set absorption model

show

save

List of absorption submodels present:
sqrt(hv-Eg) law (SCAPS traditional)

Recombination model

Band to band recombination

Radiative recombination coefficient (cm^3/s)	$0.000\text{E}+0$
Auger electron capture coefficient (cm^6/s)	$0.000\text{E}+0$
Auger hole capture coefficient (cm^6/s)	$0.000\text{E}+0$

Recombination at defects: Summary

Add a Defect 1

(no metastable configuration possible)

Add cancel Load Material Save Material

Figure 3.6: Layer Properties Panel

Table 3.1: Material properties used for simulation

Parameters (unit)	ITO[35]	MoS ₂ [35]	MoSe ₂ [36]	WS ₂ [37]	WSe ₂ [38]	Spiro-OMeTAD[66]	CdS[36]	TiO ₂ [66]	In ₂ Te ₃ [35]
Thickness (um)	0.05	0.8	1.3	1.2	1.2	0.05	0.05	0.05	0.05
Bandgap (eV)	3.6	1.23	1.41	1.29	1.19	3	2.4	3.6	2.1
Electron Affinity (eV)	4	4.2	4.4	4.05	4.5	2.2	4.2	1.7	3.47
Dielectric Permittivity (relative)	9	4	14.9	13.6	13.8	3	10	10	12
CB effective density of states (1/cm ³)	2.20×10^{18}	7.50×10^{17}	2.20×10^{18}	2.20×10^{18}	8.30×10^{18}	2.20×10^{18}	2.20×10^{18}	2.20×10^{19}	1.00×10^{16}
VB effective density of states (1/cm ³)	1.80×10^{19}	1.80×10^{18}	1.80×10^{18}	1.80×10^{19}	1.60×10^{19}	1.80×10^{19}	1.80×10^{19}	1.80×10^{18}	1.00×10^{17}
Electron Thermal Velocity (cm/s)	1.0×10^7	1.0×10^7	1.0×10^7	1.0×10^7	1.0×10^7	1.0×10^7	1.0×10^7	1.0×10^7	1.0×10^7
Hole Thermal velocity (cm/s)	1.0×10^7	1.0×10^7	1.0×10^7	1.0×10^7	1.0×10^7	1.0×10^7	1.0×10^7	1.0×10^7	1.0×10^7
Electron Mobility (cm ² /Vs)	100	100	1.0×10^2	100	100	2.10×10^{-3}	3.50×10^2	1.0×10^2	1.0×10^3
Hole Mobility (cm ² /Vs)	25	150	5.00×10^1	100	500	2.16×10^{-3}	2.50×10^1	2.50×10^1	2.00×10^2
Donor Density ND (1/cm ³)	1.0×10^{18}	0	0.00	0	0	0.00	1.0×10^{18}	0.00	0.00
Acceptor Density NA (1/cm ³)	0.00	1×10^{15}	1.0×10^{16}	1.0×10^{17}	1.0×10^{16}	1.0×10^{18}	0.00	1.0×10^{18}	1.0×10^{17}
Type of Defect	neutral	Single donor	Single donor	Single donor	Single donor	Single donor	Single acceptor	Neutral	Single donor
Energetic Distribution	single	Gaussian	Gaussian	Gaussian	Gaussian	Gaussian	Gaussian	Single	Gaussian
Capture Cross Section of Electrons (1/cm ²)	1.0×10^{-15}	1.0×10^{-15}	1.0×10^{-15}	1.0×10^{-15}	1.0×10^{-15}	1.0×10^{-15}	1.0×10^{-15}	1.0×10^{-15}	1.0×10^{-15}
Capture Cross Section of Holes (1/cm ²)	1.0×10^{-15}	1.0×10^{-17}	1.0×10^{-17}	1.0×10^{-17}	1.0×10^{-17}	1.0×10^{-15}	1.0×10^{-15}	1.0×10^{-15}	1.0×10^{-17}
Defect Density (1/cm ³)	1.0×10^{15}	1.0×10^{15}	1.0×10^{15}	1.0×10^{15}	1.0×10^{15}	1.0×10^{15}	1.0×10^{15}	1.0×10^{15}	1.0×10^{14}

Table 3.2: Interface defect parameters

Parameters (unit)	Values ^a
Defect type	Neutral
Energetic Distribution	Single
Capture Cross Section of Electrons (1/cm ²)	1.0×10^{-19}
Capture Cross Section of Holes (1/cm ²)	1.0×10^{-19}
Defect Density (1/cm ²)	1.0×10^{10}
^a Values applied to the interfaces: ITO/CdS, CdS/MoSe ₂ , CdS/WS ₂ , CdS/WSe ₂ , TiO ₂ /MoS ₂ , MoS ₂ /In ₂ Te ₃ , WS ₂ /In ₂ Te ₃ , WSe ₂ /In ₂ Te ₃ , MoS ₂ /Spiro-OMeTAD	

3.3 TRIM Calculation Procedures

Similar to SCAPS-1D, TRIM calculation requires input data of the layers from the user. This includes layer thickness (width), layer density, elements information (name, atomic number, atom stoichiometry in the crystal structure etc.), ion data (ion name, energy, angle of incidence, total number of ions to be calculated). The input panel is shown in Figure 3.7. The input parameters of the materials are presented in Table 3.3.

The screenshot shows the TRIM Setup Window with the following sections:

- Read Me**: Buttons for TRIM Demo, Restore Last TRIM Data, and ION DATA.
- TRIM (Setup Window)**: Type of TRIM Calculation (DAMAGE), Basic Plots (Ion Distribution and Quick Calculation of Damage), and Ion Distribution with Recoils projected on Y-Plane.
- ION DATA**: Fields for Symbol (PT), Name of Element (H), Atomic Number (1), Mass (amu) (1.008), Energy (keV) (10), and Angle of Incidence (?).
- TARGET DATA**: Target Layers section with Add New Layer button and a table for Layer Name, Width, Density, Compound, Corr, Gas, Symbol, Name, Atomic Number, Weight, Atom, Stoich or %, Damage (eV) Disp, Latt, Surf.
- Input Elements to Layer**: Add New Element to Layer button and a table for Symbol, Name, Atomic Number, Weight, Atom, Stoich or %, Damage (eV) Disp, Latt, Surf.
- Special Parameters**: Name of Calculation (H (10) into Layer 1), Stopping Power Version (SRIM-2008), AutoSave at Ion # (10000), Total Number of Ions (99999), Random Number Seed, Plotting Window Depths (Min 0, Max 10000), Output Disk Files (Ion Ranges, Backscattered Ions, Transmitted Ions/Recoils, Sputtered Atoms, Collision Details), Special "XYZ File" Increment (eV) (0), Resume saved TRIM calc. (checked), Save Input & Run TRIM, Clear All, Calculate Quick Range Table, Main Menu, Problem Solving, and Quit buttons.

Figure 3.7: Input panel of the TRIM software

Pressing ‘Save Input & Run TRIM’ will initiate the calculation. In the next window, the calculation will continue to run until all the incident ions are calculated (10000 in our case). Different data and plots can be activated and monitored from this window, as shown in Figure 3.8. The process can be paused and resumed, and some parameters can be changed while in paused state.

Table 3.3: TRIM input parameters for the four devices

Layer Name	Width (Angstrom)	Density (g/cm ³)	References
ITO	500	6.8	[67]–[69]
CdS	500	4.826	[70]–[72]
MoSe ₂	13000	6.9	[73]–[75]
In ₂ Te ₃	500	6.67	[76], [77]
WS ₂	12000	7.83	[78], [79]
WSe ₂	9000	9.66	[80], [81]
MoS ₂	8000	4.78	[82], [83]
TiO ₂	500	6.8	[84], [85]
Spiro-OMeTAD	500	1.26	[86]

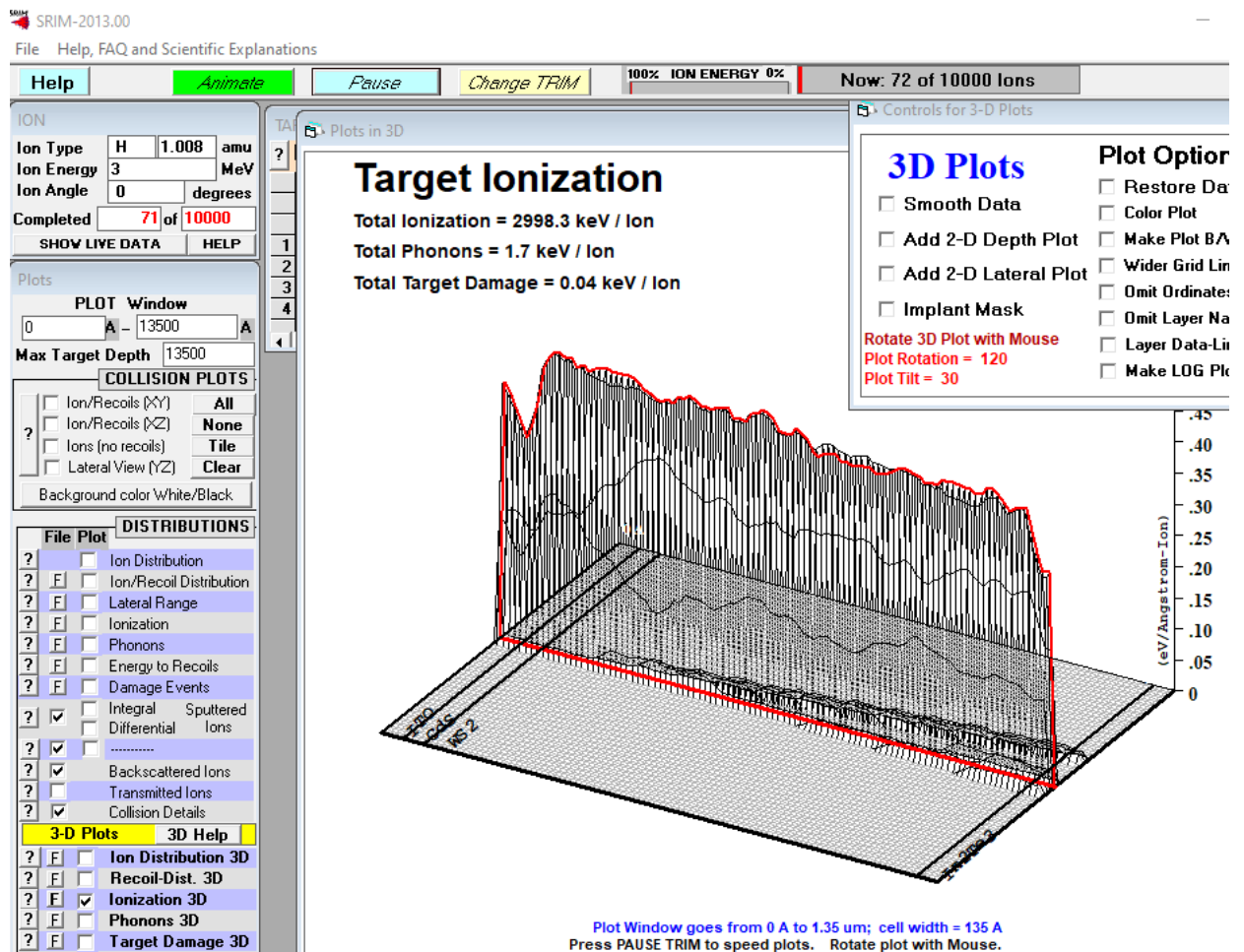


Figure 3.8: TRIM window while the calculation is active

After the calculation is complete, the desired data can be saved and retrieved for analysis.

Chapter Four

4 Results and Discussions

4.1 NIEL of the Absorber Materials

Figure 4.1 illustrates the NIEL for the four different TMDC materials: MoSe₂, WS₂, WSe₂, and MoS₂. From the graph, it appears that all four materials exhibit a peak in NIEL between approximately 2×10^{-4} to 10×10^{-1} MeV proton energies. This suggests that these materials absorb the most energy from protons within this energy range. Beyond this range, the NIEL decreases, indicating that the materials absorb less energy from protons with higher energies. Considering the thin ETL materials before these TMDC absorbers, we have chosen 0.15 MeV proton energy for the damage calculation. We also analyzed higher energy (3MeV) protons impact on the absorber layer to check the effects.

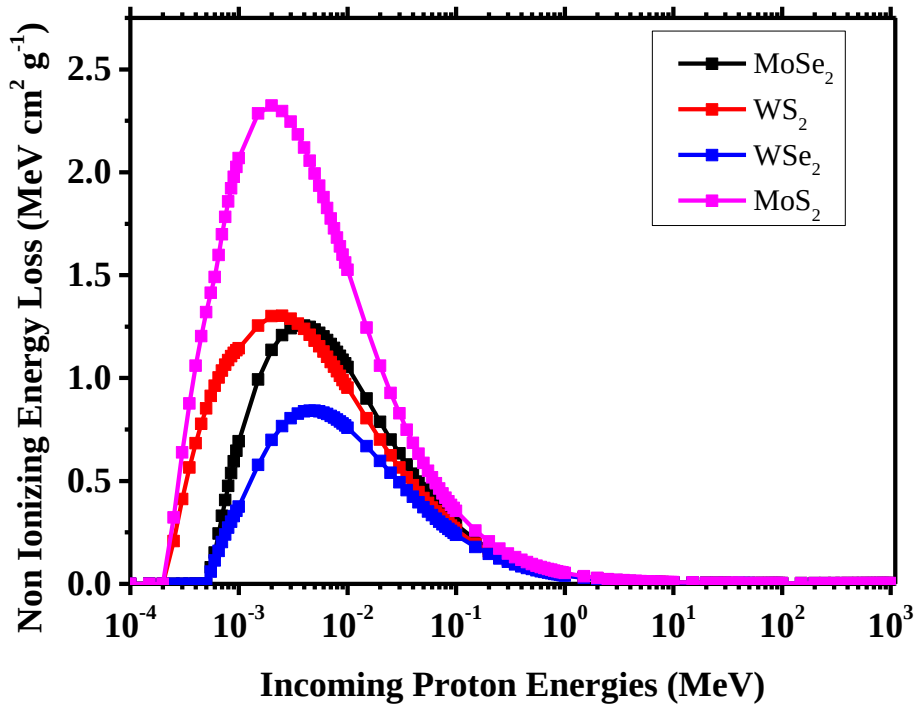


Figure 4.1: NIEL for incident proton at different energies

4.2 Initial Characteristics and PV Performances of the Selected SCs

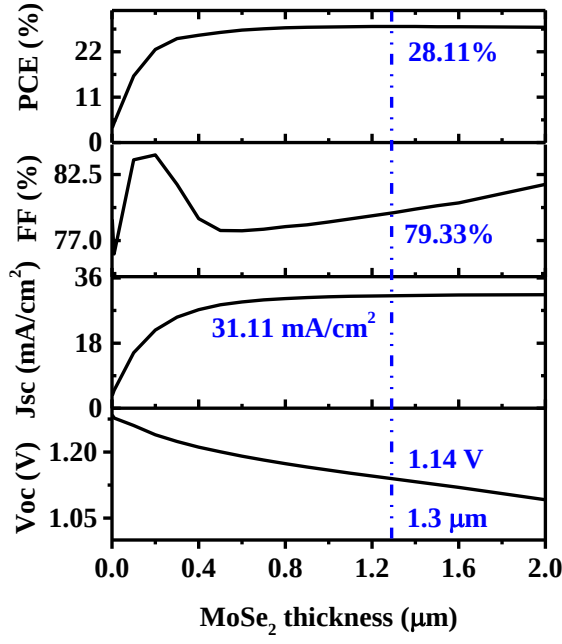
The PV performances of the four devices were measured under normal earth condition and 300K temperature. To find the optimized device performance, the optimal thickness of the absorber material should be identified. After finding the optimal thickness, the rest of the analysis results were followed.

4.2.1 Effect of Absorber Thickness on the PV Performance: Thickness Optimization

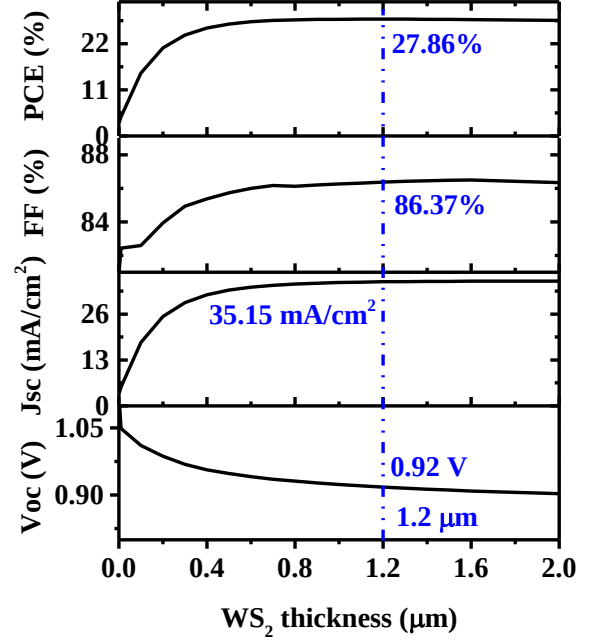
In SCs, the thickness of the absorber layer is an important factor that can greatly affect the cell's performance [87], [88]. The collection of produced carriers and the absorption of light are influenced by the thickness of the absorber layer. A coating that is too thin might not be able to absorb light well. On the other hand, the produced carriers could recombine before they can be gathered if the layer is overly thick [88].

Figure 4.2 explores the variation of photovoltaic (PV) performance with changing absorber thickness for four different materials: (a) MoSe₂, (b) WS₂, (c) WSe₂, and (d) MoS₂. In Figure 4.2(a) for MoSe₂, at a thickness of 0.0001 μm , V_{oc} is 1.27 V, J_{sc} is 7 mA/cm², FF is 76%, and PCE is 4%. As the thickness increases, FF reaches its highest value of 83% at 0.2 μm , with PCE exceeding 23%. However, V_{oc} gradually decreases while other parameters increase. At the optimal thickness of 1.3 μm , V_{oc} is 1.14 V, J_{sc} is 31.11 mA/cm², FF is 79.33%, and PCE is 28.11%. For WS₂ in Figure 4.2(b), V_{oc} reduces while other parameters increase, reaching saturation at about 0.4 μm . At 1.2 μm thickness, V_{oc} is 0.92 V, J_{sc} is 35.15 mA/cm², FF is 86.37%, and PCE is 27.86%.

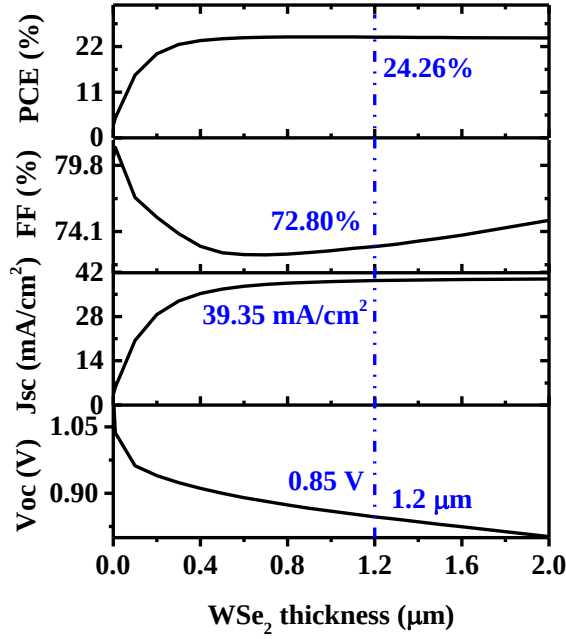
Similarly, in Figure 4.2(c) for WSe₂, V_{oc} reduces while other parameters increase. FF reduces to 71% at 0.5 μm thickness, then slowly increases. At 1.2 μm thickness, V_{oc} is 0.85 V, J_{sc} is 39.35 mA/cm², FF is 72.8%, and PCE is 24.26%. In Figure 4.2(d) for MoS₂, V_{oc} and FF increase to 1.05 V and 83%, respectively, at 0.2 μm thickness, then start to decrease. J_{sc} and PCE increase from 0.0001 μm thickness and reach saturation at 0.4 μm . At 0.8 μm thickness, V_{oc} is 1.0 V, J_{sc} is 34.54 mA/cm², FF is 81.07%, and PCE is 28.16%.



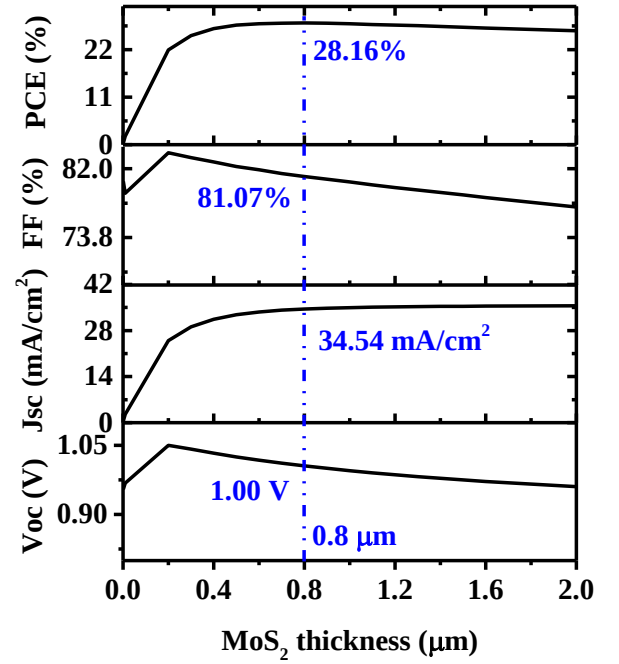
(a)



(b)



(c)



(d)

Figure 4.2: Variation of PV performance with changing absorber thickness for (a) MoSe₂, (b) WS₂, (c) WSe₂, (d) MoS₂

4.2.2 J-V Characteristics of the SCs

Figure 4.3 presents the J-V (current-voltage) curves of four different SCs fabricated with WSe₂, WS₂, MoS₂, and MoSe₂ absorber materials. For WSe₂, the J-V curve starts from 40 mA/cm² and maintains this current density until reaching 0.65 V. Beyond this voltage, the current density gradually reduces until it reaches zero at 0.85 V. Both WS₂ and MoS₂ exhibit similar J-V curves, starting from 35 mA/cm² and maintaining this current density until 0.88 V. Subsequently, the current density decreases rapidly, reaching zero shortly after. MoSe₂'s J-V curve starts from a slightly lower current density of 31 mA/cm² and maintains it until reaching a higher voltage of 0.98 V. The current density then decreases to zero at 1.15 V.

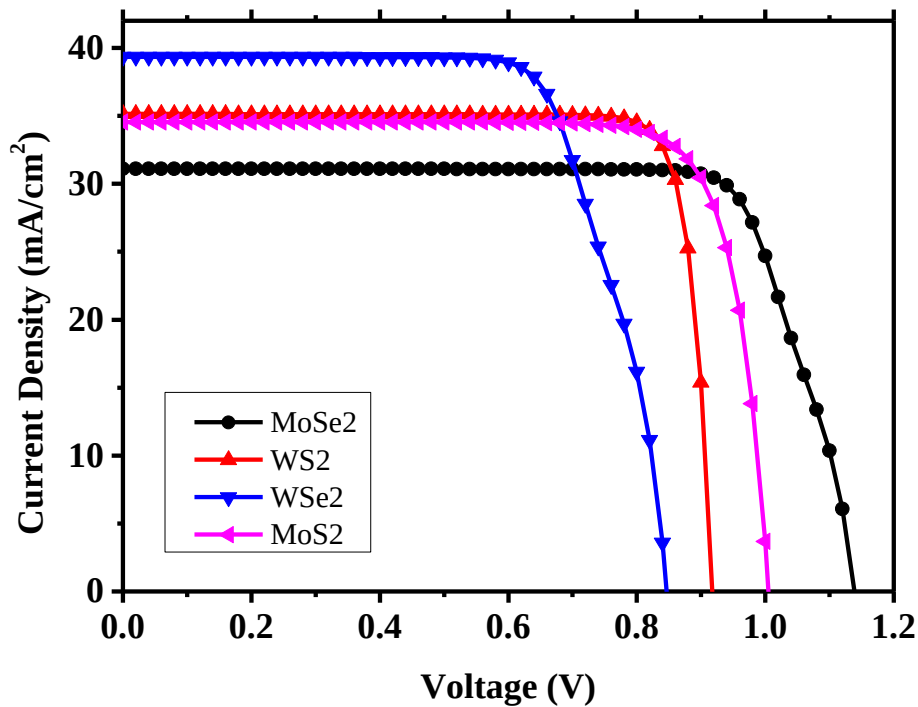


Figure 4.3: J-V curve of the four SCs

Overall, WSe₂ and MoSe₂ exhibit relatively higher initial current densities compared to WS₂ and MoS₂. However, MoSe₂ requires a higher voltage to maintain this current density compared to WSe₂. WS₂ and MoS₂, on the other hand, have similar behavior in terms of current density and voltage characteristics. Additionally, all four absorber materials show a decline in current density beyond a certain voltage threshold, with MoS₂ and WS₂ reaching zero current density more rapidly compared to WSe₂ and MoSe₂.

4.2.3 EQE of the SCs

Figure 4.4 displays the EQE (external quantum efficiency) curves of four different solar cells (SCs) fabricated with WSe₂, WS₂, MoS₂, and MoSe₂ absorber materials. In the wavelength range from 300 to 350 nm, all four absorber materials exhibit high EQE values, ranging from around 80% to 100%. This indicates efficient absorption of photons within this spectral range. Up to 800 nm wavelength, all absorbers maintain

near 100% EQE, suggesting effective utilization of photons across a broad range of wavelengths. However, specific drop-offs in EQE are observed at certain wavelengths for each material. At 880 nm, the EQE of MoSe₂ drops to zero. At 975 nm, the EQE of WS₂ and MoS₂ drops to zero. At 1100 nm, the EQE of WSe₂ drops to zero.

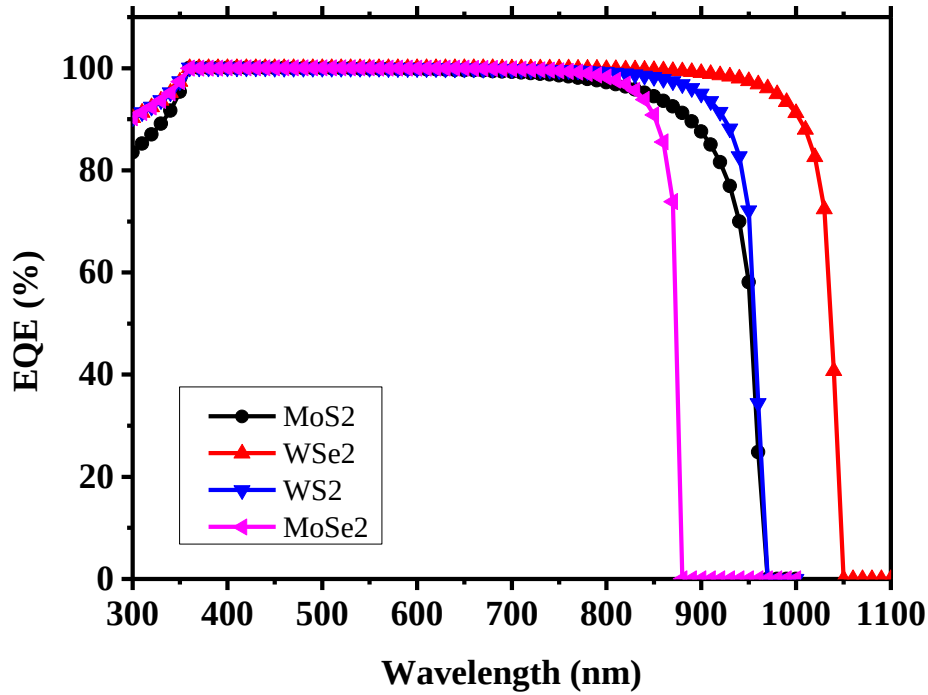


Figure 4.4: EQE curve of the four SCs

The EQE curves demonstrate that all four absorber materials are capable of efficient photon absorption and conversion over a wide spectral range, with some variations in performance at specific wavelengths. These variations could be attributed to differences in the bandgap energies and electronic properties of the materials.

4.2.4 Optimized Performance of the SCs

Before applying the proton radiation, the PV performances of the four devices was measured under normal circumstances (1000 W/m² AM 1.5 illumination, 300K temperature). The results are illustrated in Figure 4.5 and the values are tabulated in Table 4.1.

The MoSe₂ device has a comparatively high V_{oc} of 1.14 V, which suggests effective charge carrier separation and collection from photogenerated energy. Under short circuit conditions, a considerable amount of current is suggested by the J_{sc} value of 31.11 mA/cm². Good charge carrier collecting efficiency within the device is indicated by the FF value of 79.33%. All things considered, the MoSe₂ device obtains a good PCE of 28.11%, indicating efficient incident light conversion to electrical energy. In comparison to MoSe₂, the WS₂ device has a lower V_{oc} of 0.92 V, suggesting a minor restriction in charge carrier separation. But it makes up for it with a higher J_{sc} and FF of 35.15 mA/cm² and 86.37% respectively, indicating effective

creation and collection of charge carriers. The WS₂ device's high PCE of 27.86% demonstrates its efficacy as a photovoltaic material, even with its lower V_{oc}. Out of the four devices, the WSe₂ device has the lowest V_{oc} of 0.85 V, suggesting possible difficulties with charge carrier separation and collection. Nonetheless, it makes up for this with the highest J_{sc} of 39.35 mA/cm², indicating effective light absorption and charge carrier production. When compared to the other devices, the lower FF value of 72.8% results in a lower 24.26% PCE.

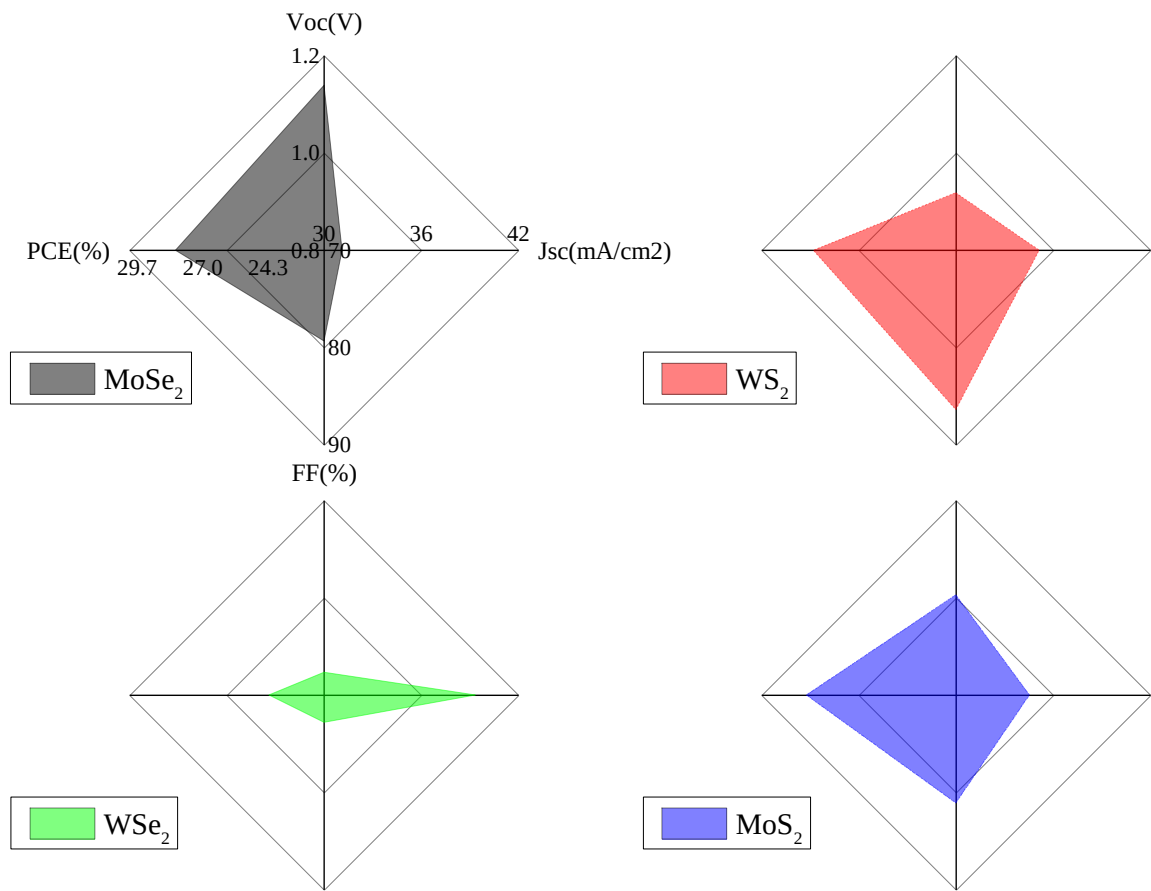


Figure 4.5: V_{oc}, J_{sc}, FF and PCE of the four optimized SCs

The MoS₂ device shows a moderate V_{oc} of 1.01 V, which suggests a reasonable level of charge carrier separation efficiency. Effective charge carrier generation and collection within the device is suggested by the J_{sc} and FF values of 34.54 mA/cm² and 81.07% respectively. Similar to the MoSe₂ device, the MoS₂ device produces a high PCE of 28.16%, demonstrating its efficacy as a photovoltaic material. Ali et al. [35] produced a simulation result of 33.32% PCE and 37.22 mA/cm² J_{sc} for MoS₂ based heterostructure. Rahmoune et al. [65] produced 35.92 mA/cm² J_{sc} and 28.54% PCE for MoS₂ based SC with different

transport layers. Haque et al. [89] produced 24.20% PCE for a WSe₂ based SC. These findings prove that our baseline structures can be improved with transport materials engineering.

Table 4.1: Optimized PV performances of the four devices

Performance parameters	MoSe ₂	WS ₂	WSe ₂	MoS ₂
V _{oc} (V)	1.13884	0.91789	0.84709	1.00555
J _{sc} (mA/cm ²)	31.11253	35.14563	39.34776	34.54023
FF(%)	79.32526	86.37265	72.79888	81.07186
PCE(%)	28.10668	27.86352	24.26456	28.1579

4.3 Monte-Carlo Simulation Results

For 0.15 MeV and 3 MeV proton radiation, calculations of several effects was performed using the SRIM Monte-Carlo toolkit. They are: energy loss to ionization by ions, energy loss to ionization by recoils, energy loss to phonons by ions, energy loss to phonons by recoils, energy from ions, vacancies by ions, and replacement collisions.

4.3.1 Energy Loss to Ionization

If the target is a metal, the energy from the recoiling atoms and fast-moving ions is absorbed by the target's electrons, which then release it as heat. Ionization from incident protons (of 0.15 MeV and 3 MeV energies) as well as from target atoms that are recoiling is depicted in Figures 4.6 and 4.7. The energy lost to the target electrons is also shown by the figures. The direct energy delivered from the ion to the target electrons is the information pertaining to "Ionization by ions". The energy transferred from the target atoms' recoiling to the target electrons is the data pertaining to "Ionization by recoils".

Figure 4.6(a) presents the energy loss to ionization by MoS₂ absorber for 0.15 MeV incident protons. The x-axis represents the target depth in Angstrom, while the y-axis depicts the energy loss to ionization by ions (eV/Angstrom) on the primary y-axis and energy loss to ionization by recoils (eV/Angstrom) on the secondary y-axis. For ionization by ions, the graph shows a decrease in energy loss from 14 to 11 eV/Angstrom as the target depth increases to 1000 Angstrom. Subsequently, there is a steady increase in energy loss, reaching 10 eV at a depth of 6000 Angstrom. Beyond this depth, there is a rapid decrease, with the energy loss becoming zero at 9500 Angstrom depth. Regarding ionization by recoils, the curve exhibits fluctuations, increasing from 0 to 0.036 eV/Angstrom with increasing absorber depth from 0 to 9500

Angstrom. This indicates the varying efficiency of energy transfer from recoils to the material as the depth increases.

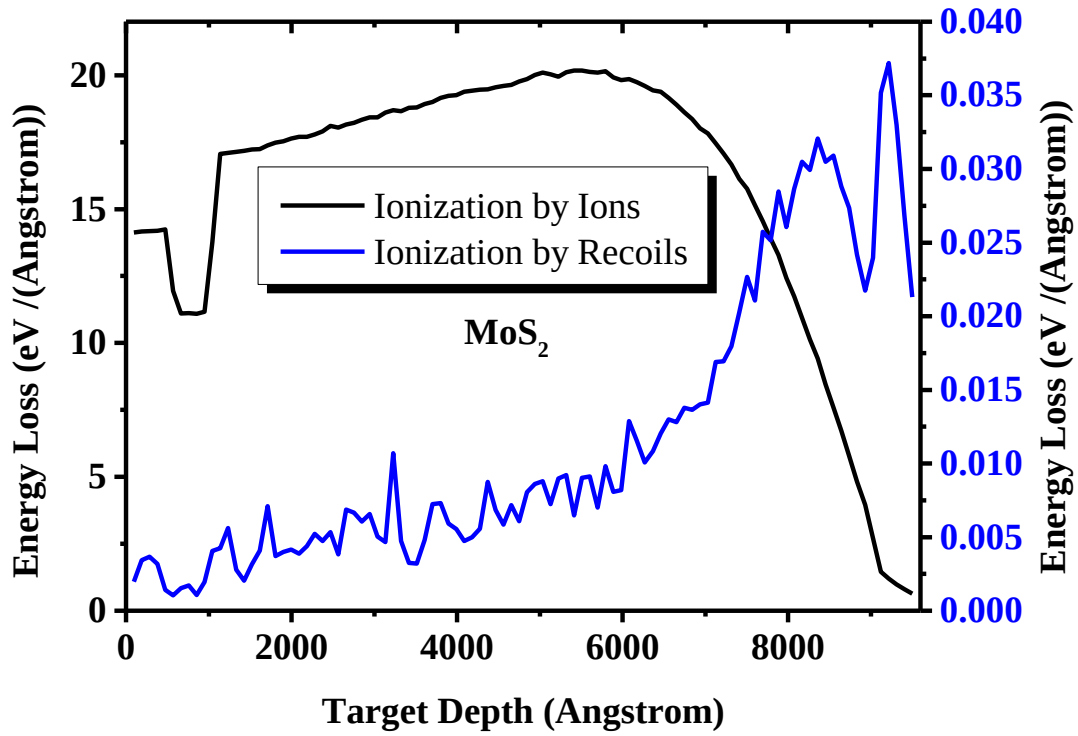


Figure 4.6(a): Energy loss to ionization by MoS_2 absorber for 0.15 MeV incident protons

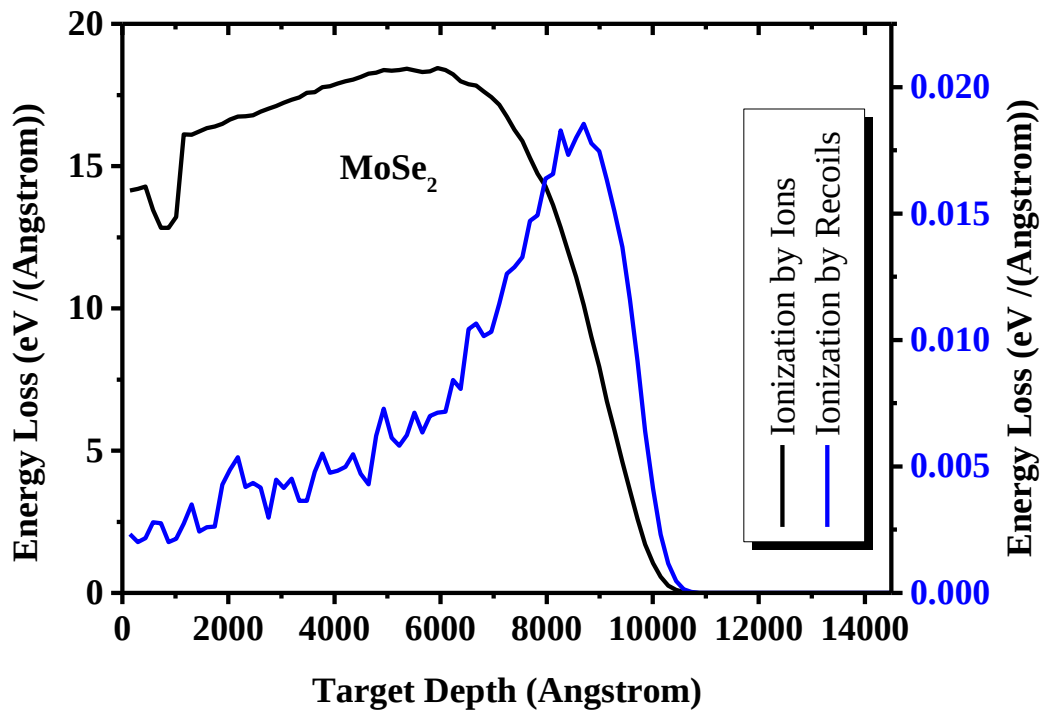


Figure 4.6(b): Energy loss to ionization by MoSe_2 absorber for 0.15 MeV incident protons

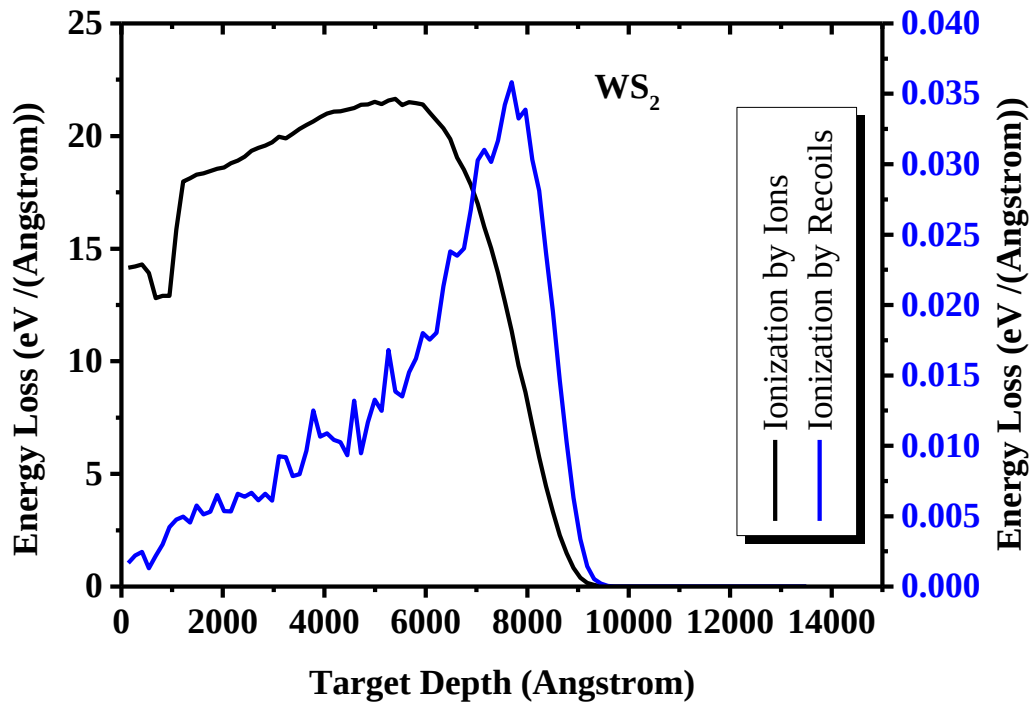


Figure 4.6(c): Energy loss to ionization by WS_2 absorber for 0.15 MeV incident protons

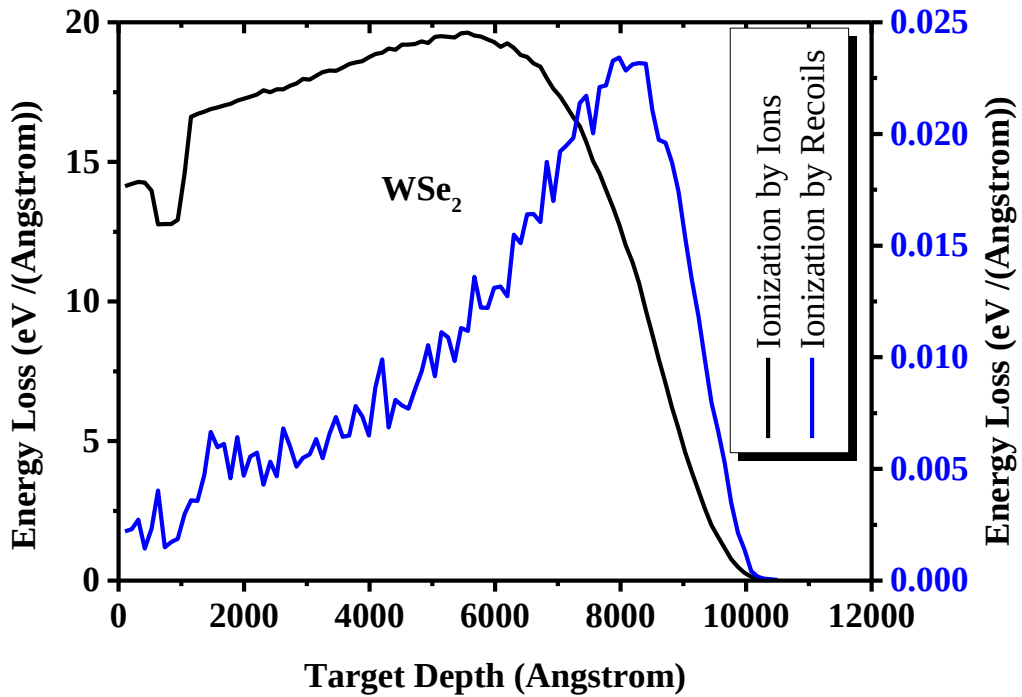


Figure 4.6(d): Energy loss to ionization by WSe_2 absorber for 0.15 MeV incident protons

Figure 4.6(b) illustrates the energy loss to ionization by MoSe_2 absorber. For ionization by ions, the energy loss decreases from 14 to 12.5 eV/Angstrom at 1000 Angstrom depth, then steadily increases to 17.5 eV at 6000 Angstrom, before rapidly decreasing to zero at 10000 Angstrom depth. For ionization by recoils, the

curve shows fluctuations, increasing from 0 to 0.017 eV/Angstrom with increasing absorber depth from 0 to 9000 Angstrom, then quickly decreasing to zero above 10000 Angstrom. Figure 4.6(c) illustrates the energy loss to ionization by WS₂ absorber. Similar to MoSe₂, for ionization by ions, the energy loss decreases from 14 to 12.5 eV/Angstrom at 1000 Angstrom depth, then steadily increases to 21 eV at 6000 Angstrom, before rapidly decreasing to zero at 9000 Angstrom depth. For ionization by recoils, the curve exhibits fluctuations, increasing from 0 to 0.035 eV/Angstrom with increasing absorber depth from 0 to 8000 Angstrom, then quickly decreasing to zero above 9000 Angstrom. Figure 4.6(d) illustrates the energy loss to ionization by WSe₂ absorber. Similarly, for ionization by ions, the energy loss decreases from 14 to 12.5 eV/Angstrom at 1000 Angstrom depth, then steadily increases to 20 eV at 6000 Angstrom, before rapidly decreasing to zero at 10000 Angstrom depth. For ionization by recoils similar to MoSe₂ and WS₂, the curve increases from 0 to 0.024 eV/Angstrom with increasing absorber depth from 0 to 8000 Angstrom, then quickly decreases to zero above 10000 Angstrom.

The energy loss for the MoSe₂, WS₂, and WSe₂ absorbers decreases from 14 to 12.5 eV/Angstrom at the beginning of the depth due to an ITO/CdS ETL. Nevertheless, the ETL for MoS₂ was ITO/TiO₂, which resulted in a decrease from 14 to 11 eV/Angstrom. All absorbers show a similar pattern of initial decrease in energy loss due to ionization, followed by a gradual increase and final drop to zero at deeper depths. This pattern suggests that the incident protons penetrate and attenuate after first interacting with the absorber material. Similar to this, ionization by recoils experiences an increase in energy loss with depth (albeit with oscillations) before it eventually drops to zero at deeper depths. This tendency points to interactions between the absorber material and the recoils, which transfer energy and ultimately dissipate it. The overall patterns in energy loss to ionization by ions and recoils are similar for all absorber materials, despite some variances in the precise energy loss values and depths at which energy loss approaches zero. Rasmetyeva et al. [90] found ionization energy loss on MAPbI₃ at a value of 0.01 eV/Angstrom.

Figure 4.7(a) presents the energy loss to ionization by MoS₂ absorber for 3 MeV incident protons. For ionization by ions, the energy loss decreases from 3.5 to 2 eV/Angstrom at 500 Angstrom depth, then increases back to 3 eV at 1000 Angstrom, remaining constant thereafter. For ionization by recoils, the fluctuating curve shows a peak of 0.0022 eV/Angstrom at an absorber depth of 3500 Angstrom, with energy loss below 0.001 eV/Angstrom for other depths. Figure 4.7(b) presents the energy loss to ionization by MoSe₂ absorber for 3 MeV incident protons. For ionization by ions, similar to MoS₂, the energy loss decreases from 3.5 to 2.75 eV/Angstrom at 500 Angstrom depth, then increases back to 3.75 eV at 1000 Angstrom, remaining constant until 14000 Angstrom thickness, where it degrades back to 3 eV. For ionization by recoils, the fluctuating curve shows a peak of 0.0045 eV/Angstrom at an absorber depth of 3500 Angstrom, with energy loss below 0.001 eV/Angstrom for other depths.

Figure 4.7(c) presents the energy loss to ionization by WS₂ absorber for 3 MeV incident protons. For ionization by ions, similar to MoSe₂, the energy loss decreases from 3.5 to 2.75 eV/Angstrom at 500

Angstrom depth, then increases back to 4 eV at 1000 Angstrom, remaining constant until 14000 Angstrom thickness, where it degrades back to 3 eV. For ionization by recoils, the fluctuating curve shows a peak of 0.0025 eV/Angstrom at an absorber depth of 7000 Angstrom, with energy loss below 0.0015 eV/Angstrom for other depths. Figure 4.7(d) presents the energy loss to ionization by WSe₂ absorber for 3 MeV incident protons. For ionization by ions, similar to MoSe₂ and WS₂, the energy loss decreases from 3.5 to 2.75 eV/Angstrom at 500 Angstrom depth, then increases back to 4.5 eV at 1000 Angstrom, remaining constant until 14000 Angstrom thickness, where it degrades back to 3 eV. For ionization by recoils, the fluctuating curve shows a peak of 0.0055 eV/Angstrom at an absorber depth of 3800 Angstrom, with energy loss below 0.0015 eV/Angstrom for other depths.

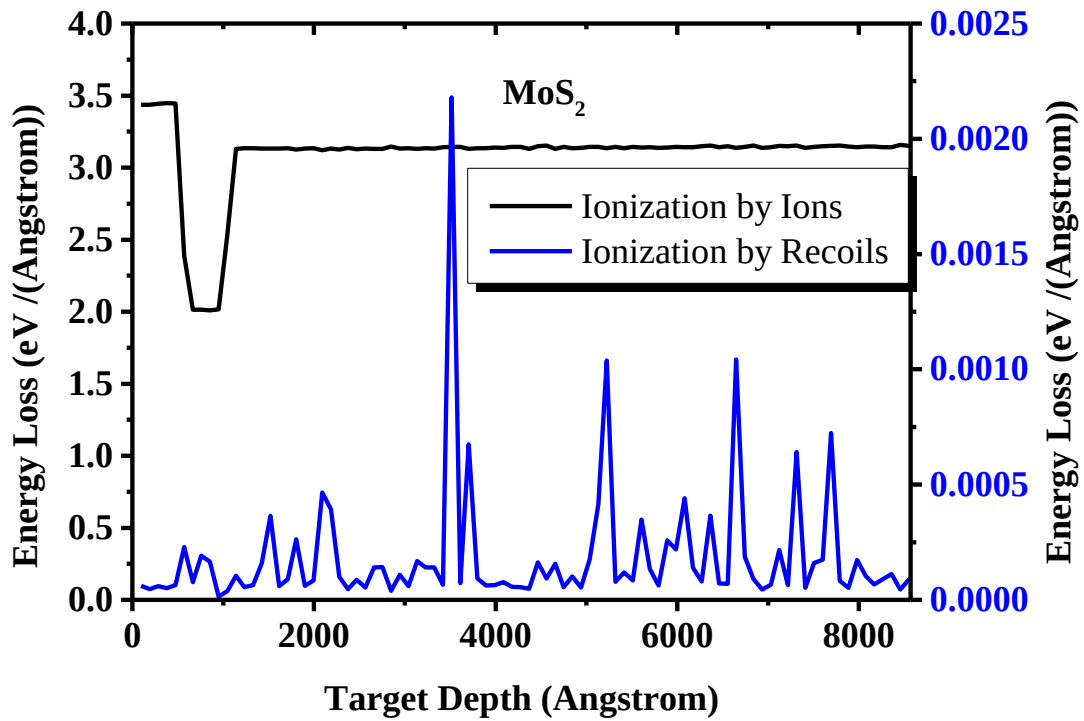


Figure 4.7(a): Energy loss to ionization by MoS₂ absorber for 3 MeV incident protons

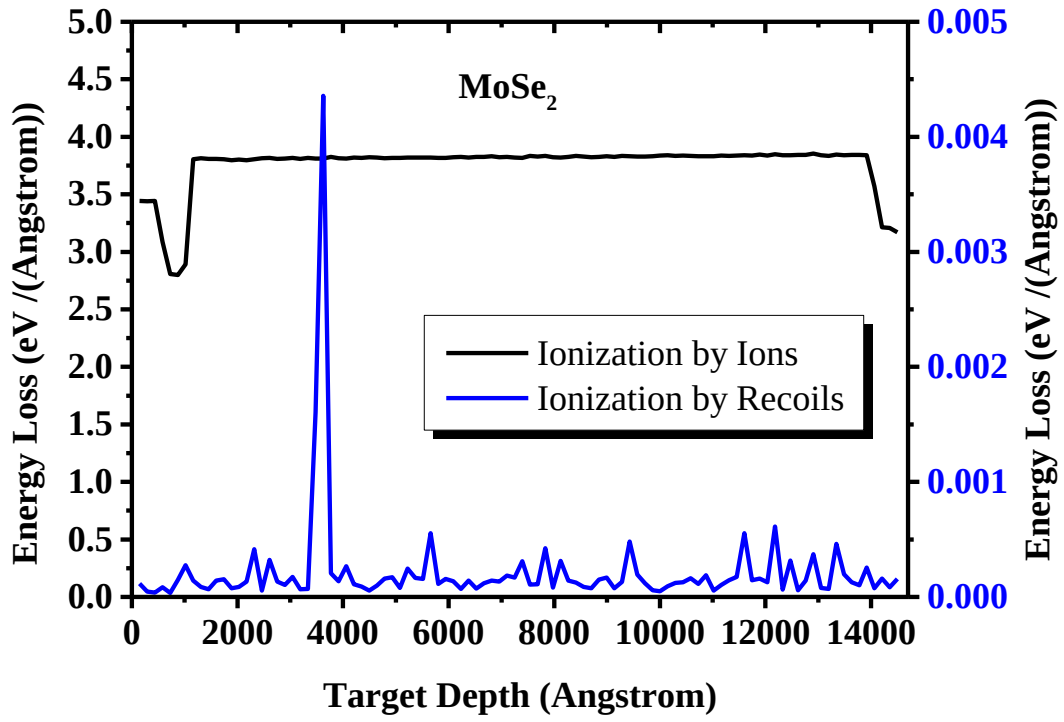


Figure 4.7(b): Energy loss to ionization by MoSe_2 absorber for 3 MeV incident protons

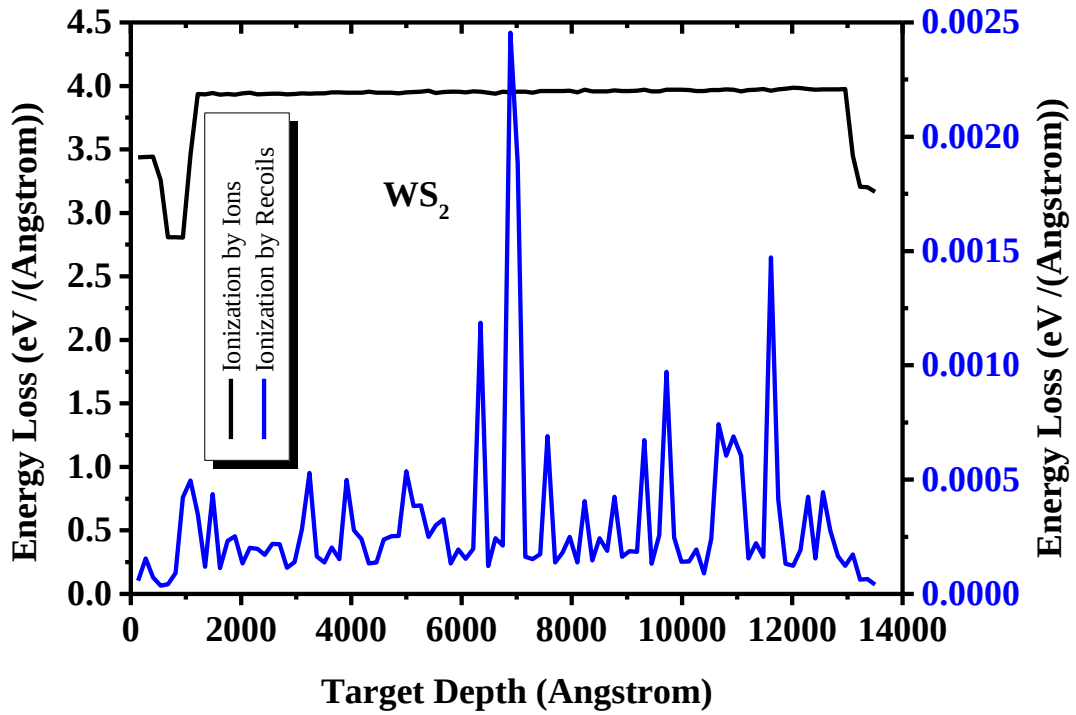


Figure 4.7(c): Energy loss to ionization by WS_2 absorber for 3 MeV incident protons

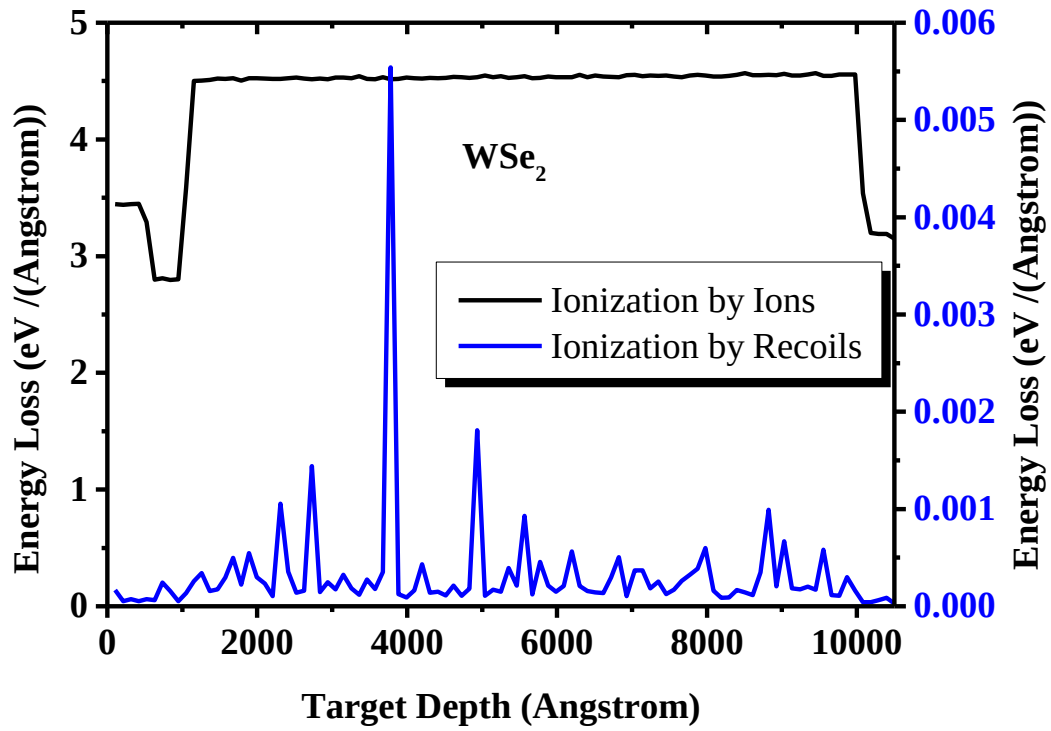


Figure 4.7(d): Energy loss to ionization by WSe₂ absorber for 3 MeV incident protons

At the beginning of the depth, there is an ITO/CdS ETL for MoSe₂, WS₂, and WSe₂ absorbers, resulting in a similar initial decrease in energy loss from 3.5 to 2.75 eV/Angstrom. However, MoS₂, with an ITO/TiO₂ ETL, experiences a higher decrease from 3.5 to 2 eV/Angstrom. Across all absorbers, there is a common trend of fluctuating energy loss to ionization by recoils, with varying peak values at different depths. Additionally, while there are fluctuations, the energy loss to ionization by ions generally stabilizes after reaching certain depths, indicating a saturation point in the interaction between incident protons and the absorber material.

4.3.2 Energy Loss to Phonon

Energy held in atomic vibrations within a crystal is called phonons. Since every atom in a crystal is connected to every other atom, when one vibrates in any way, many other atoms also begin to vibrate. Because some vibration modes are preferred over others, this mass vibration is classified as a phonon.

In Figures 4.8(a) through 4.8(d), the energy loss to phonons by different absorbers for 0.15 MeV incident protons is presented. Figure 4.8(a) presents the energy loss to phonon by MoS₂ absorber. An exponential increase is observed for energy loss to phonons by ions from 0.01 eV/Angstrom at 0 Angstrom thickness to a maximum of 0.12 eV/Angstrom at 8750 Angstrom. Afterwards, it decreases rapidly and becomes zero. A fluctuating curve is found for energy loss to phonons by recoils which gains an exponential increase from 0.01 eV/Angstrom at 0 Angstrom depth to a maximum of 0.17 eV/Angstrom at 8750 Angstrom. Similarly,

it decreases rapidly and becomes zero afterwards. Figure 4.8(b) presents the energy loss to phonon by MoSe₂ absorber. Here, energy loss to phonons by ions and recoils follows a similar pattern to MoS₂, with exponential increases from 0.01 eV/Angstrom at 0 Angstrom thickness to respective maximum values (0.1 eV/Angstrom for ions and 0.16 eV/Angstrom for recoils) at specific absorber depths, followed by rapid decreases to zero.

Figure 4.8(c) presents the energy loss to phonon by WS₂ absorber. In this scenario, energy loss to phonons by ions and recoils exhibits a similar trend as MoS₂ and MoSe₂, with exponential increases from 0.01 eV/Angstrom at 0 Angstrom thickness to respective maximum values (0.12 eV/Angstrom for ions and 0.15 eV/Angstrom for recoils) at specific absorber depths, followed by rapid decreases to zero. Figure 4.8(d) presents the energy loss to phonon by WSe₂ absorber. It is seen that energy loss to phonons by ions and recoils follows a pattern akin to other absorbers, with exponential increases from 0.01 eV/Angstrom at 0 Angstrom thickness to respective maximum values (0.1 eV/Angstrom for ions and 0.15 eV/Angstrom for recoils) at specific depths, followed by rapid decreases to zero.

For all absorbers, the energy loss to phonons by both ions and recoils exhibits an exponential increase with increasing absorber depth, reaching maximum values at specific depths before rapidly decreasing to zero. This pattern suggests efficient phonon generation and propagation within the absorber material. Additionally, the similarities in trends among different absorbers indicate commonalities in their phonon interaction mechanisms with incident protons. Rasmetyeva et al. [90] found energy loss to phonon on MAPbI₃ at a value of 0.01 eV/Angstrom.

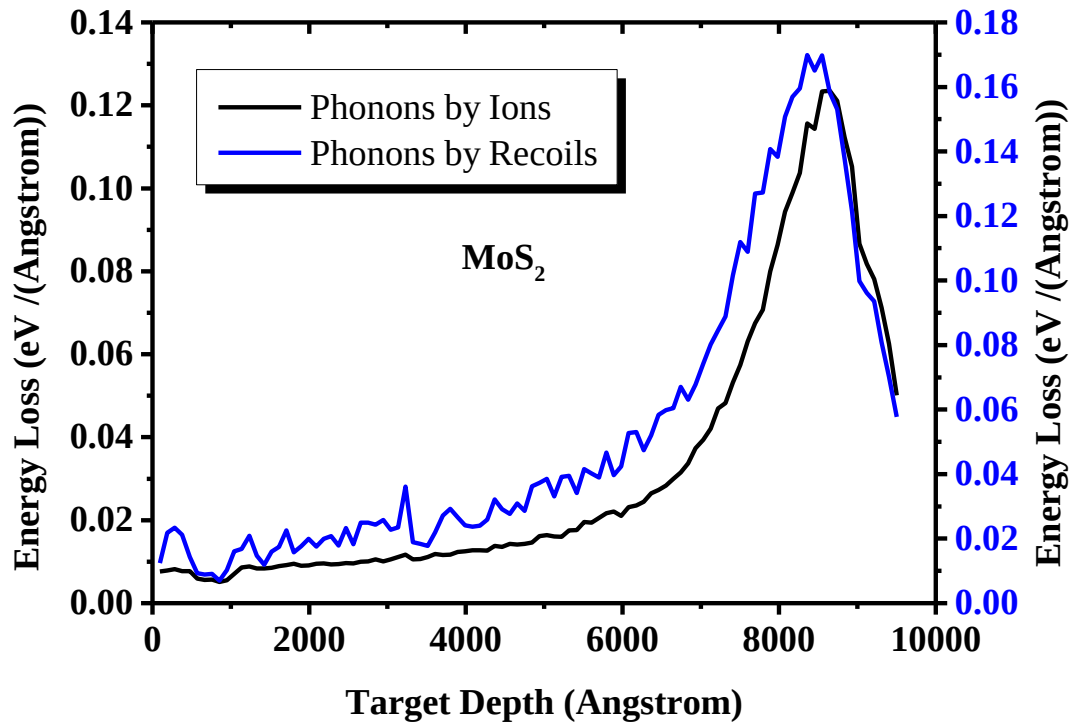


Figure 4.8(a): Energy loss to phonon by MoS₂ absorbers for 0.15 MeV incident protons

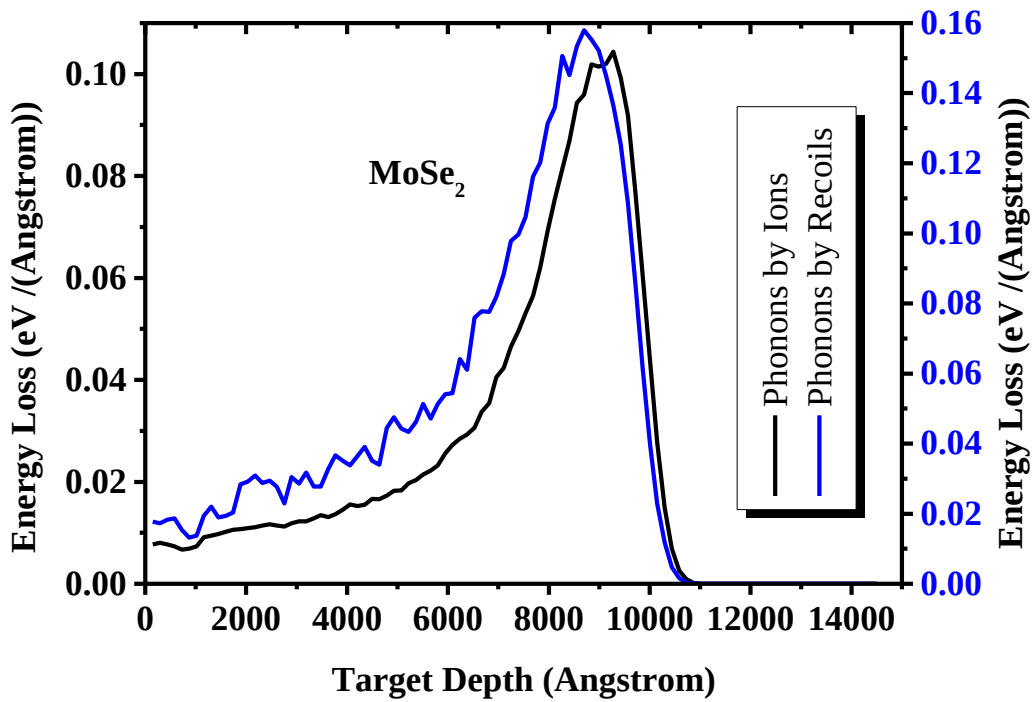


Figure 4.8(b): Energy loss to phonon by MoSe₂ absorbers for 0.15 MeV incident protons

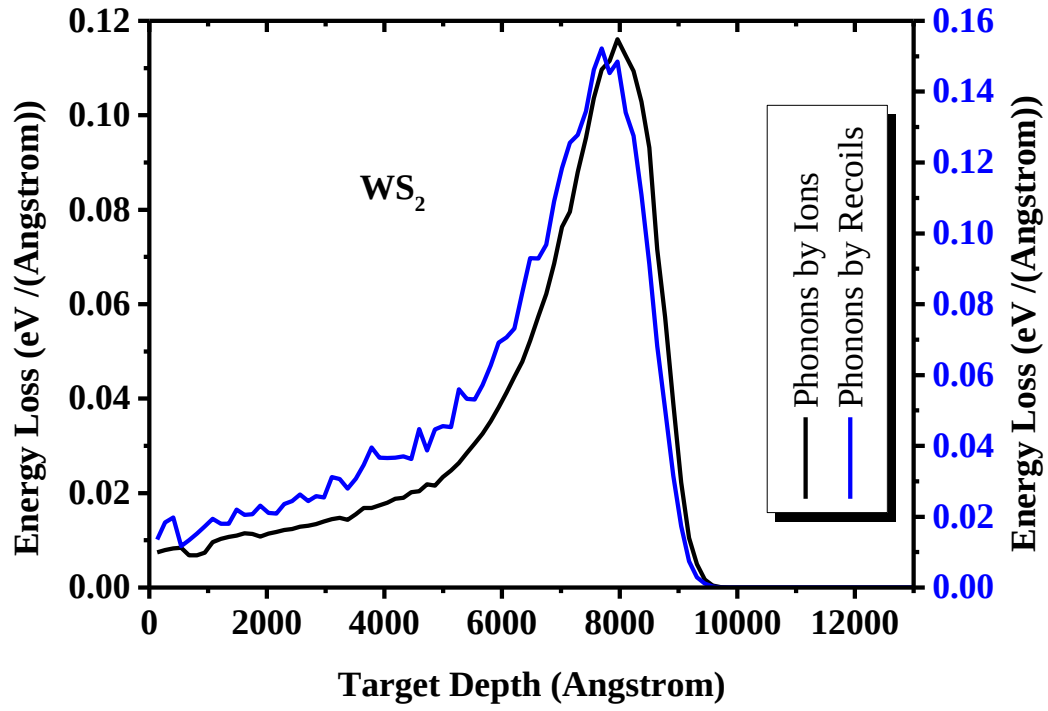


Figure 4.8(c): Energy loss to phonon by WS_2 absorbers for 0.15 MeV incident protons

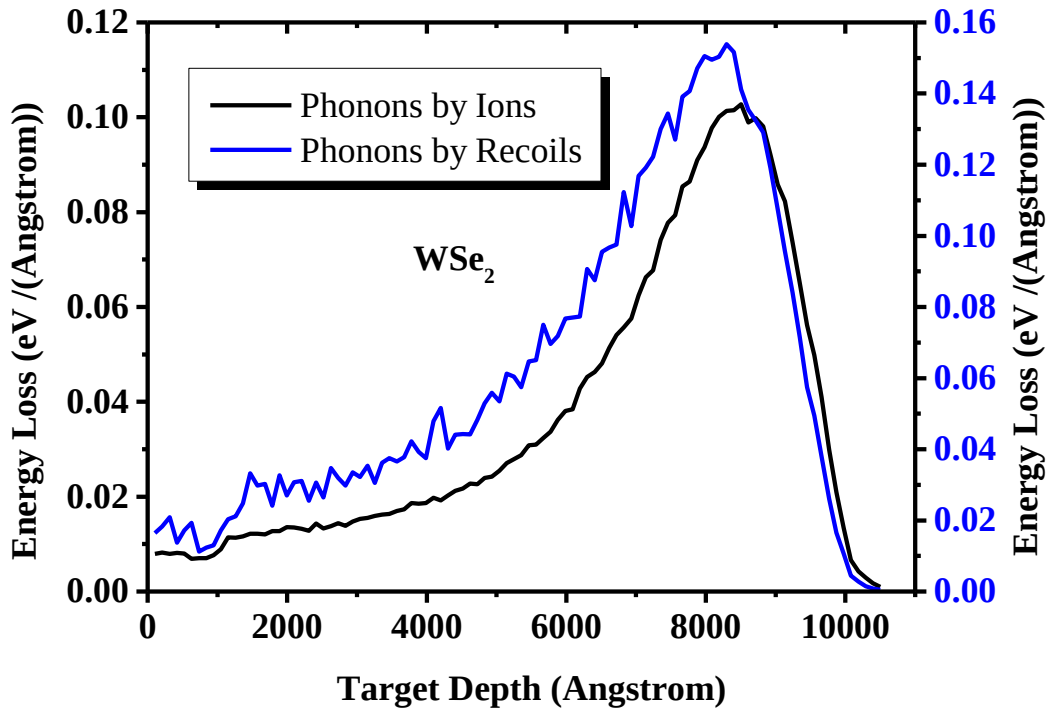


Figure 4.8(d): Energy loss to phonon by WSe_2 absorbers for 0.15 MeV incident protons

In Figures 4.9(a) through 4.9(d), the energy loss to phonons by different absorbers for 3 MeV incident protons is depicted. Figure 4.9(a) presents the energy loss to phonon by MoS_2 absorber. For energy loss to phonons by ions, the values fluctuate between 0.0006 and 0.0008 eV/Angstrom across different absorber

depths. For energy loss to phonons by recoils, fluctuations range between 0.0005 and 0.0020 eV/Angstrom, occasionally showing peaks around 0.0035 eV/Angstrom.

Figure 4.9(b) presents the energy loss to phonon by MoSe₂ absorber. For energy loss to phonons by ions, values vary between 0.0008 and 0.0010 eV/Angstrom across different absorber depths. Energy loss to phonons by recoils generally remains below 0.005 eV/Angstrom, with one peak observed at 3750 Angstrom depth, reaching 0.014 eV/Angstrom. Figure 4.9(c) presents the energy loss to phonon by WS₂ absorber. For energy loss to phonons by ions, fluctuations occur between 0.0008 and 0.001 eV/Angstrom across different depths. Energy loss to phonons by recoils Shows fluctuations between 0.001 and 0.003 eV/Angstrom, with one significant peak observed at 6900 Angstrom depth, reaching 0.007 eV/Angstrom. Figure 4.9(d) presents the energy loss to phonon by WSe₂ absorber. For energy loss to phonons by ions, values range between 0.0009 and 0.0012 eV/Angstrom across various depths. Energy loss to phonons by recoils generally remains below 0.005 eV/Angstrom, with one peak observed at 3750 Angstrom depth, reaching 0.015 eV/Angstrom.

For all absorbers in Figure 4.9, the energy loss to phonons by both ions and recoils remains relatively low, indicating minimal interaction between incident protons and the absorber material at this energy level. The fluctuations observed in the energy loss to phonons by recoils may be attributed to the stochastic nature of proton interactions within the absorber material. Additionally, the presence of peaks in some curves suggests localized energy deposition events, which could be further investigated to understand specific phonon generation mechanisms under proton irradiation.

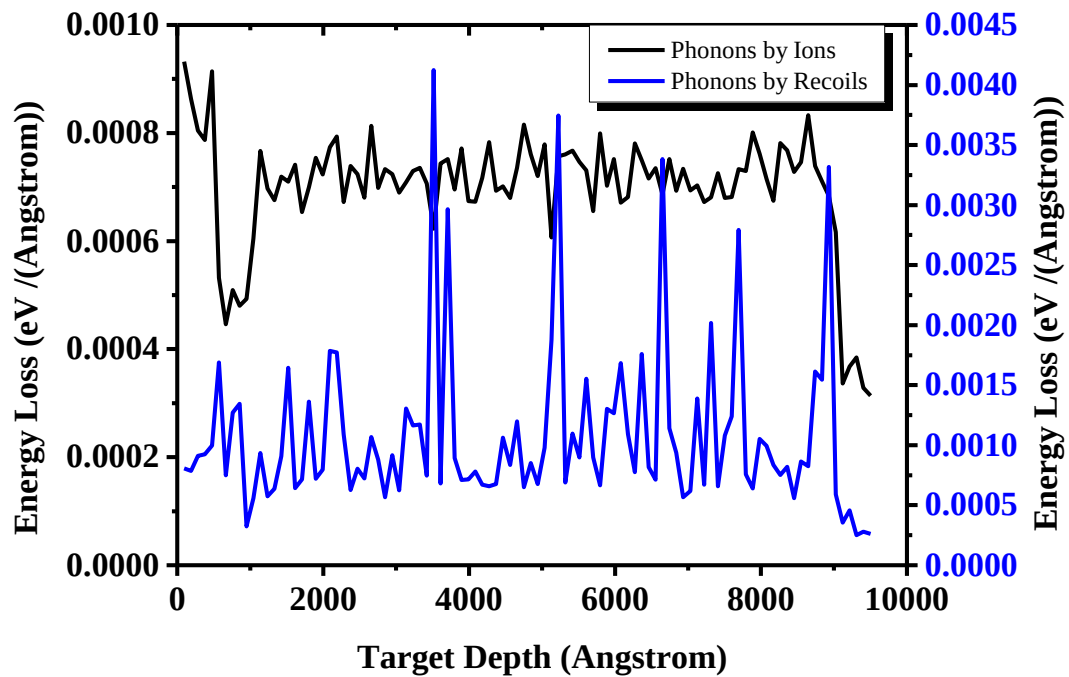


Figure 4.9(a): Energy loss to phonon by MoS₂ absorbers for 3 MeV incident protons

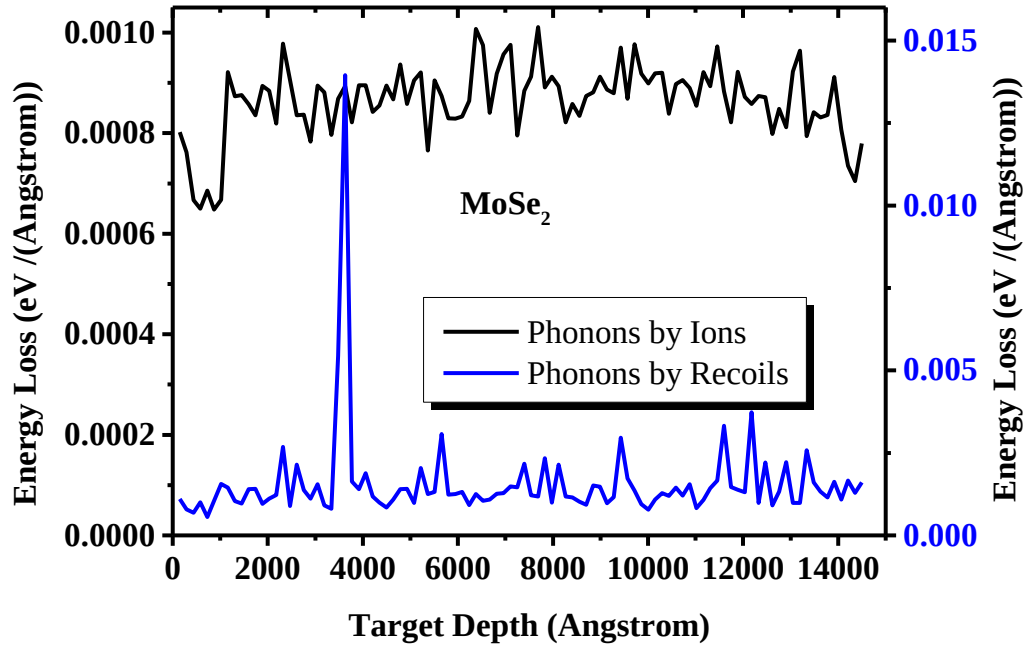


Figure 4.9(b): Energy loss to phonon by MoSe₂ absorbers for 3 MeV incident protons

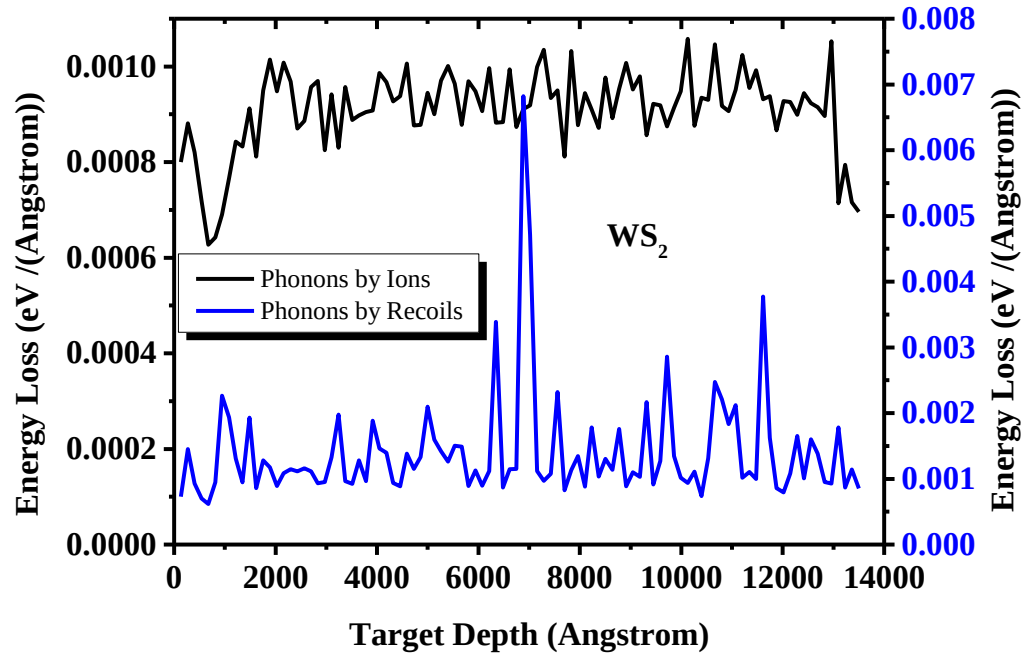


Figure 4.9(c): Energy loss to phonon by WS₂ absorbers for 3 MeV incident protons

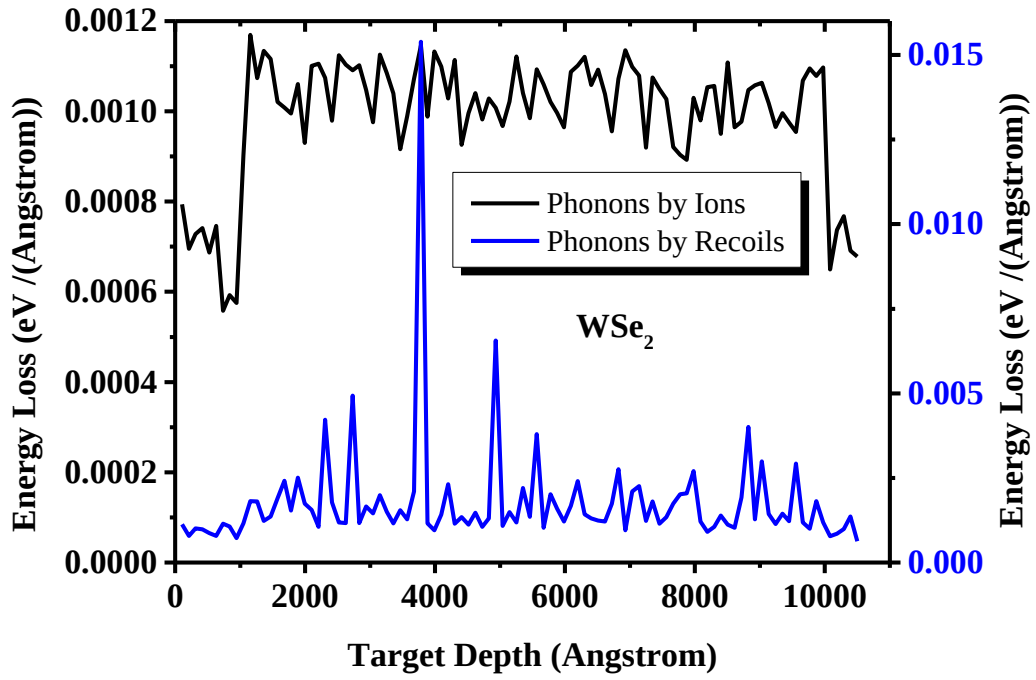


Figure 4.9(d): Energy loss to phonon by WSe₂ absorbers for 3 MeV incident protons

Figure 4.9: Energy loss to phonon by different absorbers for 3 MeV incident protons

4.3.3 Energy Loss to Recoil Atoms

This section discusses the energy loss of the ion by recoil atoms into different absorber materials. In Figure 4.10, depicting the energy loss to recoil atoms by different absorbers for 0.15 MeV incident protons, a common trend is observed across all absorber materials. Each curve fluctuates and exhibits an exponential increase from approximately 0 to varying maximum values, ranging between 0.10 and 0.13 eV, at a depth of 8000 Angstrom. Subsequently, the energy loss decreases. This pattern suggests that as the incident protons penetrate deeper into the absorber materials, they interact with the atoms, leading to the generation of recoil atoms and the subsequent energy loss.

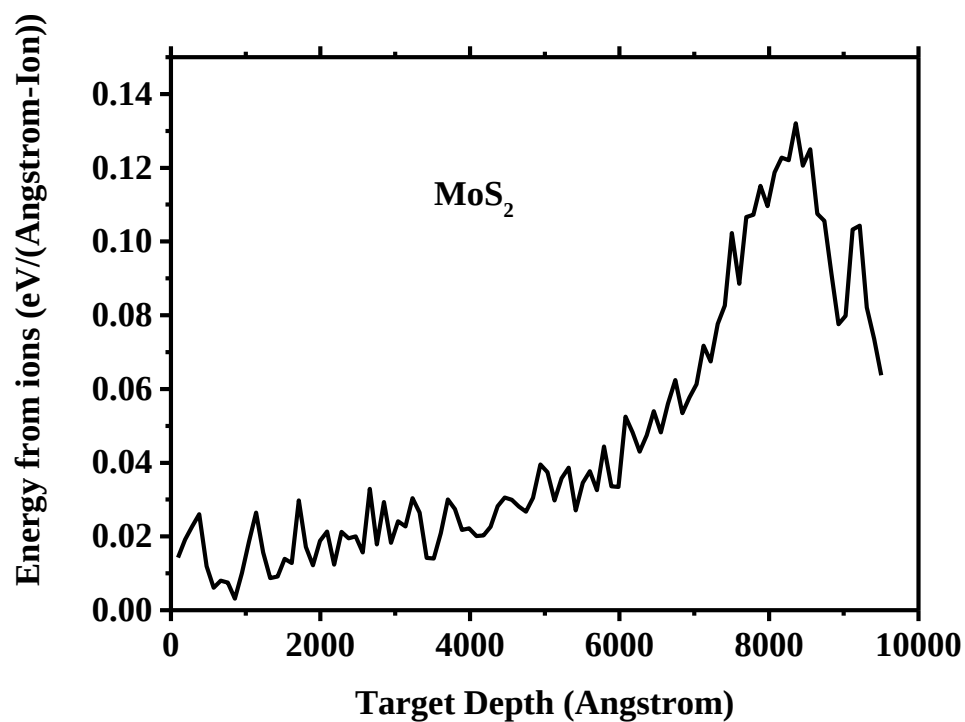


Figure 4.10(a): Energy loss to recoil atoms by MoS₂ absorber for 0.15 MeV incident protons

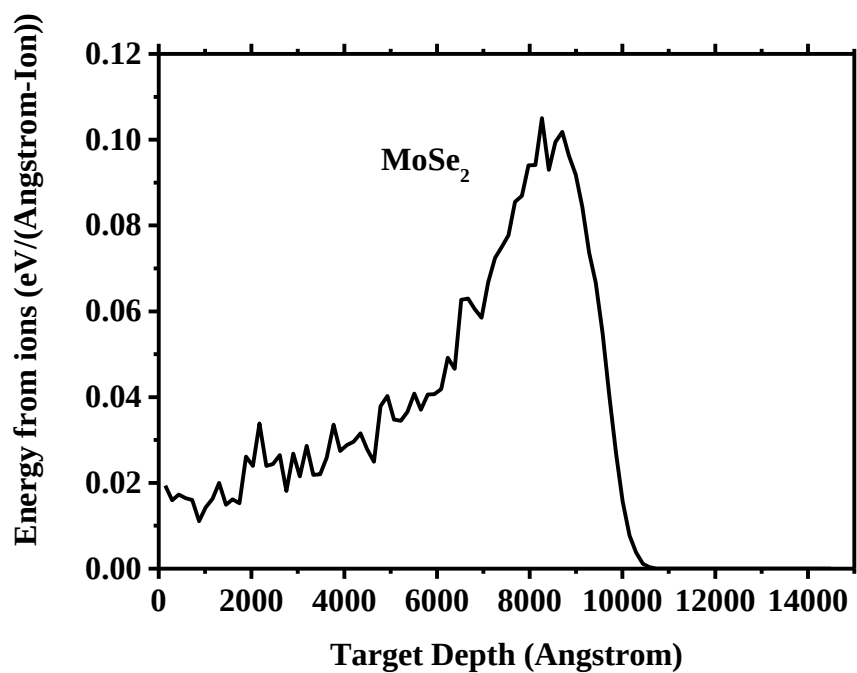


Figure 4.10(b): Energy loss to recoil atoms by MoSe₂ absorber for 0.15 MeV incident protons

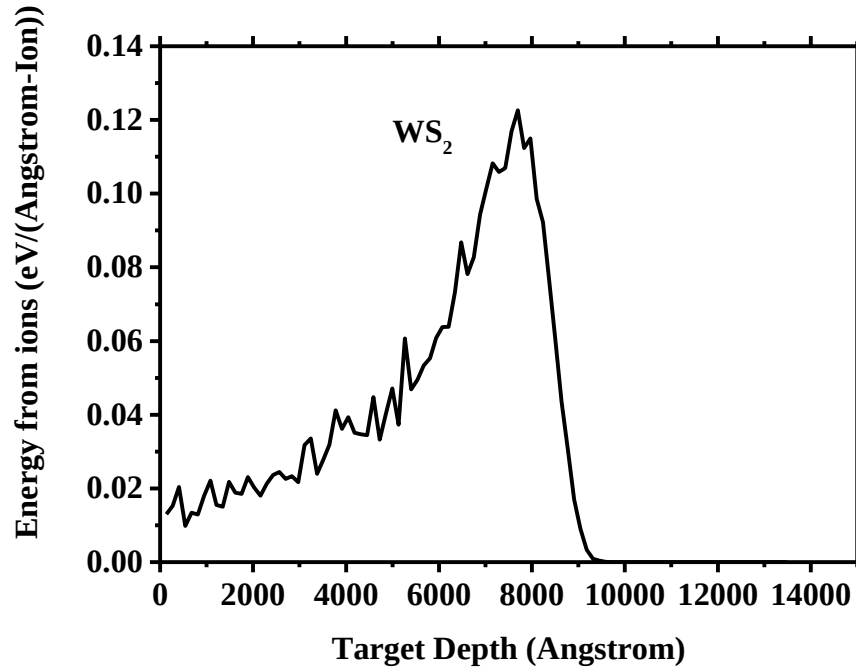


Figure 4.10(c): Energy loss to recoil atoms by WS_2 absorber for 0.15 MeV incident protons

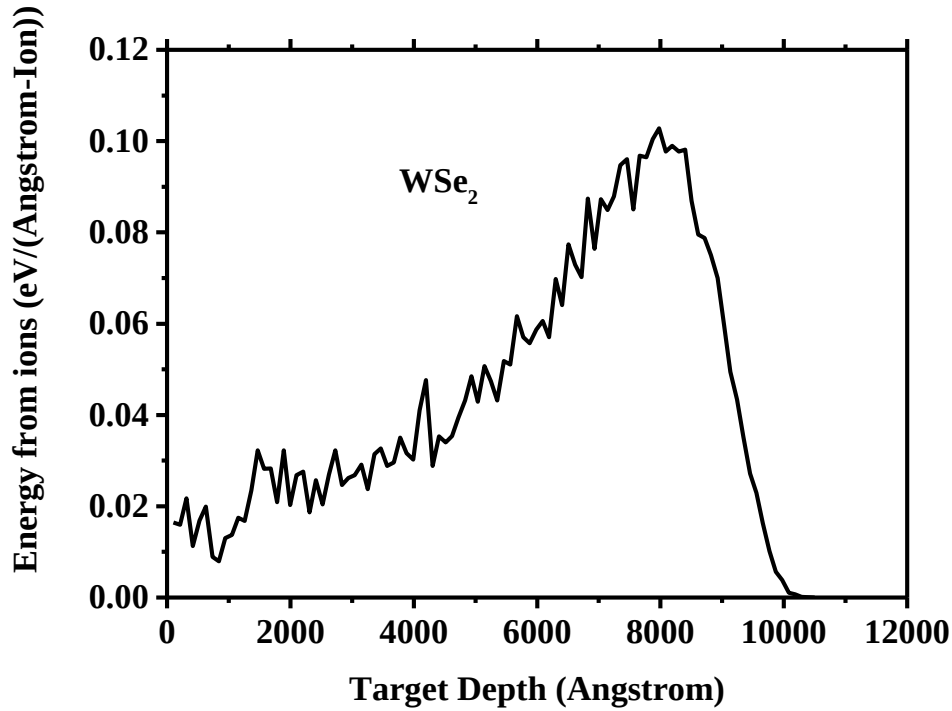


Figure 4.10(d): Energy loss to recoil atoms by WSe_2 absorber for 0.15 MeV incident protons

In Figure 4.11, illustrating the energy loss to recoil atoms by different absorbers for 3 MeV incident protons, minor fluctuations in the values are observed across all absorber materials, ranging between 0 and 0.005 eV/(Angstrom-Ion). Additionally, each material exhibits one or multiple major peaks at various absorber

depths, indicating localized energy deposition events. For MoSe_2 , a significant peak is observed at 3250 Angstrom with a value of 0.025 eV/(Angstrom-Ion), while WS_2 shows a major peak at 7000 Angstrom with a value of 0.013 eV/(Angstrom-Ion). WSe_2 displays two major peaks at 3750 Angstrom and 5000 Angstrom, with values of 0.012 and 0.008 eV/(Angstrom-Ion), respectively. These findings suggest that the interaction of 3 MeV incident protons with the absorber materials leads to the generation of recoil atoms, resulting in localized energy deposition and significant variations in energy loss across different depths.

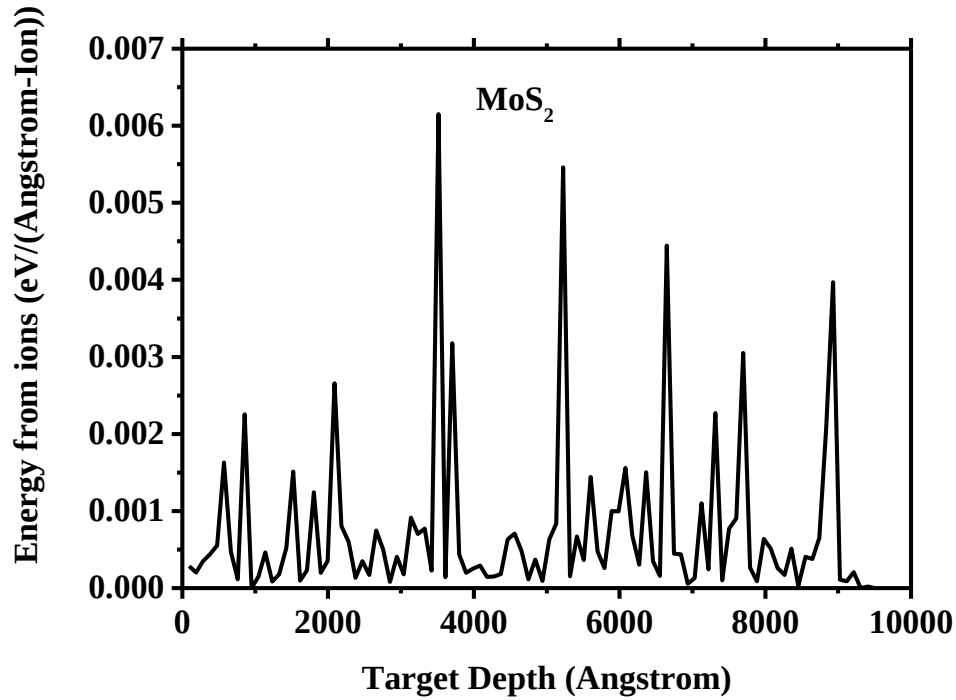


Figure 4.11(a): Energy loss to recoil atoms by MoS_2 absorber for 3 MeV incident protons

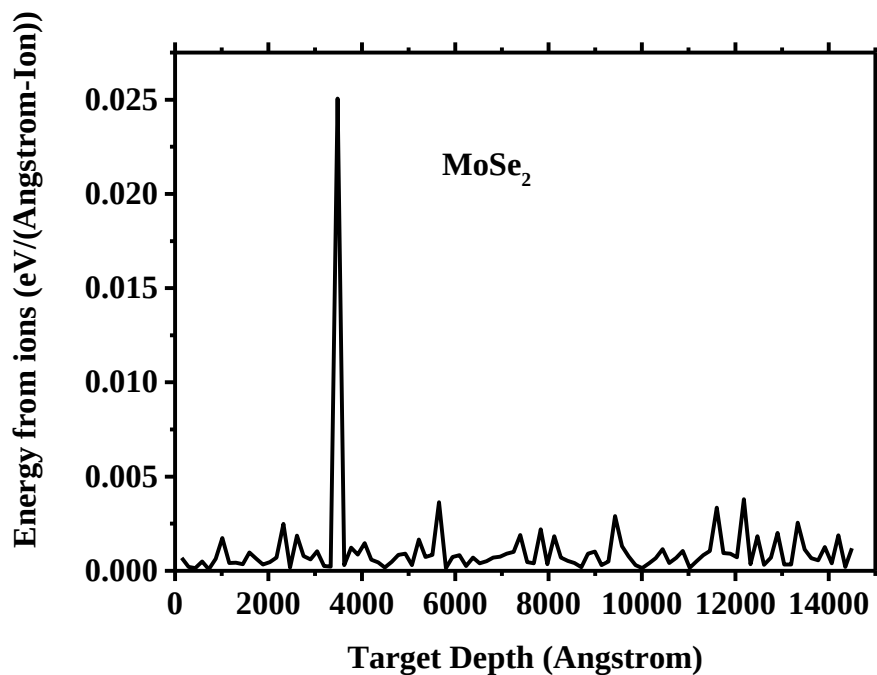


Figure 4.11(b): Energy loss to recoil atoms by MoSe_2 absorber for 3 MeV incident protons

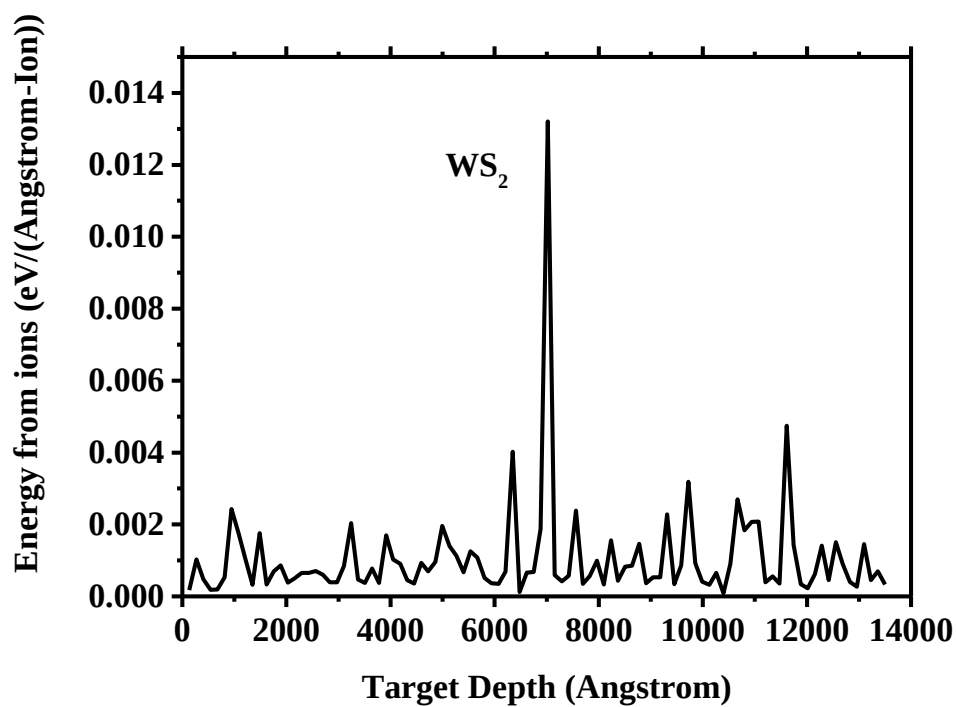


Figure 4.11(c): Energy loss to recoil atoms by WS_2 absorber for 3 MeV incident protons

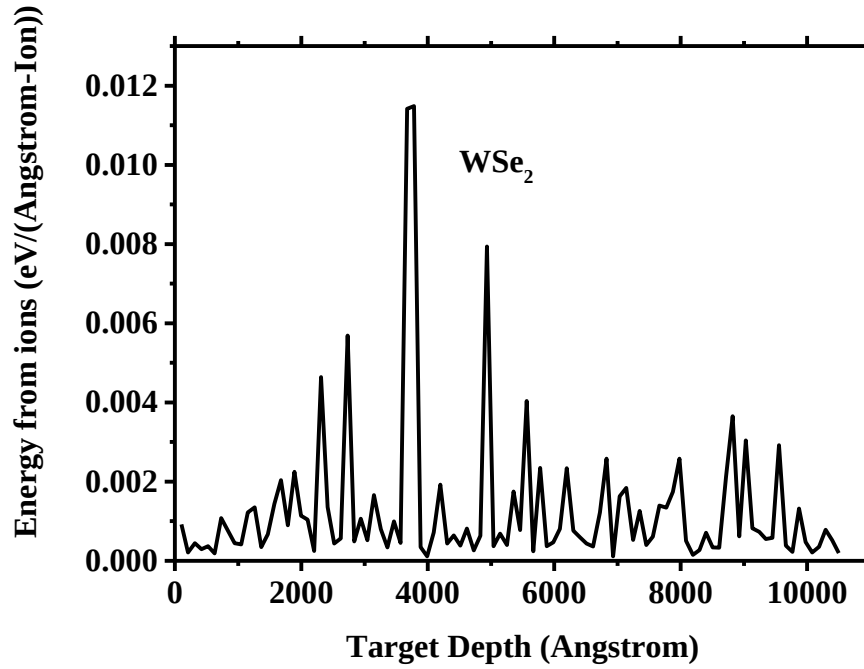


Figure 4.11(d): Energy loss to recoil atoms by WSe₂ absorber for 3 MeV incident protons

4.3.4 Energy Loss to Vacancy Production

This section examines the generation of target vacancies, as does the accompanying Figure 4.12(a-d) and Figure 4.13(a-d). The amount of displacement energy allotted to each target atom determines the number of vacancies. In this part, we also talk about replacement collisions. These are a unique kind of collision where the traveling atom hits an identical target atom, transmits more energy than the displacement energy of that atom, and is unable to continue moving out of the lattice site due to a lack of energy. Because both atoms belong to the same atomic species, there is no ultimate damage when the target atom goes on and is replaced by the original moving atom. Although the two atoms swap locations, there is no discernible difference because they belong to the same species. Target vacancies are produced by collisions between revolving target atoms and ions as well as by collision cascades of these atoms.

In Figure 4.12, depicting the vacancy production by different absorbers for 0.15 MeV incident protons, a clear trend emerges across all materials. Vacancies generated by ions and replacement collisions both exhibit exponential increases with absorber depth, indicating a progressive buildup of vacancies within the materials as the incident protons penetrate deeper. Specifically, MoS₂, MoSe₂, WS₂, and WSe₂ all display similar patterns of vacancy production, with exponential increases observed in both types of interactions across various absorber depths. The average target displacements and vacancies per incident ion, calculated based on 10,000 incident ions, remain consistent across the materials, suggesting uniform behavior in vacancy production mechanisms.

In MoS₂, vacancies due to ions expand exponentially from 0.0001 to 0.0017 vacancies/(Angstrom-Ion) at a depth of 8250 Angstrom. In the same depth range, replacement collisions also show an exponential growth. It is found that both the average target displacements and the average number of vacancies per occurrence are 11, indicative of a consistent vacancy production mechanism. Similarly, over a depth of 9000 Angstrom, MoSe₂ shows exponential increases in vacancies caused by replacement collisions and ions, reaching values of 0.00010 and 0.0015 vacancies/(Angstrom-Ion), respectively. The material exhibits consistent vacancy formation behavior, as evidenced by the computed average target displacements and vacancies per incident ion of 13.

The tendency of exponential vacancy formation persists in WS₂, where the accumulation of vacancies is made possible by both replacement collisions and ions. Over a depth of 8000 Angstrom, vacancies created by ions grow from 0.0001 to 0.0017 vacancies/(Angstrom-Ion), and replacement collisions follow a similar pattern. Ten target displacements and vacancies on average per incident ion are still present. Finally, WSe₂ has a comparable vacancy production pattern, with exponential increases noted in replacement collisions as well as ions. Over a depth of 8750 Angstrom, vacancies created by ions grow from 0.0001 to 0.0014 vacancies/(Angstrom-Ion), and replacement collisions behave similarly. In line with the other materials examined, the average target displacements and vacancies per incident ion are found to be 13.

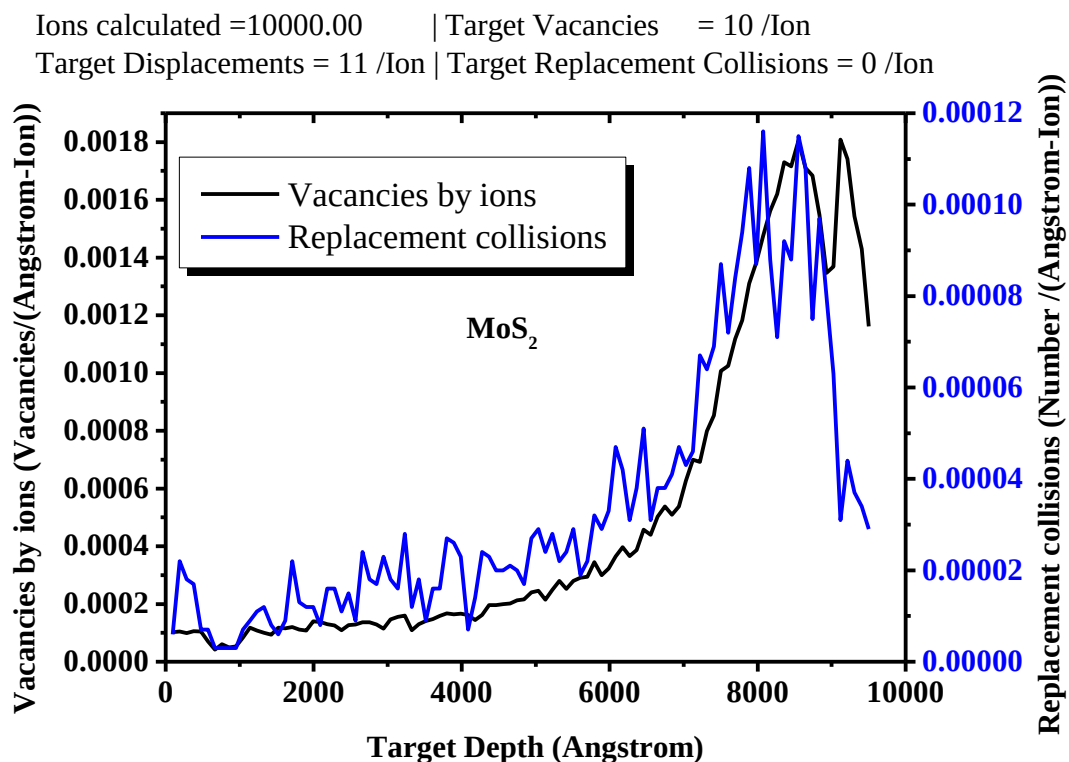


Figure 4.12(a): Vacancy production and replacement collisions by MoS₂ absorber for 0.15 MeV incident protons

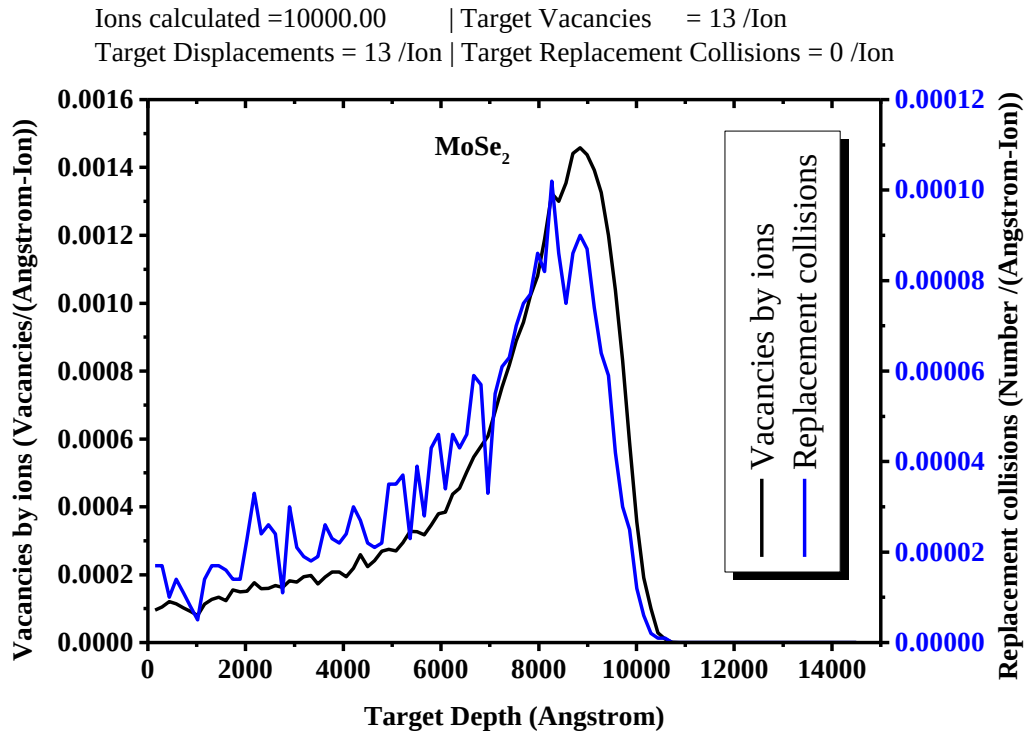


Figure 4.12(b): Vacancy production and replacement collisions by MoSe_2 absorber for 0.15 MeV incident protons

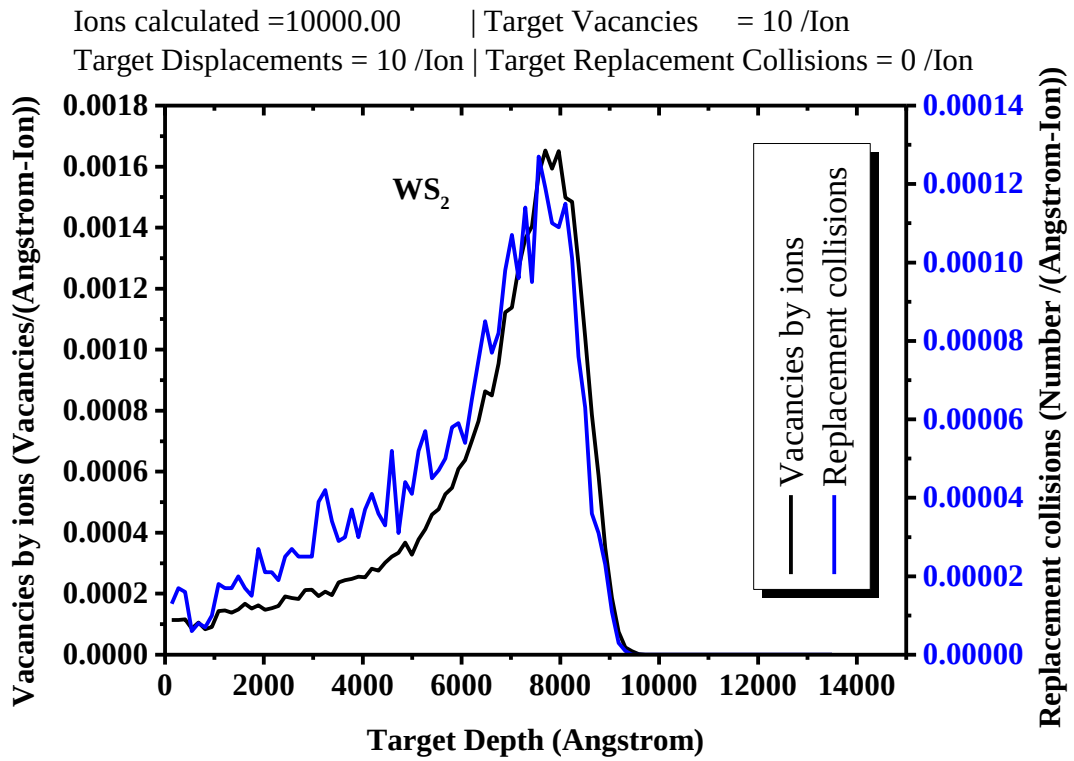


Figure 4.12(c): Vacancy production and replacement collisions by WS_2 absorber for 0.15 MeV incident protons

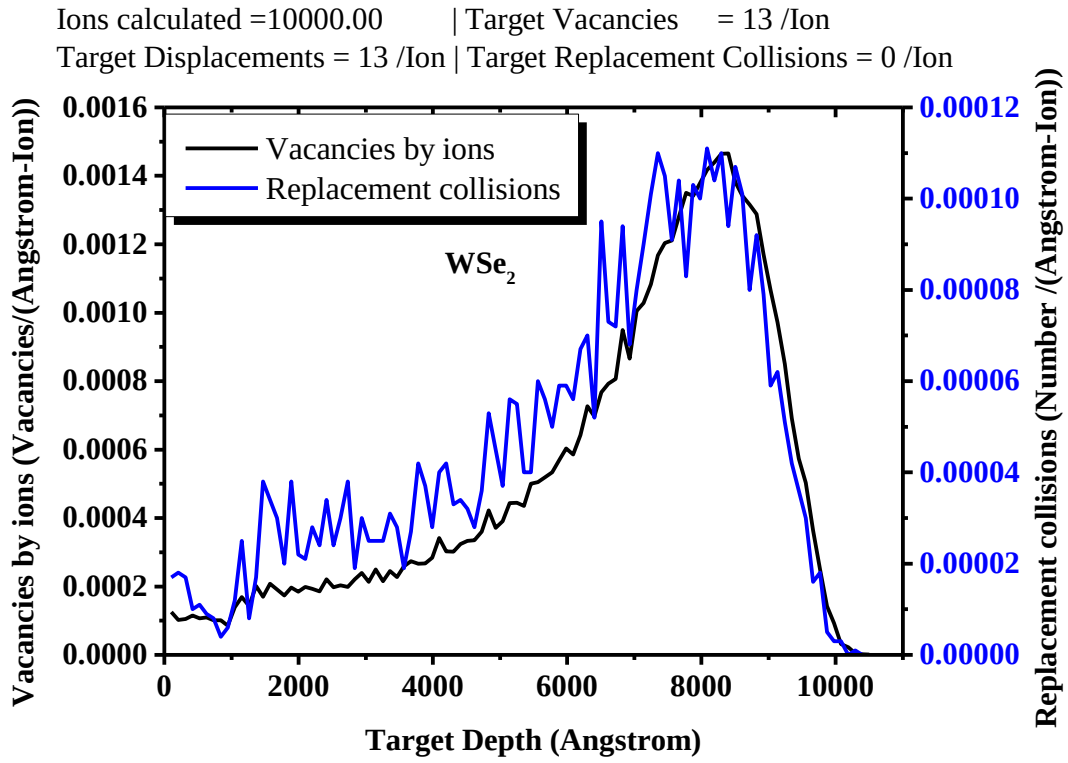


Figure 4.12(d): Vacancy production and replacement collisions by WSe₂ absorber for 0.15 MeV incident protons

In Figure 4.13, which illustrates vacancy production and replacement collisions by different absorbers for 3 MeV incident protons, notably low values are observed across all materials, indicating minimal vacancy generation and replacement collision events.

For MoS₂, both vacancies generated by ions and replacement collisions exhibit values ranging from 1×10^{-6} to 1×10^{-5} Vacancies/(Angstrom-Ion) and do not exceed 5×10^{-6} collisions/(Angstrom-Ion), respectively. The absence of significant peaks suggests a lack of substantial vacancy production or replacement collision events within the material. Similarly, MoSe₂ and WS₂ display comparable patterns, with vacancies by ions and replacement collisions remaining in the range of 2×10^{-6} to 1.2×10^{-5} Vacancies/(Angstrom-Ion) and not exceeding 4×10^{-6} collisions/(Angstrom-Ion). While MoSe₂ shows one major peak in replacement collisions at a depth of 3750 Angstrom, WS₂ exhibits two major peaks at depths of 7000 and 11750 Angstrom. However, these peaks are still relatively low compared to the overall range of values. WSe₂ follows a similar trend, with vacancies by ions and replacement collisions fluctuating within the range of 2×10^{-6} to 1.5×10^{-5} Vacancies/(Angstrom-Ion) and not surpassing 6×10^{-6} collisions/(Angstrom-Ion). One major peak in replacement collisions is observed at a depth of 3750 Angstrom, indicating a slightly higher incidence of replacement collisions compared to the other materials.

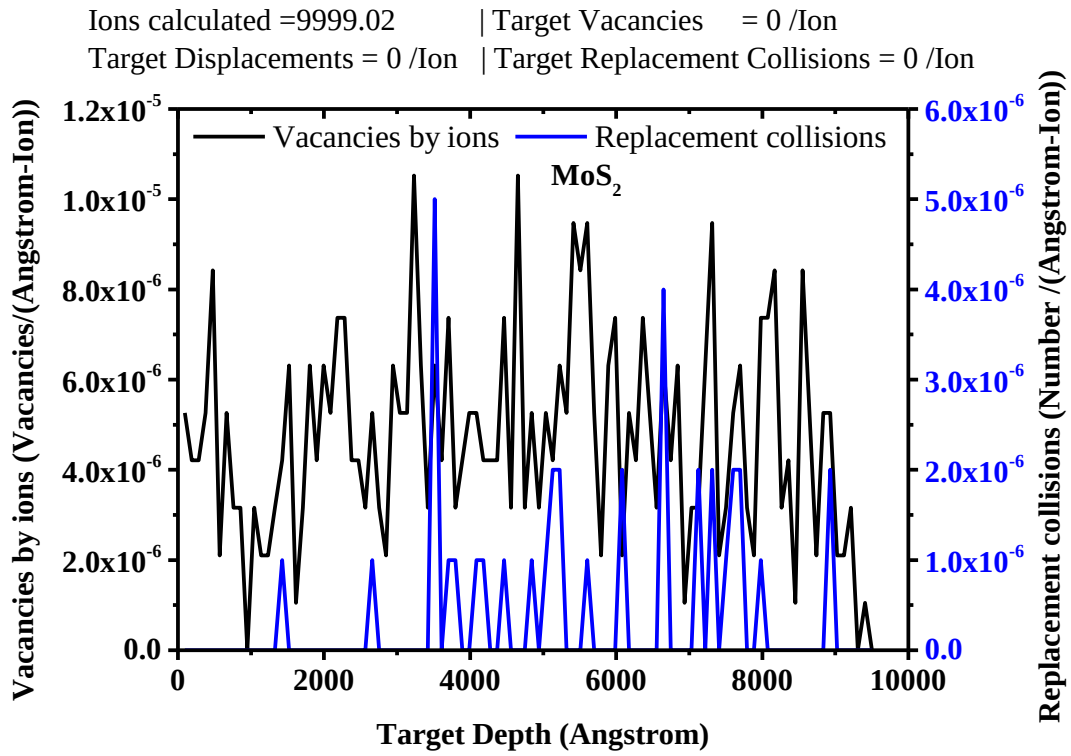


Figure 4.13(a): Vacancy production and replacement collisions by MoS₂ absorber for 3 MeV incident protons

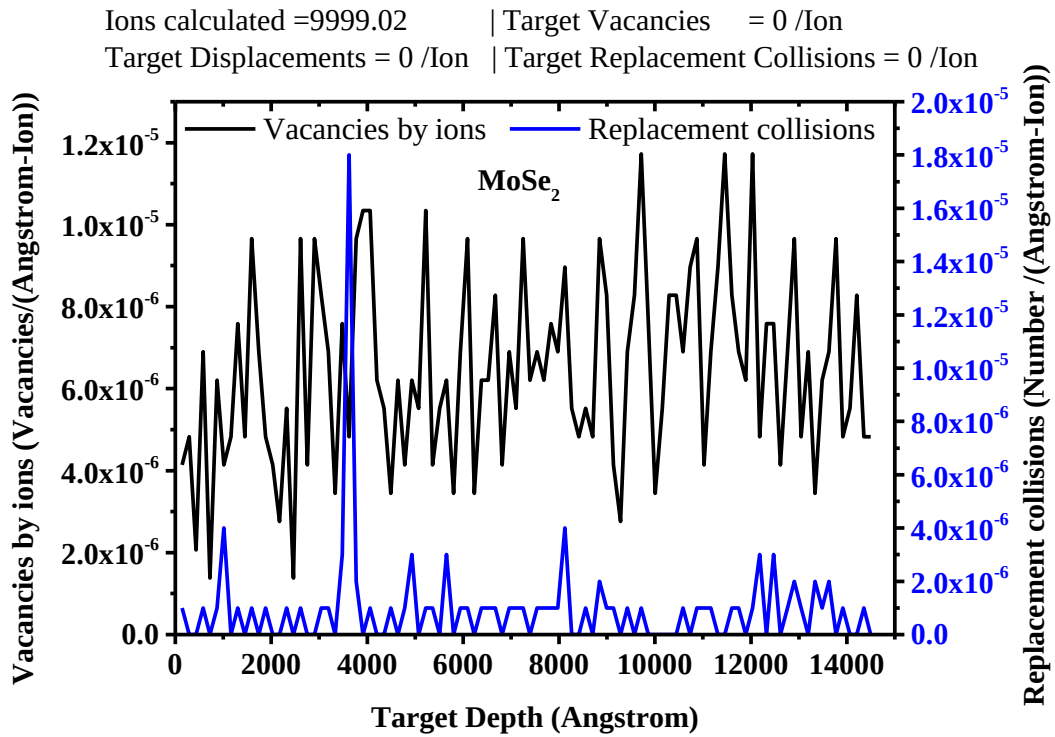


Figure 4.13(b): Vacancy production and replacement collisions by MoSe₂ absorber for 3 MeV incident protons

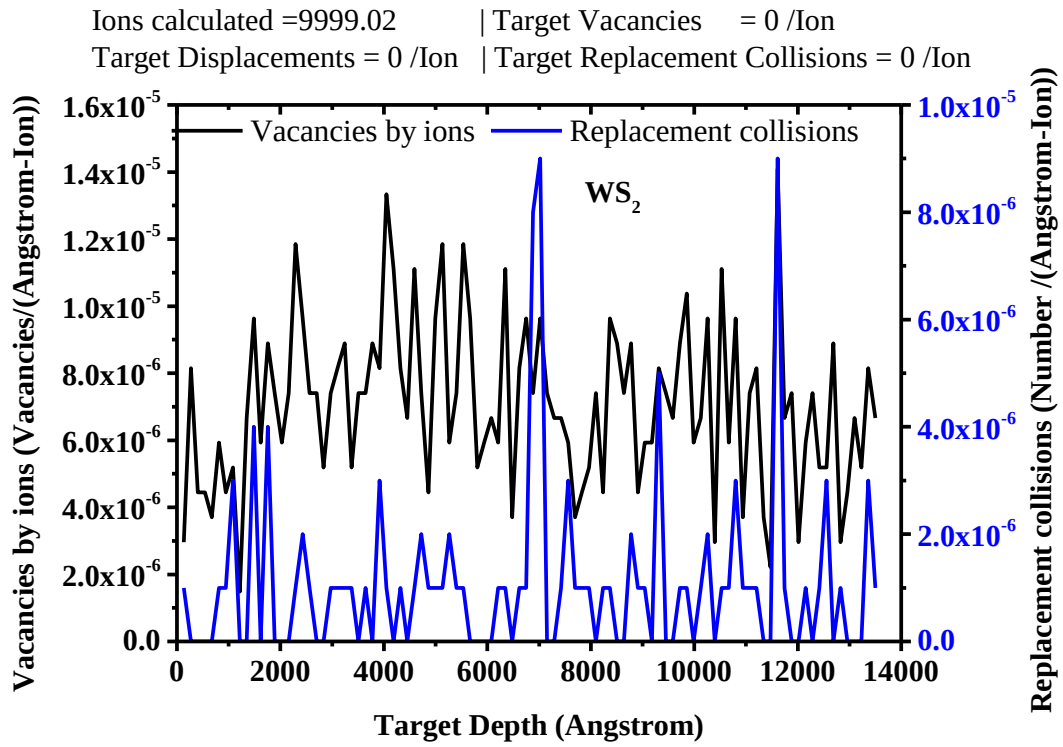


Figure 4.13(c): Vacancy production and replacement collisions by WS₂ absorber for 3 MeV incident protons

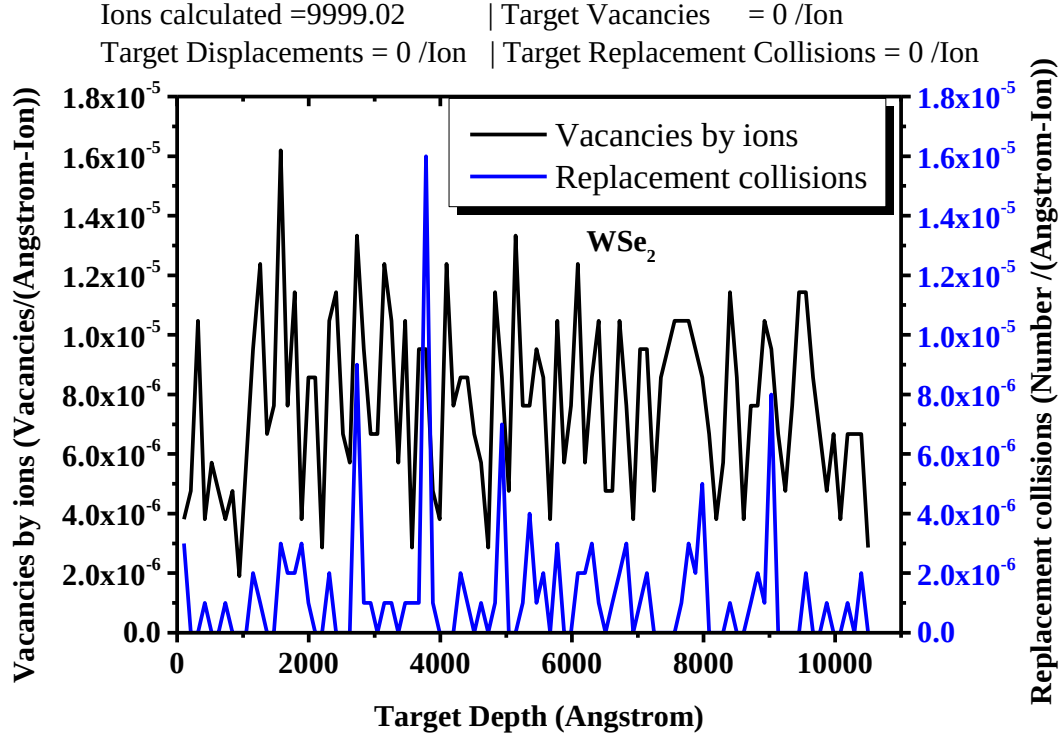


Figure 4.13(d): Vacancy production and replacement collisions by WSe₂ absorber for 3 MeV incident protons

The higher energy of the incident particles accounts for the much lower vacancy generation and replacement collision rates found for 3 MeV incident protons compared to 0.15 MeV incident protons. Protons interact less with the atomic structure of the absorber material at higher energies because they can enter the substance more deeply before losing energy. As a result, the observed decline in the rates of vacancy and replacement collisions is caused by a drop in the probability of vacancy production and replacement collisions. For 3 MeV incident protons, the vacancy creation and replacement collision analysis show very little activity in the absorber materials, with values that are constantly very low. In contrast, exponential increases in vacancy formation and replacement collisions were seen throughout a range of absorber depths for 0.15 MeV incident protons.

4.4 Defect Density Conversion for Performance Calculation

The total number of vacancies created by the ion irradiation is calculated by multiplying the number of vacancies created per ion by the total number of ions (10,000 ions). This gives the total number of vacancies created in the target. The volume of the target material is calculated by cubing the length of one side of the target. This length was converted to centimeters (since 1 Angstrom = 10^{-8} cm), and then cubed to get the volume in cm^3 . The defect density (in vacancies/ cm^3) is then calculated by dividing the total number of vacancies by the volume of the target. This gives the average number of vacancies per unit volume in the target material.

$$\text{Defect density} = \frac{\text{vacancies per ion} \times \text{total ions}}{(\text{target depth in Angstrom} \times 10^{-8})^3} \text{ cm}^{-3} \quad (4.1)$$

Table 4.2 presents defect density conversion data for the MoS₂, MoSe₂, WS₂, and WSe₂ absorbers. The table includes information on vacancies per ion, the number of ions, the length of the affected target sides in Angstrom, and the total defect density in cm^{-3} for each device. The defect density values provide insight into the structural integrity and performance characteristics of the materials, aiding in the understanding of their suitability for specific applications.

Table 4.2: Defect density conversion data

Device	Vacancies/Ion	Number of Ions	Length of the affected target sides (Angstrom)	Total Defect Density (cm^{-3})
MoS ₂	10	10000	9500	1.166×10^{17}
MoSe ₂	13	10000	10730	1.05×10^{17}
WS ₂	10	10000	9585	1.136×10^{17}
WSe ₂	13	10000	10500	1.123×10^{17}

4.5 Performance Analysis of the Damaged Devices

Table 4.3 displays the photovoltaic (PV) performance parameters of devices damaged by 0.15 MeV proton radiation, including MoSe₂, WS₂, WSe₂, and MoS₂. We did not include performance of the SCs by 3 MeV radiation because the defect parameters were negligible. Comparing the values in Table 4.3 with those in Table 4.1, which represents the optimized PV performances of the same devices, reveals the impact of radiation damage on their performance. In Table 4.3, all devices exhibit lower values for V_{oc}, J_{sc}, FF, and PCE compared to Table 4.1. This suggests that the radiation damage has negatively affected the efficiency and overall performance of the devices. Notably, the decrease in PCE indicates a reduction in the ability of the devices to convert incident light into electrical energy, reflecting the impact of radiation-induced defects on their operation.

Table 4.3: PV performances of the devices damaged by 0.15 MeV proton radiation

Performance parameters	MoSe ₂	WS ₂	WSe ₂	MoS ₂
V _{oc} (V)	0.87	0.76	0.57	0.645
J _{sc} (mA/cm ²)	29.03	30.24	36.8	32.71
FF(%)	76.84	74.21	71.74	72.66
PCE(%)	19.47	17.01	15.1	15.32

Figure 4.14 presents a comparison of the PV performance parameters of four devices, MoSe₂, WS₂, WSe₂, and MoS₂, before and after exposure to 0.15 MeV irradiation. The parameters include V_{oc}, J_{sc}, FF, and PCE. Prior to irradiation, the values of V_{oc}, J_{sc}, FF, and PCE were higher in every device than they were afterwards. This suggests that all four devices' performance was adversely affected by the irradiation. The decline in all parameters subsequent to irradiation indicates the deleterious impact of faults caused by radiation on the overall performance and efficiency of the devices. For every parameter and device, there is a different degree of decline. For instance, following irradiation, MoSe₂ showed decreases of 0.26884 V in V_{oc}, 2.08253 mA/cm² in J_{sc}, 2.48526% in FF, and 8.63668% in PCE. In a similar vein, but to varying degrees, WS₂, WSe₂, and MoS₂ also showed reductions in all metrics. Among the parameters, the FF experienced the most significant reduction for all devices, indicating a notable decrease in the devices' internal efficiency and ability to utilize generated power. This reduction in FF directly contributes to the decrease in the overall PCE of the devices after irradiation.

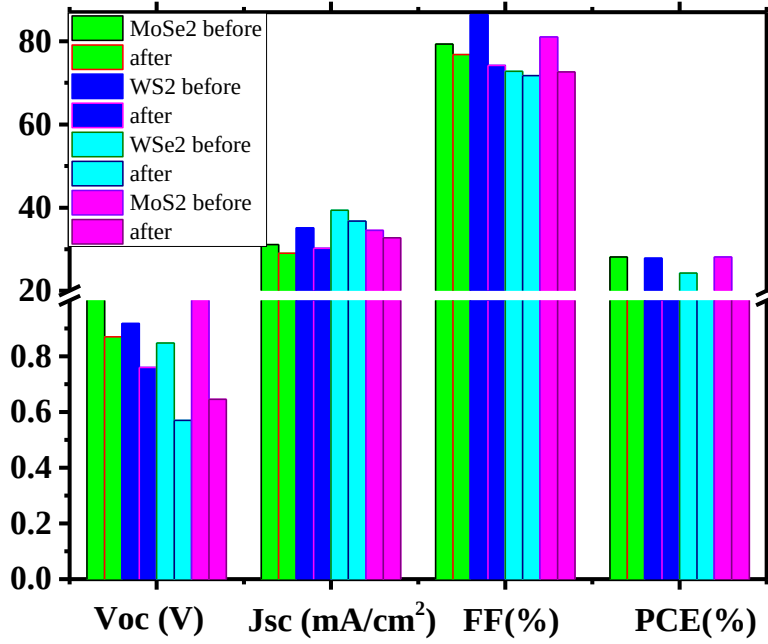


Figure 4.14: Performance comparison diagram of the four devices before and after 0.15 MeV irradiation

4.6 Machine Learning Analysis of the Devices: Influence of the Collision Parameters

To understand which collision parameters were responsible for the reduction of performance, we applied two different state-of-the-art ML techniques: RF regression, and XGB regression. Our dataset involved 390 rows and 8 independent variable vectors (Absorber Material, Energy Loss to ioniz by ions, Energy Loss to ionization by recoils, Energy loss to phonons by ions, Energy Loss to phonons by recoils, Energy from ions, Vacancies by ions, Replacement collisions), and one dependent variable vector (PCE). For both the models, we first split the dataset as training set with 80% data, and test set with 20% data. Then we trained the two models with our data. Finally, the model predicted the PCE of test set, which we then compared with the actual values. The R^2 score, which determines accuracy of the trained models, was found to be 0.958 for RF regression and 0.98 for XGB regression. Figure 4.15(a) and Figure 4.16(a) depicts the predicted and actual PCE of the test set for RF regression and XGB regression, respectively. It is observed that, for higher values of PCE, the prediction gained more accuracy than the lower values of PCEs for both models. It is important to note that the thickness of the absorbers was not included as the independent variable vector. If thickness were to be included, the model would exploit this parameter to predict the PCE, and we would lose insights for the 7 collision parameters involved. This procedure inclines with the aim of this research.

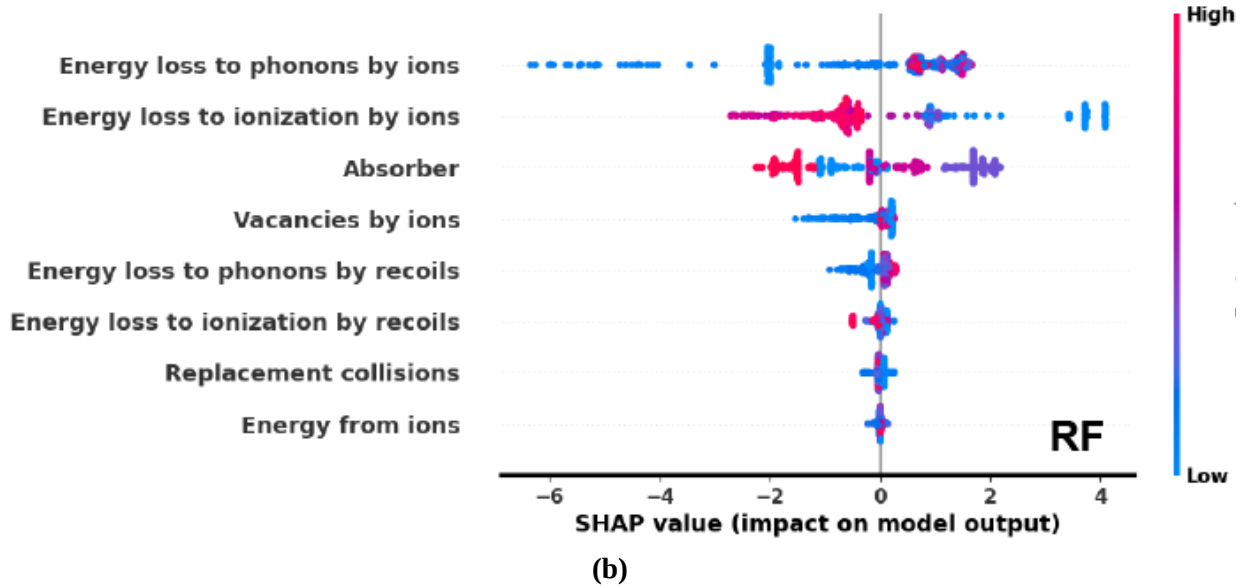
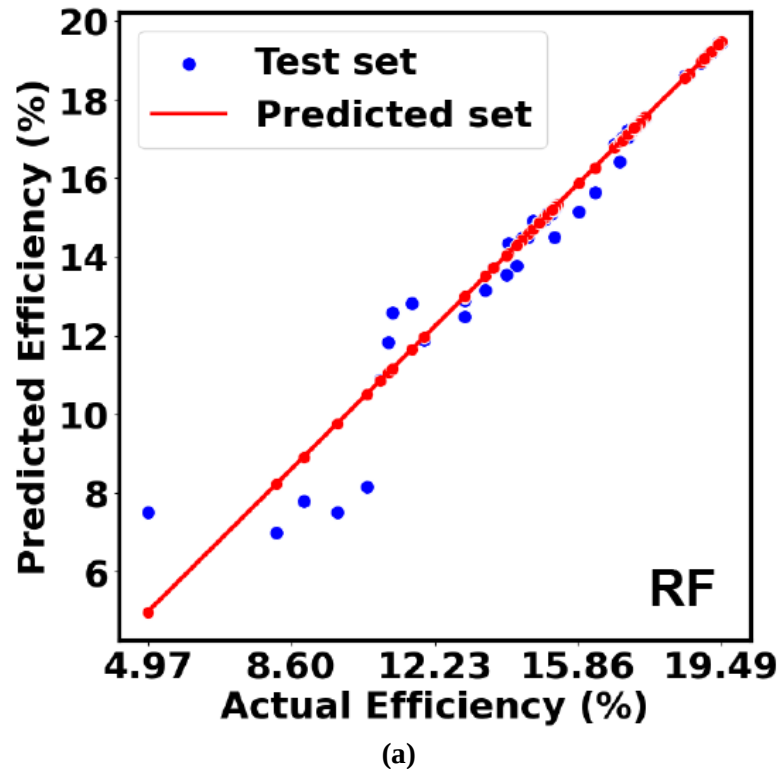


Figure 4.15: (a) RF regression, (b) SHAP values for RF regression

The SHAP plot depicted in Figure 4.15(b) and 4.16(b) shows the impact of various collision parameters on the PCE of the devices. The feature of energy loss to phonons by ions shows a wide range of SHAP values, suggesting that its influence on PCE is not constant. Since most of the SHAP values are negative, it appears that a rise in this characteristic is typically accompanied by a fall in PCE. There is a large range of SHAP values in the energy loss to ionization by ions characteristic, the high values are responsible for declination of PCE while the low values are responsible for increase in PCE. The absorber type in question has a comparatively narrow spread of SHAP values around zero, suggesting that its effect on PCE is negligible.

It is a categorical data where red represents WSe_2 , violet represents WS_2 , deep blue represents MoSe_2 , and sky blue represents MoS_2 . WSe_2 and MoS_2 absorbers tend to lower the PCE. Whereas WS_2 and MoSe_2 absorbers positively impact the PCE. The high values of energy loss to phonons by recoils increase has minor positive impact on PCE where low values play a major role in reduction of the PCE. The other parameters have insignificant impact on the PCE.

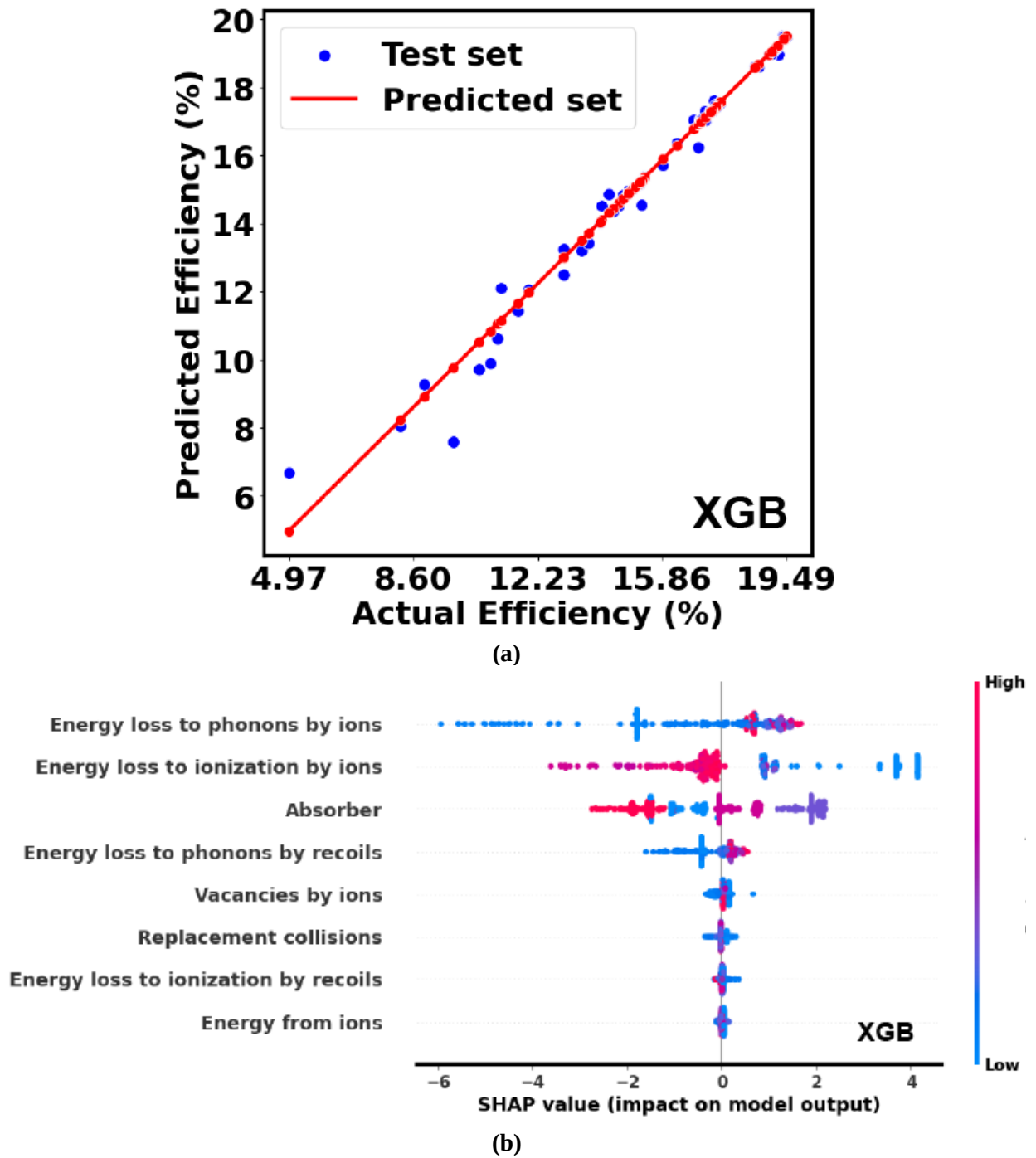


Figure 4.16: (a) XGB regression, (b) SHAP values for XGB regression

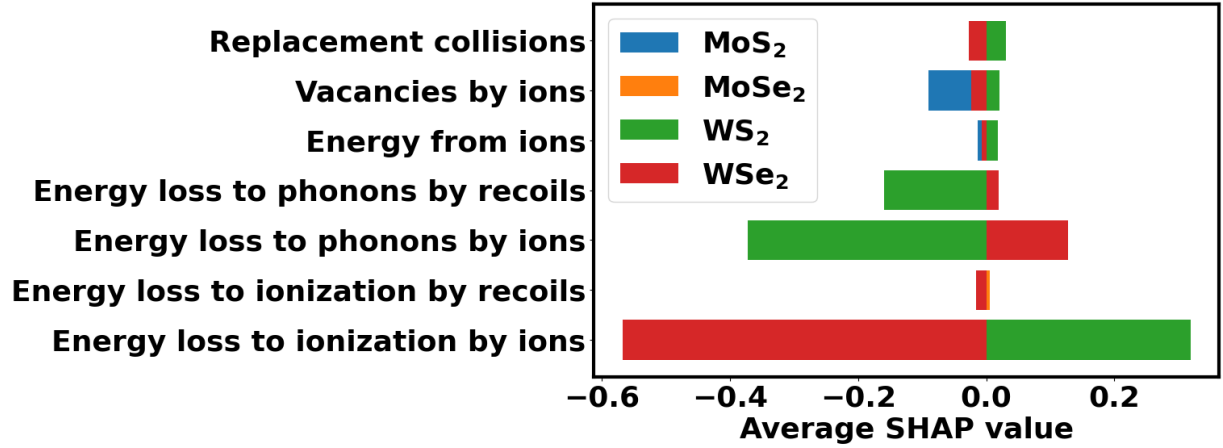


Figure 4.17: XGB Average SHAP values representing the influence of various defect parameters on the PCE of four different absorber materials (MoS₂, MoSe₂, WS₂, and WSe₂) under 0.15 MeV proton radiation.

The bars in Figure 4.17 represent the average impact of each feature (such as energy loss to ionization by ions, energy loss to phonons by recoils, etc.) on the PCE for each material. Notably, WS₂ and WSe₂ show a more significant influence across most features compared to MoS₂ and MoSe₂. It is important to note that the atomic number for Mo is 42 and 74 for W. WSe₂ has the highest mass density of 9.66 g/cm³ and WS₂ has the second highest mass density of 7.86 g/cm³ (Table 3.3 contains detailed data about mass densities). PCE is reinforced by energy loss to ionization by ions for WS₂, other parameters degraded it. Similar phenomenon happens for WSe₂. Absorbers with lower mass densities (MoSe₂ and MoS₂) did not participate in the energy loss significantly, indicating that these absorbers might withstand 0.15 MeV radiation efficiently. MoSe₂ and MoS₂ also showed high PCE under default condition. Hu et al. [91] studied structural designs for performance improvement in TMDC materials for solar applications, taking into account the production problems associated with large-area photovoltaic technologies.

Chapter Five

5 Conclusions

The ever-growing space explorations demand efficient solar energy technology to power-up the operations. The revolutionary development in materials science help us engineer newer materials that can withstand a specific environment while maintaining an outstanding performance. Hence, a new search for energy materials worthy of next generation solar cell absorbers is necessary, which can replace the costly silicon solar cells. In this simulation research, we have selected four candidates of TMDC absorber materials and analyzed them under 0.15 MeV and 3 MeV proton radiation, a common occurrence in space environment. We have used Monte-Carlo method-based software SRIM, SCAPS solver, and ML methods to investigate the effect of such radiation on the performance of the TMDC solar cells. We also have done a NIEL calculation to identify impactful proton energies that will cause more damage. MoS₂ and MoSe₂ produced higher PCE (28.16%, 28.11%) while WSe₂ and WS₂ produced high J_{sc} (39.36 mA/cm², 35.15 mA/cm²) under normal circumstances (AM 1.5G, 1000 W/m² incident photon). With 0.15 MeV proton radiation the performance dropped significantly. In comparison to the other two, MoSe₂ and WS₂ maintained high PCE of 19.47% and 17.01% respectively. Interestingly, the ML results predict that, WS₂ and WSe₂ are vulnerable to proton radiation more than MoSe₂ and MoS₂ absorbers. This tells us that more intense proton radiation with many energy variants can degrade the performance of WS₂ and WSe₂ based solar cells quickly. Although WS₂ and WSe₂ are promising as high J_{sc} and generating options, they are less suitable for proton radiation environments. The MoSe₂ and MoS₂ absorber-based solar cells are more effective against such environments.

Our research predicts that other materials with same features might follow this pattern. These findings are valuable and can act as a precautionary guidance for manufacturing space based TMDC solar cells. The space-based solar cells encounter other types of radiations as well. Future studies might explore those paths to add new insights to our research.

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