



## Synthesis of Structured Molybdenum Disulfide for Optoelectronic Applications

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### Abstract

#### Keywords:

Electrodeposition, Thin Film, Characterization, Deposition time variation

*In this paper, synthesis of molybdenum disulfide based photovoltaic materials deposited by electrode position method. The material films have been characterized for their optical properties using UV-VIS spectrophotometer with wavelength range of 300 nm – 900 nm and electrical conductivity using photoelectrochemical (PEC) cell measurement. The conductivity type of the electrodeposited materials was investigated together with the tuning of the optical phenomena. The materials deposited were obtained by varying deposition time from 5 minutes to 15 minutes for MoS<sub>2</sub>. It was observed that the optical properties of the materials increased with an increase in the time of deposition. The optical band gap of MoS<sub>2</sub> was found to be in the range 1.87 - 2.17 eV. The PEC signal results revealed MoS<sub>2</sub> as a p-type material.*

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### INTRODUCTION

Solar energy which is a free and abundant form of energy has the potential to provide sufficient power to the growing number of industries and population especially in the developing world (Akimoto *et.al*, 2006). Its maximum exploitation has however been hindered by the high cost of silicon based solar cells which currently dominate the market (Asaduzzaman *et.al* 2017). The available fossil fuels that currently power society will not meet up with demand over the long term, and the continued use of these conventional energy resources causes harmful side effects such as pollution that threatens human health and greenhouse gases (GHG) associated with climate change (Xia *et.al* 2015). It has been stated that the warming and precipitation trends due to anthropogenic climate change during the past 30 years already claim over 150,000 human lives annually (Slonopas *et.al* 2017). The sun is Earth's natural power source, driving the circulation of global wind and ocean currents, the cycle of water evaporation and condensation that creates rivers and

lakes, and the biological cycles of photosynthesis and life (Balitskii *et.al* 2013). Presently, solar and other alternative energy resources are being harnessed for various applications such as power generation, air-conditioning, space heating, domestic hot water system (Ikhioya. *et al*, 2020). In order to meet up with the world energy demand using the eco-friendly method (Mittal *et.al*, 2017), this work takes a look at how we can effectively harness the Molybdenum Disulfide (MoS<sub>2</sub>) for optoelectronic devices. Molybdenum disulfide (MoS<sub>2</sub>) is an inorganic compound that belongs to the transition metal dichalcogenides (TMDCs) class of materials and it has one atom of molybdenum and two atoms of Sulfur (S – M – S). The choice for this compound (MoS<sub>2</sub>) lies on the fact that its physical, chemical, and electronic properties makes it a promising material to substitute previously used semiconductor and graphene devices (Beck *et.al* 2005 and Manoharan,*et.al* 2016). The constituent materials are nontoxic and abundantly available (Salim *et.al* 2015) and (Khan *et.al* 2016), and that the MoS<sub>2</sub> has a high

absorption coefficient in the wavelength range 350-800 nm and low-cost of production (Olusola *et.al* 2020). This makes it a good absorber layer in solar cell devices. MoS<sub>2</sub> seems to solve many problems facing many semiconductor materials used for solar cell devices (Echendu *et.al* 2016). It has a wide energy band gap of 1.8 eV which changes from an indirect band gap to a direct one in thin structures (Ceviz *et.al* 2013). Thus, it is ideal for thin-film transistors with excellent on/off switching characteristics and high efficiency (Pandey, 2015), electrical and optoelectronic applications. Its fabrication is simple which means large production yield and low cost (Khan *et.al*, 2016). The covalent bonds between molybdenum and Sulfur and the Van der Waals bonds between its layers make it optimal for gas sensing and a lubricant in aerospace industry. It has a direct energy band gap, better charge transport, good absorption coefficient and highly transmittance material (Al-Hadeethi *et.al*, 2019). Olubosede . *et al*, (2020). In the study, Aluminum Selenide (Al<sub>2</sub>Se<sub>3</sub>) thin films were synthesized electrochemically using cathodic deposition technique in which graphite was used as a cathode while carbon as an anode. Synthesis was done at 353 K temperature from an aqueous solution of analytical grade selenium dioxide (SeO<sub>2</sub>), and Aluminum chloride (AlCl<sub>3</sub>.7H<sub>2</sub>O). The films are characterized for their optical properties and electrical conductivity. The optical properties of the films at varied voltages showed that the films are good materials in the formation of optoelectronic devices. Farami. *et, al* (2021) worked on optoelectronics applications of electrodeposited p- and n-type Al<sub>2</sub>Se<sub>3</sub> thin films. In the report, energy band gaps and electrical conductivity based on aluminum selenide (Al<sub>2</sub>Se<sub>3</sub>) thin films were synthesized electrochemically using cathodic deposition technique, with graphite and carbon as cathode and anode, respectively. Synthesis was done at 353 K from an aqueous solution of analytical grade selenium dioxide (SeO<sub>2</sub>), and aluminum chloride (AlCl<sub>3</sub>.7H<sub>2</sub>O). Junctions-based Al<sub>2</sub>Se<sub>3</sub> thin films from a controlled medium of pH 2.0 were deposited on fluorine-doped tin oxide (FTO) substrate using potential voltages varying from 1,000 mV to 1,400 mV and 3 minutes -15 minutes respectively. The films were characterized for optical properties and electrical conductivity using UV-vis and photoelectrochemical cells (PEC) spectroscopy. The PEC reveals a transition in the conduction of the films from p-type to n-type as the potential voltage varies. The energy band gap reduces from 3.2 eV to 2.9 eV with an increase in voltage and 3.3 eV to 2.7 eV with increase in time. These variations indicate successful fabrication of junction-based Al<sub>2</sub>Se<sub>3</sub> thin films with noticeable transition in the conductivity type and energy band gap of the materials. Consequently, the fabricated Al<sub>2</sub>Se<sub>3</sub> can find useful applications in optoelectronic devices.

It has been reported that molybdenum disulfide (MoS<sub>2</sub>) based thin film solar cell technology is known to be 40% cheaper than silicon based solar cells (Wang *et.al*, 2014). In order to effectively exploit solar energy, research into new materials for production of cheaper and efficient solar cell must be intensified (Olusola *et.al*, 2020). This paper, studies the properties molybdenum disulfide (MoS<sub>2</sub>) for possible applications in optoelectronic devices, determine the conductivity type of the material and improve and optimize optical properties of materials by the variation of time of deposition.

## MATERIALS AND METHODS

### Methodology

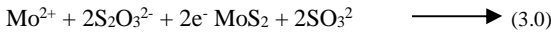
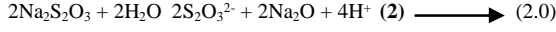
These materials and experimental methods used on MoS<sub>2</sub> were analyzed in this section. The materials used in this research work are potentiostat, magnetic stirrer, electrodes, substrate, pH meter and weigh balance. The reagents used consist of ammonium molybdate (NH<sub>4</sub>MoO<sub>4</sub>), Sodium thiosulfate (Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub>). All these reagents were of analytical grade, purchased and used without further purification. The FTO substrate of 2.3 cm<sup>2</sup> by 2.5 cm<sup>2</sup> was washed to remove oil substances and any other dirt from the surface of the substrate, so the substrate was washed with liquid soap, methanol, and acetone. After washing, the substrate was rinsed off with methanol and acetone. A graphite plate was attached to one of the electrodes, this electrode was taken as the working electrode, as the adhesive surface of the substrate was attached to the graphite plate after these three (carbon rod, graphite plate, and substrate) have been joined together with the PTFE, a multimeter is used to test the conductivity of the working electrode by putting negative pin of the multimeter at bottom of the carbon rod and the positive pin of the multimeter on any part of the adhesive surface of the substrate the figure below, a reading from the multimeter shows that current can pass through from the substrate to the bottom of the carbon rod. A buffer solution was prepared using a buffer of 4. The buffer of 4 was mixed and stirred with 200ml of deionized water for 30 minutes for the pH meter calibration and pH for the MoS<sub>2</sub> electrolytic bath was 4.6±0.1. The molarity of the chemical reagent was first calculated to ascertain the amount of the chemical reagent needed to achieve the desired molarity in the solution. For this research, the desired measurement for the deionized water which was the solvent used was 400ml.

$$\text{Molarity of solute} = \frac{\text{Mass of solute} \times 1000\text{m}}{\text{Molar mass of solute} \times \text{volume of solvent}} \quad (1.0)$$

### Synthesis of MoS<sub>2</sub>

Electrolytic bath of MoS<sub>2</sub> was prepared by dispensing 3 grams of ammonium molybdate (NH<sub>4</sub>MoO<sub>4</sub>) as a

source of molybdenum in a 500 ml beaker containing 400 ml of de-ionized water in a to form 0.06 mole. Also, 19.8 grams of sodium thiosulfate (Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub>) as a source of Sulphur was dispensed in a 500 ml beaker containing 400 ml of de-ionized water to form 0.2 mole and was added to the solution and the admixed solution was placed on the magnetic stirrer. A magnetic bar was added to the solution to increase the rate of stirring. The reactions can be described as follows:

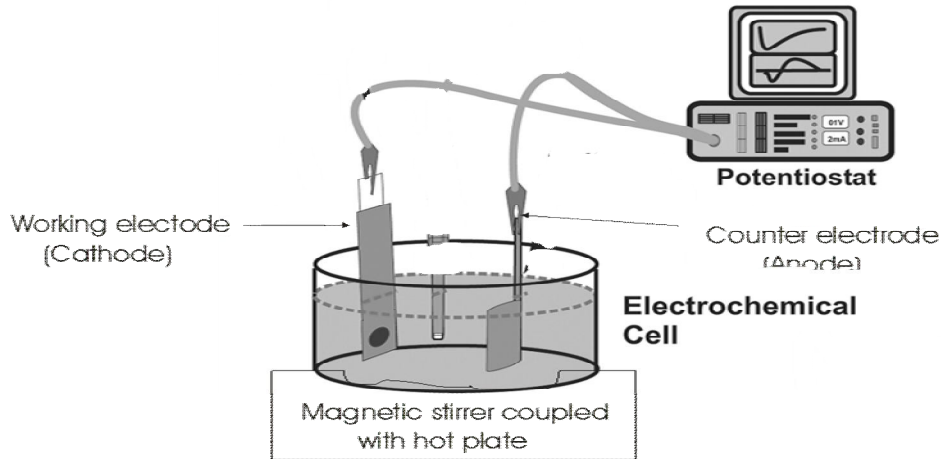


The magnetic stirrer was switched on and stirring of the solution was done for 1 hour to ensure homogeneous solution. The films were prepared at room temperature; the rinsed pH meter was used to

measure the pH level of the electrolyte and was found to be 4.6 pH values which was considered since the synthesis technique used is favored in acidic medium. The electrochemical deposition technique was adopted in depositing the films. Deposition took place at bath temperature of 70°C in 5, 10, 15 and 20 minutes of deposition durations. The prepared films were therefore cleaned and dried and subjected to optical analysis and electrical conductivity type examination using ultraviolet photospectrometer (UV-visible) and photoelectrochemical cell (PEC) measurement, respectively. The optical phenomena and optical constant were extracted using equations 4 to 11. The electrical conductivity type was deduced using equation 12.

**Table 1: The molarity, mass and molar mass of solutes in the electrolytic bath of ZnSe and MoS<sub>2</sub>**

Solute	Molarity (mol)	Mass (g)	Molar mass (g/mol)
Ammonium Molybdate	0.06	3	125
Sodium Thiosulfate	0.2	19.8	248



**Fig. 1.0** Schematic diagram of two-electrode System used for electrodeposition of MoS<sub>2</sub>

$$\text{Absorbance (A)} = \frac{\tau}{\ln 10} \quad (4.0)$$

$$\text{Transmittance } T = 10^{-A} \quad (5.0)$$

$$\text{Reflectance } R = 1 - (A + T) \quad (6.0)$$

$$\text{Photon energy (eV)} E = h\nu = \frac{hc}{\lambda} \quad (7.0)$$

$$A + T + R = 1 \quad (8.0)$$

$$\alpha = \frac{2.303A}{t} \quad (9.0)$$

$$k = \frac{\alpha\lambda}{4\pi} = \frac{\alpha\lambda}{12.57} \quad (10.0)$$

$$(\alpha h\nu) = A(h\nu - E_g)^n \quad (11.0)$$

$$\text{PEC Signal} = V_L - V_D \quad (12.0)$$

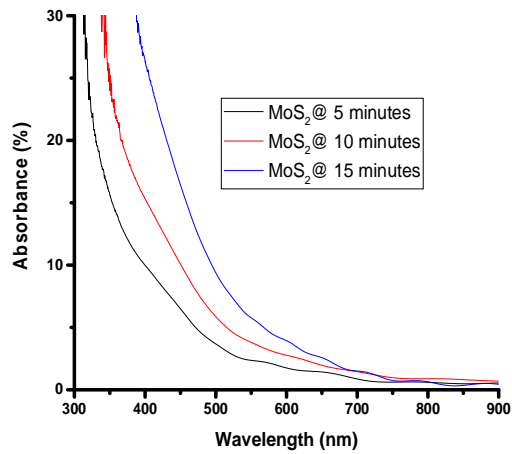
where  $\tau$  is the optical depth,  $h$  is plank constant,  $\nu$  is frequency,  $c$  is the speed of light and  $\lambda$  is wavelength,  $A$  is absorbance,  $T$  is transmittance,  $R$  is reflectance,  $\alpha$  is absorption coefficient,  $t$  is thickness of the film,  $A$  is absorbance,  $k$  is extinction coefficient,  $\lambda$  is wavelength of photon,  $h\nu$  is photon energy,  $A$  is a constant usually equal to 1,  $E_g$  is energy band gap,  $n$  is transition between the valence band and conduction band ( $n$  is 0.5 for direct transition and 2 for indirect), and  $V_L$  is voltage under light and  $V_D$  is voltage under dark.

## RESULT AND DISCUSSION

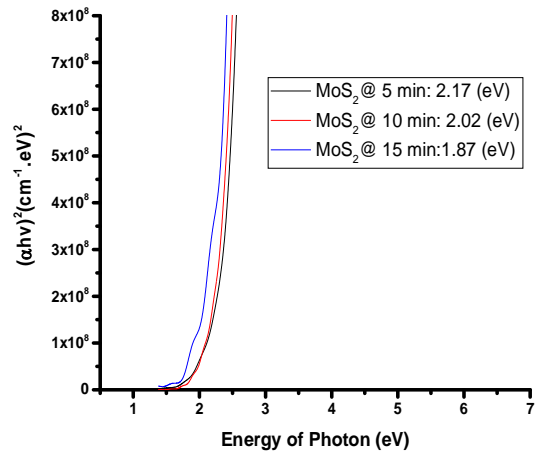
### Optical characterization of electrodeposited MoS<sub>2</sub> thin films

The absorbance spectral of the films obtained in UV-visible region with wavelength ranged from 300 nm - 900 nm is revealed in figure 2. The absorbance spans through visible region (400 nm – 700 nm) which is an indication the materials possess good absorption edge and such a good absorption edge characterized good absorber layers suitable for optoelectronic applications. The percentage of the materials' absorbance as a function of wavelength, as depicted, followed the occurrence of electromagnetic radiation on a transparent object. When a beam of light is impinged on a transparent object, part of the beam is transmitted, part is reflected and part is absorbed. The films transmittance was also observed which is an integral part of the optical phenomena that characterize the materials transparency. The films percentage of transmittance increase proportionally with the wavelength as depicted in figure 3. The transmission of light by the materials still spanned within the visible region. From figure 4, it could be seen that part of the electromagnetic beams reflected. In the figure, the materials percentage of reflectance reveal non-zero reflectance despite the variation of

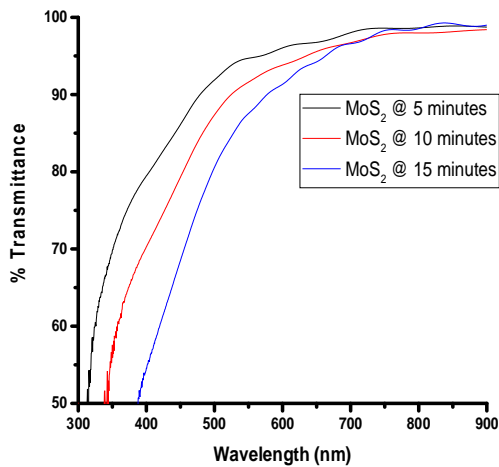
deposited time as spectra followed the same trend which means the material can reflect light. The average value of reflectance, absorbance and transmittance as a function of wavelength as depicted in table 2 were summed up and the result obtained showed that the materials is transparent. The energy band gap of Molybdenum Disulfide thin films prepared at different deposition time of 5, 10 and 15 minutes is depicted in figure 5. The obtained energy band gap through the horizontal axis of the plot by extrapolating the linear parts of the graphs using Tauc equation at absorption coefficient is zero ( $\alpha = 0$ ) is revealed in table 2. The energy band gap of the films decreases as the deposition time increases due to increase in the films thickness. It could be inferred that the energy band gaps of the films is inversely proportional to the thickness as a result of the varied preparative parameters arising from the quantum confinement effect. Absorption coefficient is a characteristic that describes how far light travels in materials before it is being absorbed. The dependence of absorption coefficient of MoS<sub>2</sub> thin film on wavelength (ranges from 300 nm to 900 nm) was investigated at different deposition time of 5, 10 and 15 minutes and the result were shown in figure 6. The absorption coefficient of good photovoltaic materials is not zero which means that the higher the absorption coefficient, the more photon energy absorbed. This shows that MoS<sub>2</sub> is a very good absorber layer material capable of absorbing more photon energy which is suitable for heterostructured based devices. The extinction coefficients of MoS<sub>2</sub> thin film as depicted in figure 7 showed a good optical characteristic which is corresponded to the absorption coefficient obtained. The relationship between the extinction and absorption coefficients of MoS<sub>2</sub> as established by the mathematical equation used revealed the suitability of MoS<sub>2</sub> material in fabrication of solar cells. The non zero ( $k \neq 0$ ) extinction coefficient showed how strong the materials absorb or reflect light at particular wavelength.



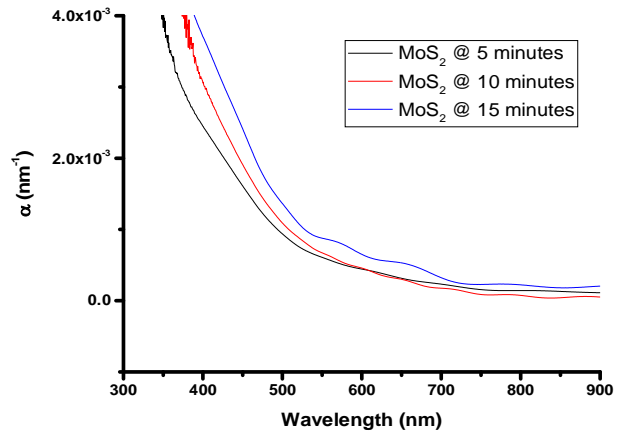
**Figure 2:** Percentage of absorbance of electrodeposited MoS<sub>2</sub> films at varied time of deposition as function of wavelength..



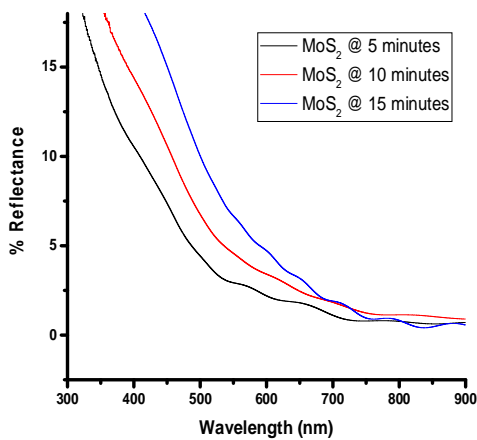
**Figure 5:** Energy band gap of MoS<sub>2</sub>



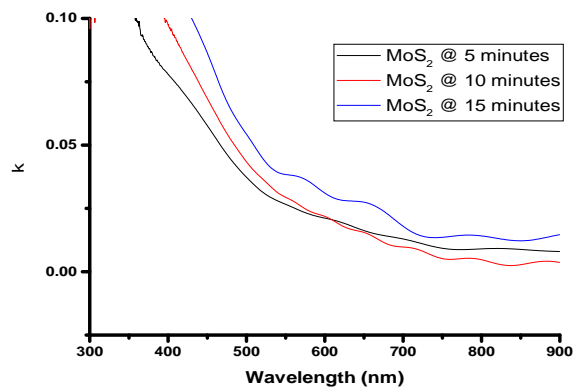
**Figure 3:** percentage of transmittance of MoS<sub>2</sub> thin films as a function of wavelength.



**Figure 6:** Graph of absorption coefficient versus wavelength for MoS<sub>2</sub>



**Figure 4:** Reflectance versus the wavelength of the MoS<sub>2</sub>



**Figure 7:** Graph of Extinction coefficient versus wavelength for MoS<sub>2</sub>

**Table 2. Optical measurements of MoS<sub>2</sub> at deposition time**

Time of Deposition	Absorbance	Transmittance	Reflectance	Total
5 minutes	0.1006	0.8293	0.0700	0.9999
10 minutes	0.1218	0.7945	0.0838	1.0001
15 minutes	0.1483	0.7558	0.0958	0.9999

**Table 3. Energy band gap for MoS<sub>2</sub>**

Time of deposition (minute)	Thickness (nm) MoS <sub>2</sub>	Energy band gap (eV) MoS <sub>2</sub>
5	62	2.17
10	144	2.02
15	198	1.87

**Photoelectrochemical (PEC) cell Analysis of MoS<sub>2</sub> thin films**

The PEC signals analysis was done to characterize the semiconductor type of the materials which gave access to the type of semiconductor the materials exhibited. The PEC was formed by forming a liquid junction between the substrate and reference electrode. When light is onto the liquid junction, the voltage reads and when light was on off, the voltage was also taken. When the light was switched on for 5, 10, 15 and 20 minutes, the voltage was taken.

In the same process as the light was switched off 5, 10, 15 and 20 minutes, the voltage was also taken. The voltages taken for 5, 10, 15 and 20 minutes when the light was switched off were subtracted from the voltages taken at the same time intervals when the light was switched on as depicted in table 4. The qualitative PEC signal of MoS<sub>2</sub> as depicted in figure 8, revealed the material is positive which is an indication of p-type layer materials.

**Table 4: PEC results for electrodeposited MoS<sub>2</sub>**

Substrate	Deposition time (minute)	V <sub>L</sub>	V <sub>D</sub>	V <sub>L</sub> - V <sub>D</sub> (V)	PEC signal (mV)
A1	5	-0.420	-0.422	+0.002	+2
A2	10	-0.416	-0.418	+0.002	+2
A3	15	-0.415	-0.416	+0.001	+1
A4	20	-0.414	-0.415	+0.001	+1

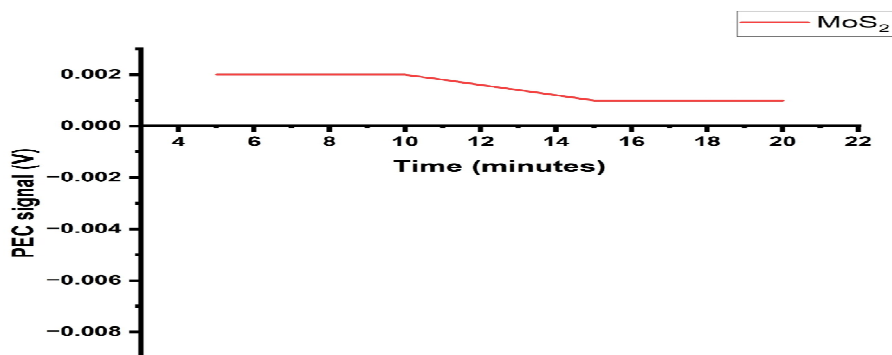


Figure 8: Graph of PEC signal as a function of time.



## CONCLUSION

The various characterizations carried out in the analysis of both the optical and conductivity type of the materials reveal the successful fabrication of MoS<sub>2</sub> thin film through the application of sophisticated electrodeposition technique. The optical phenomena such as reflectance showed clearly that MoS<sub>2</sub> thin film has less reflectance properties of light which is good for the absorption of light energy from the sun suitable for solar cells applications. Also, the low reflectance values make the thin films of MoS<sub>2</sub> an important material for anti-reflection coating. The energy band gap of MoS<sub>2</sub> and the thin film at deposition time of 5, 10 and 15 minutes are 2.17 eV, 2.02 eV and 1.87 eV which provided information about the proportionality of the materials energy band gap to both the time of deposition and the thickness of the films. The electrical conductivity type of the materials through the PEC analysis showed that the materials is p-type semiconductor suitable for junction-based devices. Since solar cells works on the principle of photovoltaic effect which is about the absorption of photon energy with direct conversion into useable energy, electricity required both p-type and n-type and our findings has shown that the materials conductivity type is not only dependent on cathodic potential but also depend on the time of deposition. Given this, the study has provided useful information about electrodeposition technique and tunability of Molybdenum Disulphide properties as the materials characteristics matches that of Cadmium Telluride. Since CdTe thin films are known to be poisonous despite their promising optoelectronic potentials, the electrodeposited materials could be used as a best alternative to CdTe.

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