

Comparative study of electrical and optical properties of SrPrFeTiO₆ double perovskite ceramic: A potential candidate for solar cells applications

AbuSandal A. AbuSandal¹, Muawya M. Elhadi^{1,2*}, Abdulsakhi H. Suliman¹,
Abdelrahman A. Elbadawi¹,

¹ Department of Physics, Faculty of Science and Technology, Al Neelain University, Khartoum 11111, Sudan

² Department of Physics, Faculty of Science and Humanities, Shaqra University, P.O. Box 1040, Ad-Dawadimi 11911, Saudi Arabia

Abstract

In this research three samples were prepared of double perovskite compound (SrPrFeTiO₆) by using eosin (Red color), yamidine (blue color), and blue Nile (blue color) dyes. The effects of this dye increase the efficiency of solar cell, we found that the yamidine dye is more efficient than eosin and blue Nile dyes, that is, $\eta = (3.73) \%$ yamidine and $(3.29, 3.48) \%$ eosin and blue Nile respectively, then this increase of efficiency to increase the absorption of color of yamidine. Then the energy band gaps were calculated, that is 3.789 eV, this range of band gap is good for semiconductor material. The electronic transition and molecular vibration were studied by using FTIR Spectroscopy, and studied optical properties using UV spectroscopy, and calculated the efficient of the solar cells due to the unique curve (I-V), $(3.29-3.48-3.73) \%$ the result show that increased in the efficiency of the cell due to compare with the previous study that found $(0.32-0.42-1.18) \%$, about all this studies materials can be used to industrial electronic devices and other using in the future.

Keywords: Double Perovskite, Optical Properties, Solar Cell.

Date of Submission: 04-12-2022

Date of Acceptance: 16-12-2022

I. Introduction

The mineral perovskite was discovered and named by Gustav Rose in 1839 from the sample obtained in the Ural Mountains. Perovskite, is named after a Russian mineralogist, Count Lev Aleksevich von Perovskite, whom was appointed Russian secretary of the interior in 1842. The term perovskite was originally reserved for the mineral CaTiO₃, and the first synthetic perovskite, were produced by Goldschmid (1926) of the university of Oslo leading to the use of the term perovskite as a description of a class of compounds sharing the same general stoichiometry and connectivity found in CaTiO₃. The technologic development and the more demands of the tomorrows society in material science field, puts continues the need for developed material with 2 improved properties. The perovskite structure has continuous attraction and highly interest, and this has proven its suitability for industrial application [1]. Then the term perovskite was used to describe the class of compounds sharing the same general stoichiometry and connectivity with perovskite oxide (CaTiO₃), which was first synthesized perovskite by Goldschmidt at 1926 in the University of Oslo [2].

In the last years, a high interest is focused on perovskite type compounds which show a large variety of interesting function properties such as Ferro, piezo, pyro-electricity magnetic order colossal magnetic resistance superconductivity etc.) due to their compositional and structural diversity. As a result, many compounds that belong to this group have been synthesized the general formula of perovskites is ABO₃ where (A and B) might be almost or semimetal from the periodic table. The perovskite structure has many types, single, double, and treble, the general formula is (ABX₃) nearly all stable elements in the periodic table have been studied in the perovskite framework A is an alkali, alkaline earth metal or rare earth metal element, B is usually a transition metal element, while X is anion such as F, Cl, Br, I and even H, etc. but usually oxygen. Several combinations of A- and B-site cations can form a stable perovskite-like structure, additionally A- B-site cations as well as oxygen anions can be partially substituted by other suitable elements [3].

Partial substitution allows the control of the valence state of A- and B-site cation as well as the non-stoichiometry (cation or anionic vacancies) in the mixed oxide based on electro neutrality arguments. The presence of a multiplicity of oxidation states is the major responsible for the catalytic properties of perovskite-type [4]. Perovskite compounds and related structures represent a large family of important inorganic materials which have been widely used in industry and comprehensively studied in the laboratory due to their wide

variation of useful and exotic properties samples under study have been studied before but in the form of single perovskite structures. The perovskite-like compounds AVO_3 where A is a three or divalent cation are widely studied due to their simple structures which allow a deep understanding of the relationship between structure and properties in these systems. AVO_3 oxides were reported for most of the divalent elements as A-cation for alkali-earth elements (except Mg) their structures are three-dimensional frameworks consisting of corner-shared VO_6 Octahedra in these structures are regular or slightly distorted and no formation of a short vanadyl bond is observed. Thus $SrVO_3$ is an ideal cubic perovskite and $CaVO_3$ is an orthorhombically distorted perovskite ($GdFeO_3$ type) [5].

While $BaVO_3$ forms trigonal 5H close packing in a wide range of oxygen nonstoichiometric; 4 Stoichiometric $CaVO_3$ and $SrVO_3$ compounds exhibit metallic-like conductivity down to 2-4 and Pauli paramagnetic behavior these properties can be changed by the variation of oxygen content [6] As now just a few compounds of ideal cubic structure were found based on the known compounds of perovskite McGaw and her colleagues pointed out that ion size difference between A and B atoms may lead to distorted structures Years earlier, Goldschmidt at the University of Oslo introduced the tolerance factor "t" which is an indicator for the stability and distortion of crystal structures and this pioneering work provided a basis for the further exploration of the structure of the perovskite family [7].

To obtain high energy from the solar cells that are still not effectively available, many researchers tend to use different methods to improve the performance of the solar cells to obtain a relatively efficiency that can be used in the field of industry and education. And the other by using perovskite as semi-conductive material in the manufacture of solar cells. Perovskite has been used as a semiconductor material to convert solar energy into electrical energy by making it a solar cell.

Many researchers have tried to obtain a high efficiency solar cell by grafting on two different elements to the study perovskite with the formula $SrPrFeTiO_6$ to know its structural and optical properties by using some of the techniques used such as infrared and FTIR and UV and IV characterization then making a solar cell from this compound and study of optical and electrical properties.

Elbadawi, A.A., Yassin, O.A. and Siddig, M.A. (2015) studied the effect of negative ion size on the disorganization of the Structural properties at position (A) of the sample ($SrPrFeTiO_6$) where the following elements (A=La, Pr, Nd) concluded that placing (Pr) in the position (A) double perovskite led to the study of this property by using the X-ray diffraction (XRD) and Fourier Transform Infrared FTIR samples have the same structure (orthorhombic) with Pnma space group. There are also some differences in the lattice parameter where differ from $SrLaFeTiO_6$ up to $SrNdFeTiO_6$ as follows $a=5.557 \text{ \AA}$, $b=7.824075 \text{ \AA}$, $c=5.537659 \text{ \AA}$ for La and $a=5.52728 \text{ \AA}$, $b=7.79671 \text{ \AA}$, $c=5.52395 \text{ \AA}$ for Pr, and $a=5.51584 \text{ \AA}$, $b=7.79255 \text{ \AA}$, $c=5.5131 \text{ \AA}$ for the Nd. The patterns were subjected to careful analysis by means of the standard Reitveld method using the Full Prof suite [17]. Three structural models were selected instead of the refinement processes for accurate determination of the best crystal structure matching the data. The anti-site effect of the Fe and Ti atoms is considered by their shared occupation between the Band B' sites. The XRD characterization showed that all samples are single phase, the best fitting results are achieved, the FTIR spectra results of the samples under study, the FTIR spectrum resembles the general appearance of the double structure. A shift in the peak position in going from La up to Nd sample in the group has been noticed. In the last studied and the results they reached will be compared with ours.

Maha A. Mohamad (2018) et al. used devices such as infrared and XRD to know some of the physical and optical properties of this sample and a simplified model was made as an applied work for this material in order to know the scalability of the material as a good solution for a simplified solar cell as the practical application for this sample. The relative efficiency of it was also calculated by reading the voltage and current as well, as identifying some of the structural and optical properties of the perovskite.

The double perovskite oxide with formula $CaLaMn_{1-x}FeTiO_6$ were ($x = 1, 0.33, 0.67$) was successfully prepared. The samples showed variation in crystal structure from monoclinic to cubic, the band gaps of the samples from the absorption edges were found to be closer to the value that calculated by Tauc plot. The absorption and optical band gap energy classified the series as semiconductor material, double perovskite solar cell based on a Thin Film double perovskite active layer of solar cells sandwiched between FTO and graphite on FTO electrodes were fabricated. The three FTO, double perovskite, and graphite of FTO solar cell were produced and characterized, which provided η of (1.18, 0.42, and 0.32%), FF of (0.84, 0.89, and 0.95) Jsc of (9.91, 19.12, and 14.6).

II. Materials and Methods

Preparation of double perovskite oxide is usually conducted through a multi-stage procedure [86] because it is difficult to prepare by the direct solid state reaction, and this is because there is a possibility of a growth of a single perovskite structure as a second phase along with the double perovskite phase. Thus, Here it is aimed to outline the series of samples while keeping in mind the relation between them when we look in to

their physical properties, the compound SrLaFeTiO₆ is considered as the core sample. The following diagram shows the guide of the sample sequences.

The raw metal carbonate and oxide's materials SrCO₃, Fe₂O₃, TiO₂, and Pr₇O₁₁ are all from Alfa Aesar of purity 99.9%, two heating schemes were used to prepare the samples. The first one is the conventional solid reaction in which all starting raw materials are mixed and heated up to 1200°C. This method we will name the direct method. The second route is to mix and heat the 3d oxide materials together at the first beginning and then mix and heat with the alkaline earth carbonate and the rare earth oxide. The last method we will call it precursor method. In the following sections, the details are given, the general scheme is illustrated. All the heat treatments are carried out inside Carbonites Furnace Model 1700 (Aston lane, hope Sheffield, S 30 2RR England)

In this method, the appropriate amounts of the starting materials are mixed, dry and ground and for a few minutes. A small amount of acetone was added after that hand ground and left to dry in air, subsequently heated in the furnace at 900°C for 12 hours to remove carbon dioxide. This calcination step is next followed by dry grinding and pressing, the powder was pressed in to pellets under 1.9×10^8 N/m² pressure for 30 seconds. Then heated for 24 hours with intermediate grinding. Finally, the samples were ground again and pressed as before and sintered at 1200°C hours using a heating rate of 10°C/min.

The ferrous and titanium oxides were first mixed carefully and ground manually to 45 minutes continuously in agate mortar with a little amount of acetone for homogeneity. After that, the mixture was put into high density alumina crucible and heated up to 900 °C for 12 hours. After cooling to room temperature, the alkaline earth carbonate and rare earth oxides were added, grind, and then pressed in to pellet form at pressure 1.9×10^8 N/m² and heated at 900 °C with a rate of 10 °C /min for 12 hours. This calcinations step was repeated twice to remove the carbonates from the sample. Finally, the samples were ground again and pressed as before and sintered at 1200 °C for 12 hours at a rate of 10 °C /min. All samples were cooled to room temperature with the same rate as that of heating.

In the beginning, I prepared the double perovskite ores by cleaning the tools and FTO glass plates by using distilled water and ethanol nitric acid, then I took a period to dry, then the ends were tested using an voltmeter to ensure their work after that I poured a quantity of the sample on the surface of the glass plates with chlorine by to precipitate. The sample entered the electric furnace for an hour under the frounce of temperature 100°C. In the second step, the sample was cooled for a period of time the rest of the other glass panels were coated with yam dine dye the other with dye the other with Eriochrom- black T dye and the last plate with lead well, and the eosin dye was used on the other end.

These panels were combined with each other to form a conductive layer, and the prince's device, voltmeter and light source were used to increase the intensity of illumination.

Finally, the prince and the voltmeter were read together and then the results were recorded.

III. Results and Discussion

Different characterization techniques were used following the preparation of the samples to investigate their structure and optical properties. The detail information about the structure of the samples can be obtained from FTIR measurement, and the optical properties were investigated using Ultraviolet visible spectroscopy and Fourier Transform infrared spectroscopy (FTIR). This chapter represents the results that take from the powder for the sample of double perovskite oxide were collected in order to get the formation of sample studied by three devices. FTIR result are show in figure (1) and Uv results in figures (2) and Energy band gap, figure (3) Transmission and figure (4) Reflection, figure (5) Absorption coefficient, figure (6) I-V curve of double perovskite SrPrFeTiO₆ solar cells sample (1) and figure (7) double perovskite SrPrFeTiO₆ solar cell sample (2). Figure (8) double perovskite SrPrFeTiO₆ solar cell sample (2).

Figure (8) double perovskite SrPrFeTiO₆ solar cell sample (3) and table (1) show the basic of electrical properties of proposed perovskite solar cell and the table (1) result of relation between the voltage and current (I) Table, (2) result of relation between Voltage and Current (II) Table (3) result of relation between Voltage and Current (III).

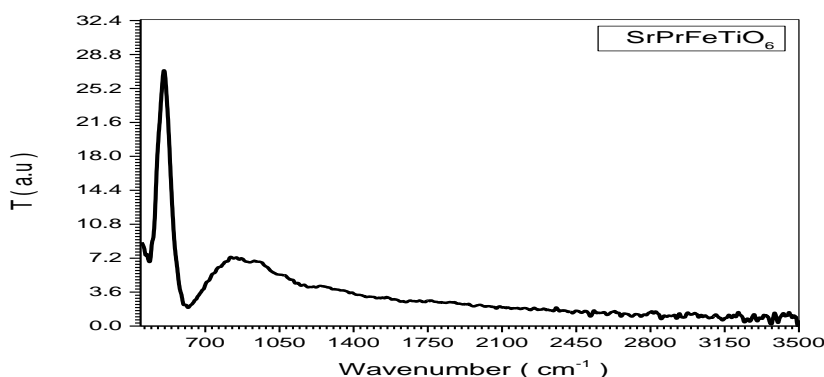


Figure (1) FTIR spectrum of SrPrFeTiO₆

Table 1 FTIR wavenumber of SrPrFeTiO₆

Wave number	Absorption range	Functional group	Type of vibration
436	500-436	Aryldisulfides	S-S stretch
607	690-515	alkyl Iahabides	S-S stretch
907	910-665	1,2 amines	N-H wag
1200	1300-1000	Ethers	C-O stretch
2520	3300-2500	Carboxylic acids	O – H stretch
2850	2800-3000	Aldehydes CH ₂ C=OH	C-H Stretch off C=O
3140	3300-3200	Alkynes CH≡ OCH ₃	C-H stretch
3260	3500-3100	Amides	N-H stretch similar to amines
3380	3500-3200	Alcohols, phenols	O-H stretch, H- Bonded

The chemical structure and bonds of samples were verified. Several bands due to combinations double perovskite SrPrFeTiO₆ of S-S, N-H, C-O, O-H, C-H, C=O, entities appear in the range(700-3500)cm⁻¹The obtained FTIR results are shown in table(1) in the S-S stretch appeared at 436,607 cm⁻¹, N-H stretch appeared in the region between 907 to 3260 cm⁻¹ in 3260 similar amines and wag in 907 cm⁻¹ strong and broad, C-O appeared in region between1000 to 1300 cm⁻¹ in 1200cm⁻¹ belong to ether, O-H appeared between 2520 to 3380 cm⁻¹ medium carboxylic acid in 2520 and alcohols, phenols in 3380 cm⁻¹, C-H appeared between 2800-3000 cm⁻¹ belong to Alkanes exactly in 2850 cm⁻¹ and C=O appeared between 2800 to 3000 exactly in 2850 cm⁻¹ of double bond as carbonyl.An infrared spectrum characterizes a fingerprint of a sample with absorption peaks s, which corresponds to the frequencies of vibrations between the bonds of the atoms making up the material. Because each different material is a unique blend of atoms, not a y, two compounds produce the same infrared spectrum. For that reason, infrared spectroscopy can result in a positive identification (qualitative analysis) of every different kind of material. In addition, the size of the peaks in the spectrum is a direct sign of the amount of material present [24].

The ultraviolet-visible spectroscopy (UV-Visible) was used to determine some optical properties and energy band gap of the synthesized samples.

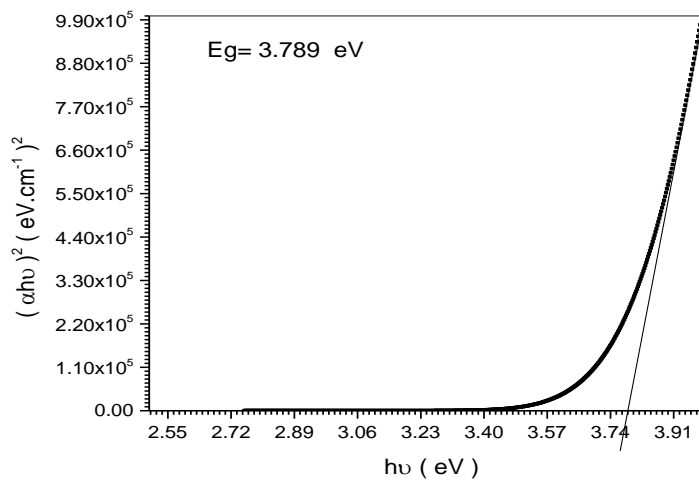


Figure (2) optical energy band gaps of double perovskite SrPrFeTiO₆

The optical energy gap (E_g) was calculated by the relation: $(\alpha h\nu)^2 = C (h\nu - E_g)$ Where (C) is constant. By plotting $(\alpha h\nu)^2$ vs photon energy ($h\nu$) as shown in fig (2) for the double perovskite SrPrFeTiO₆, the value of the energy gap has been calculated. In fig (2) the value of (E_g) of sample was obtained (3.789) eV). The transition is indirect and this uses for the industrial devices en route for convert materials from insulator to semiconductors.

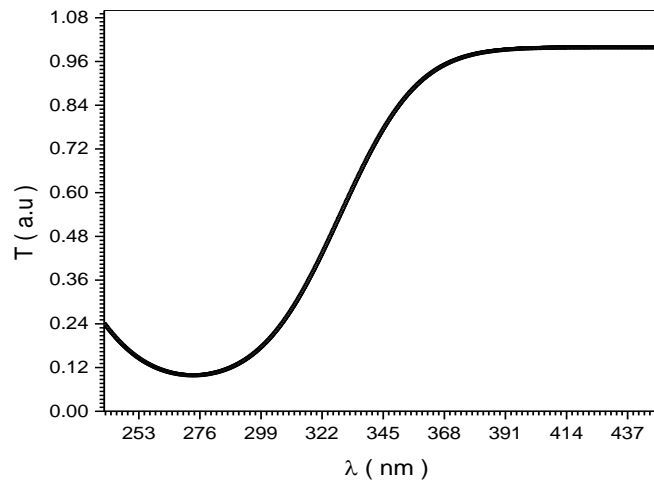


Figure (3) transmission of double perovskite SrPrFeTiO₆

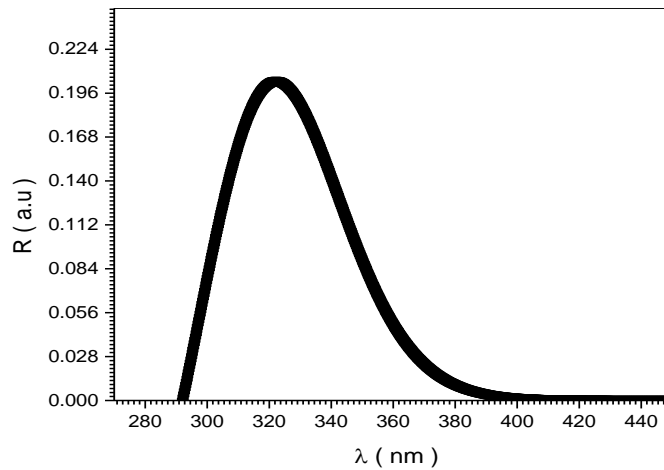


Figure (4) reflection spectrum of double perovskite SrPrFeTiO₆

The optical reflectance (R) spectra in the (280 – 440) nm wavelength range for the double perovskite SrPrFeTiO₆ samples are depicted in Fig (4). The maximum reflection is observed at (290.55 - 416.12) nm range for all samples, in this range the samples will be mirror.

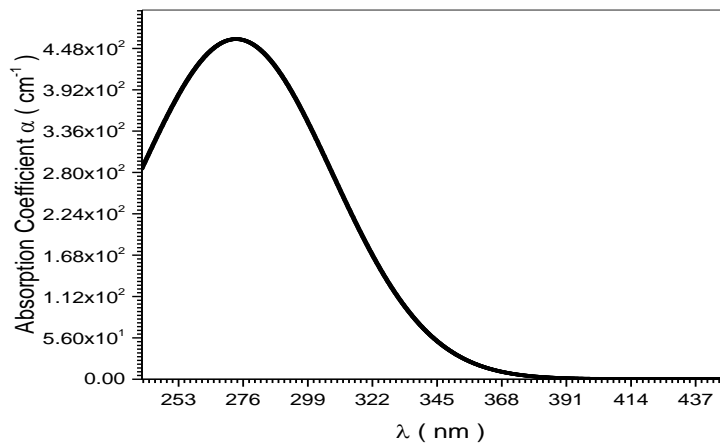


Figure (5) absorption coefficient spectrum of double perovskite SrPrFeTiO₆

Absorption coefficient (α): The absorption coefficient (α) of the double perovskite SrPrFeTiO₆ were found from the following relation $\alpha = \frac{2.303 \times A}{t}$ Where (A) is the absorbance and (t) is the optical length in the samples. In fig (5) the plot of (α) with wavelength (λ) of the samples was shown for the double perovskite SrPrFeTiO₆. The absorption coefficient obtained for the sample at $\alpha = 46170 \text{ cm}^{-1}$ at UV region (273.5 nm). This means that the transition may be corresponding to a direct electronic transition, and the properties of this state are important since they are responsible for electrical conduction.

Table 1 shows the basic electrical properties of the proposed perovskite solar cells

Sample	Area(cm ²)	I _{sc} (mA)	V _{oc} (volt)	J _{sc} mA/cm ²	F.F	PCE%
SrPrFeTiO ₆	0.33	26.78	0.563	4.114	0.78	3.23
		20.39	0.761	3.132	0.86	3.73
		27.27	0.578	4.189	0.79	3.48

Table 4.1.1 result of relation between Voltage and Current (I)

Voltage (V)	Current (mA)
0	27
0.11	27
0.24	27

0.31	27
0.39	26
0.45	25
0.52	21
0.56	12.6
0.56	0

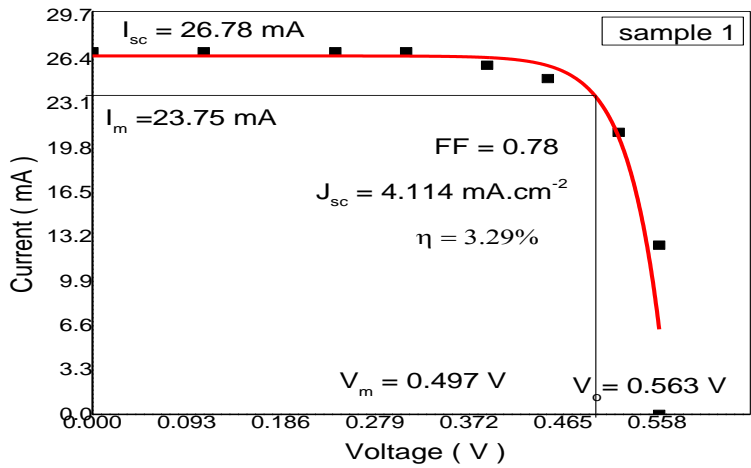


Figure (6) I-V curve of double perovskite SrPrFeTiO₆ solar cells

Table 4.1.2 result of relation between Voltage and Current (II)

Voltage (V)	Current (mA)
0	21
0.17	21
0.38	21
0.52	21
0.68	17
0.75	12
0.75	5.5
0.76	0

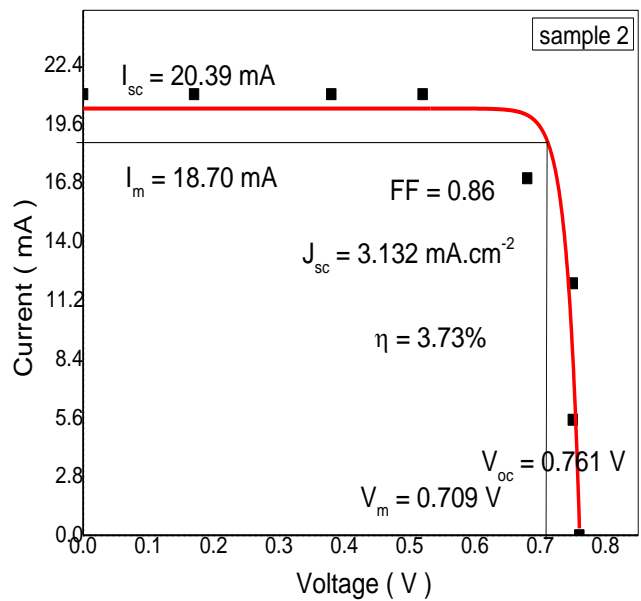


Figure (7) I-V curve of double perovskite SrPrFeTiO₆ solar cells

Table 3 result of relation between Voltage and Current (III)

Voltage (V)	Current (mA)
0	27.54
0.1133	27.54
0.2472	27.54
0.3193	27.54
0.4017	26.52
0.4635	25.5
0.5356	21.42
0.5768	12.852
0.5768	0

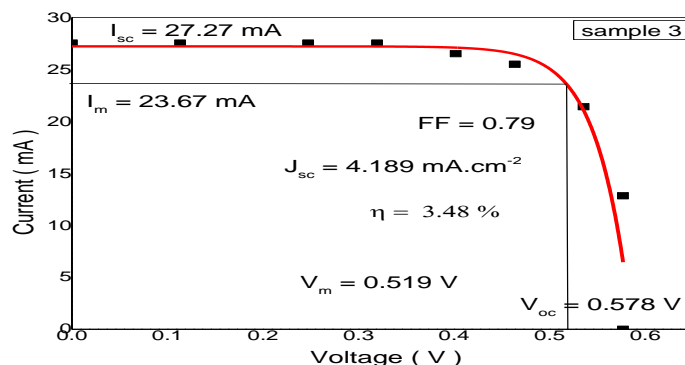


Figure (8) I-V curve of double perovskite SrPrFeTiO₆ solar cells

IV. Discussion Of The I-V Characteristics Result:

The I-V reading for the three sample of double perovskite solar cell are fabricated in the table (1) below is used to find (I_{sc}), (V_{oc}), (I_{max}), and (V_{max}) it is found that these parameters have the J_{sc} of samples. the fill factor(FF) is found by dividing maximum out power (P_{max}) by the product of short-current and the open-circuit voltage equation to calculate the maximum power is given by max volt(V_{max}) and max current (I_{max}) the power conversion efficiency (η) of the double perovskite solar cell is determined by the photocurrent density measured at short-circuit V_{oc} the F.F of the cell .and the open-circuit and J_{sc} as shown in equation these results for the three samples are recorded in table (1) the varied in efficiency for the three samples is often due to the doping rates I-V reading are displayed graphically in the figures (6, 7 and 8).

References:

- [1]. E.A. Perianu., Ioana. Aurodea., Rev. (Bucharest), 62 (2011), 17-22.
- [2]. A.A. Elbedawie, O. A Yassin., Abbasher. A. Gismelseed., Magnetism and Magnetic Material 32, (2013),1-6.
- [3]. Dhahri, Ahmed, Laifi, J., Gouadria, Soumaya, Elhadi, M., Dhahri, E., Hlil, E. K., RSC Advances, Issue 7, 2022. <https://doi.org/10.1039/D1RA07059B>
- [4]. A.S. Bhalla, Guo, R. and R. Roy, (2000). The Perovskites Structure- a Review of its Role in Ceramic Science and Technology, Mat. Res. Innovat. 4,3-26.
- [5]. H. Inoue; Marikina, K; Fukuchi, H.; Ts uji, T., Ige, F., Nishihara, Y. Physical B. 194-196, 1067, (1994).
- [6]. R. V. Shpanchenko, V. Chenaya, A.M. Abakumov, J Hadermann, G. Van Tendeloo, E.E. Kaul, C. Geibel, D. S heptyakov, and A. M. balagurov.. Chem.627, 2143-2150, (2001).
- [7]. Y. J. Ueda. Solid State Chem. 135,36.(1998).
- [8]. Full Prof Suite, Juan Rodrigues-Carbajal, Laboratoires Brillouin (CEA-CNRS) EA /Saclay,91191 Gif sur Yvette Cedex. (2011).
- [9]. A.S. Bhalla. Guo, R.and R. Roy, the Perovskite Structure-review of its Role in Ceramic Science and Technology, Mat.Res. Innovat.4,3-26, (2000).
- [10]. Al. Singh et.,J.Appl. Phy.107,09D917. (2010).
- [11]. R.M. Silverstein,and Bassler, T.C., Morrill, Spectrometer Identification of Organic, Compounds 4th ed., New York: Wiley,166. (1981)
- [12]. D.A. Skoog. Holler, F. J, Crouch, S, R., Principles of Instrumental Analysis,6th ed, Thomson Brooks/Cole: Belmont, CA, pg.434. (2007).
- [13]. A.R. West, Solid state Chemistry and its Application, John Willey Sons Singapore. (1887).
- [14]. A. Awad Allah, M. Elhadi, O.A. Yassien, Synthesis and Characterization of ALaFeNi_{0.5}W_{0.5}O₆ (A= Sr or Ca), a New Structure Distorted Double Perovskite, Advanced Materials Research Vol. 717 (2013) pp 133-138.
- [15]. Adel Ben Ali; E. M. Benali; SoumayaGouadria; M. Elhadi; ah. Dhahri; M. P. F. Graça; M. A. Valente; B.F.O. Costa, Journal of Materials Science: Materials in Electronics volume 33, pages16236–16250 (2022).
- [16]. D.R. lide, Handbook of Chemistry and physics, 75th ed.,BoceaRaton,FL:CRC Press,9-97, (1994).
- [17]. Ahmed. Dhahri , Arwa Belkahla , J. Laifi , SoumayaGouadria , M. Elhadi , J. Dhahri , E. Dhahri, Inorganic Chemistry Communications, V141,109570,July 2022,
- [18]. R, E. Newnham ,MRS Bulletin May. 20 -34, (1997).

- [19]. Song Zhen –Wen and Liu Bang-Gui, Chin Phys.BVol.22, No.4047506, (2013).
- [20]. V. Luana, Costalesz, A and Martin Pendas A. Phys.RevB.55(7) 4285-4287. 5-4287, (1997)
- [21]. Hoffman, M, Martin, S., Choi and Hahnemann D., chemical Review, vol. 95, 69-96, (1995).
- [22]. J. Jpank0ve. Optical Processes in Semiconductors', Prentice-Hall Englewood Cliffs, New Jersey, (1971).
- [23]. Klaus Jger, et, al, Solar energy, fundamentals, Technology and systems Copy-right Delft university of technology 2014.
- [24]. Coates J., interpretation of infrared Spectra, A Practical Approach Encyclopedia of Analytical Chemistry pp.10815-10837, (2000).

AbuSandal A. AbuSandal, et. al. "Comparative study of electrical and optical properties of SrPrFeTiO₆ double perovskite ceramic: A potential candidate for solar cells applications." *IOSR Journal of Applied Physics (IOSR-JAP)*, 14(6), 2022, pp. 16-24.