Review Article

A Brief Review of the Optoelectronic Properties of Delafossite Materials for Solar Cell Applications

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Delafossite materials have excellent properties making them highly sought after for the next-generation solar cells. They are based on abundant and non-toxic elements, and since environmental and economic factors are crucial in pursuance of discovering a new solar energy harvester, extensive research has been done. This paper reviews various synthesis methods, crystal structure and optoelectronic properties of delafossite materials. The calculated solar cell parameters such as short-circuit current (J_{sc}), open circuit voltage (V_{oc}) and efficiency (η) for solar cells fabricated through diverse conditions are reported. The findings indicate that these materials are ideal for use in solar cells as they can function as photocathodes or photoanodes in p-type dye-sensitised solar cells (DSSCs) and also serve effectively in absorber layer and hole transport layers. Their unique crystal structure with tunable band gap allows for maximizing power conversion efficiency. However, there are still limitations in synthesizing the nanoparticle structures to achieve desired properties, and improvement in various aspects and higher efficiency are still required.

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1. Introduction

In recent years, interest in solar cells as an alternative energy source elevated more intensely[1]. Solar cells harness energy from the sun, which is an abundant and renewable source unlike fossil fuels[2]. Compared to traditional energy sources, solar energy is clean and it reduces air and water pollution helping combat climate change. It provides a reliable energy solution improving access to electricity

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and enhancing the quality of life. Huge advancements have been made in photovoltaic technology, however, improvements in various aspects such as efficiency, costs, sustainability etc. are still very much needed[3]. Solar cell technology is classified into three main generations indicated in ***Table 1***. The working principle was based on the photoelectric effect. Silicon wafers are used for the production of first-generation solar cells[4]. They remained dominant due to non-toxicity, abundant and high-power conversion efficiency. The main drawback was its high cost and energy-intensive manufacturing. The thin film-based solar cell was reported later and they are cheaper than crystalline silicon as they require less amount of construction materials. However, efficiency is lower than that of the first generation. High power conversion efficiency exhibited by third-generation solar cells shows promise for use in next-generation solar cells but is not commercially investigated in detail[5].

In 1873, Charles Friedel first discovered the delafossite compound. It was named 'delafossite' after Gabriel Delafosse, a French mineralogist and crystallographer[6]. Delafossite materials with the general formula ABO_2 can display various electrical properties based on their composition. Additionally, they can exhibit p-type conductivity without intentional doping[7]. Silver-based Delafossites have conductivities similar to or lower than that of copper-based Delafossites with wider optical band gaps and lower visible light absorption[8]. Indirect fundamental band gaps from 1 – 2 eV have been reported for $CuAlO_2$, $CuGaO_2$ and $CuInO_2$[9]. Further research to find delafossite using Density Functional Theory (DFT) results in variety of properties like metals, magnetic metals and p-type conductivity.[10]. Among the p-type candidates, $CuCrO_2$ is a good material for achieving a required p-type transparent conducting oxides (TCO) properties[11].

Delafossite materials are considered to be a good candidate for solar cell applications because of their exceptional electronic as well as optical properties. A low-cost $CuAlO_2$ nanoparticle of ~ 20 nm in size shows good use in solar energy converter[12]. With Shockley-Queisser limit (SQ) and Spectroscopic Limited Maximum Efficiency (SLME), efficiencies of 14% and 12.5% for CuAlO2 were observed respectively[13]. Theoretical analysis of $CuFeO_2$ shows a maximum achievable efficiency of 28% in SQ limit which is comparable to modern-type solar cells[1]. Delafossite nitrides like $CuTaN_2$, $CuNbN_2$, $AgTaN_2$, and $AgNbN_2$ show good light absorption ranging from 1.0 to 1.7 eV, while $AuTaN_2$ and $AuNbN_2$ have band gaps and onset of absorption close to the ideal value for higher efficiency, which suggests that they are good candidates for an absorber material in solar cell[14]. Copper-based Delafossites have been incorporated into DSSCs to enhance their solar cell performances. One of the

highest open circuit voltages (357mV) for p-DSSCs has been achieved for $CuGaO_2$ nanoparticles. Compared to NiO which has a dark colour, these nanoplates are white presenting an attractive advantage[15][16]. High cathodic photocurrents (0.954mA cm^{-2}) were also observed when fabricated using $CuAlO_2$[17]. The $CuMO_2$ (Al, Ga, Cr) compound has a lower valence band edge, higher optical bandgap and conductivity making them useful for alternative materials over commonly used NiO in p-DSSCs[18]. A successful synthesis of heterojunctions between ZnO and $CuCoO_2$ showed an efficiency of 6.27% resulting in $CuCoO_2$ acting as a promising photoanode[19]. Doping of delafossite can enhance their performance as well[20][21], however, it is important to note that the impact of doping depends upon the number of valence electrons of the dopants[22]. Delafossite oxides are attractive candidates for hole transport layers (HTL) in perovskite solar cells because of their wide band-gap, suitable energy band alignment with the perovskite absorber and simple fabrication exceeding 14% in efficiency[23].

In this paper, we review the crystal structure, synthesis methods, electronic properties and optical properties of different delafossite materials and their solar cell parameters. Compared to other materials, delafossite materials are less explored. A limited understanding of their optical properties, defect physics and interfaces restricts their optimization for solar cell applications.

2. Structural Characteristics of Delafossite Materials

Delafossites, a cuprous meta ferrite, with the general formula ABO_2 is a class of ternary oxides characterized by edge-sharing octahedra and A atoms arranged in O-A-O dumbbell structure[24]. The A cation typically includes Cu, Ag, Pd or Pt, while B is a trivalent cation, often a transition metal as well as p-block metal and rare earth elements[7]. Delafossite structure have two alternating layers, one with triangularly arranged A cations and the other with edge-sharing BO_6 octahedra aligned along the c-axis. The arrangement allows for two structural polytypes depending on the stacking of the planar layer. The hexagonal 2H type is formed by 'AaBbAaBb' stacking with $P6_3/mmc$ space group while the rhombohedral 3R type consists of 'AaBbCcAaBbCc' stacking with space group $R^{-}3m$. Both polytypes are shown in ***Figure 1***. Structural data of various delafossite materials are presented in ***Table 2***. The a-axis is mainly determined by the B site ionic radii and the c-axis by the atomic radii of A atoms[11]. The hexagonal structure of delafossite exhibits only *a* and *c* lattice parameters[14]. Numerous delafossite structures have been reported including copper-based Delafossites $CuMO_2$ (M=Al, Sc, Ga, In, Y, Cr, Co,

La, Nd)[7], delafossite nitrides ABN_2 (A=Cu, Ag, Au and B=Ta ,Nb ,V)[14] and silver based Delafossites $AgBO_2$ (B= Al, Ga, Sc and In)[8].

Solar Cells	Cell type	Efficiency	Description
First generation	Monocrystalline	17% - 18%	• Oldest and most popular • High power efficiencies • High cost of production
	Polycrystalline	12% - 14%	
Second generation	Amorphous silicon	4% - 8%	• More economical than first generation • Thin light absorbing layers • Less efficient compared to first generation
	Cadmium Telluride	9% - 12%	
	Copper Indium Gallium Di-Selenide	10% - 12%	
Third generation	Nanocrystal	7% - 8%	• High efficiency potential • Innovative materials and designs • Tunable properties • Limited investigation in detail
	Polymer	3% - 10%	
	Dye Sensitized	10%	
	Concentrated	40%	
	Perovskites	31%	

Table 1. The first, second and third generations of solar cells

3. Synthesis methods

Several methods have been reported for synthesising delafossite materials. Copper-based Delafossites have been efficiently synthesized using solid-state reactions. This method involves solid reactants mixing in stoichiometric proportions using methods such as ball milling and then pressing into pellets. The mixture is then treated with high temperatures ranging from 600-1500°C carried out in a nitrogen atmosphere[22][25][26][27].

Various low-temperature synthesis methods have been applied to synthesize Delafossites and among them, hydrothermal reactions are one of the most common methods. This technique starts with

reacting parent precursors in HCl or NaOH solution, transferred to an autoclave heated with the desired temperature for a set duration. The autoclave is then cooled at room temperature and the resulting precipitate is filtered, washed and dried[8][19][20][23][28][29]. Another low-temperature synthesis technique is the sol-gel method. This method involves combining metal oxides or salts with an alpha-hydroxycarboxylic acid like citric acid and adding polyhydroxy alcohol. The solution is allowed to dry for a few days at room temperature followed by thermal treatment at the desired temperature to remove the chelating organics[3][17].

Compound	Space Group	a (Å)	c (Å)	Ref.
$CuCrO_2$	$R^{-}3m$	0.29772	1.7113	[25]
$CuAlO_2$	$R^{-}3m$	2.86	17.21	[13]
$CuTaN_2$	$R^{-}3m$	3.156, 3.152	17.565, 17.518	[14]
$CuNbN_2$	$R^{-}3m$	2.895	17.520	[14]
$CuVN_2$	$R^{-}3m$	3.159	18.999	[14]
$AgTaN_2$	$R^{-}3m$	3.154	18.946	[14]
$AgNbN_2$	$R^{-}3m$	2.917	18.932	[14]
$AgVN_2$	$R^{-}3m$	3.164	18.806	[14]
$AuTaN_2$	$R^{-}3m$	3.161	18.746	[14]
$AuNbN_2$	$R^{-}3m$	2.921	18.76	[14]
$AuVN_2$	$P6_3/mmc$	2.850	16.903	[14]
$CuAlO_2$	$P6_3/mmc$	2.832, 2.854	11.10, 11.274	[30]
$CuScO_2$	$P6_3/mmc$	3.181, 3.207	11.107, 11.281	[30]
$CuYO_2$		3.488, 3.514	11.122, 11.277	[30]

Table 2. Structural Characteristics of Delafossite Materials

The ultrasonic process for synthesizing delafossite nanoparticles involves mixing parent materials

followed by titration with an aqueous solution of $NaHCO_3$ at 25 ℃ under ultrasonic waves with frequencies 60 kHz and 117 V for 3 hours. The resulting precipitates were then centrifuged, subsequently washing with demineralized water followed by drying at the desired temperature for a set of duration[12]. Thin film deposition by sputtering method uses a high-energy laser pulse to transform a sintered disc target into vapour for depositing a thin film onto different substrates like sapphire, quartz, and yttria-stabilized zirconia with the range of 300 to 700℃and 10^6 Pa pressure[27] [31].

Synthesis of delafossite materials has been reported to be challenging. While solid-state reactions are simple, cost-effective and suitable for large-scale production, they require high temperatures which leads to high energy consumption. Sol-gel method synthesised a film directly on the substrate and the thickness can be easily controlled by repeating the process. However, it requires a high temperature and inert gas flow, and a substrate that can withstand high temperatures is necessary. Precursor deposition was also reported to be time-consuming[3]. From the preceding overview of the synthesis of delafossite material, hydrothermal methods are often preferred due to their high quality, phase-pure delafossite materials for application in electronics and optoelectronics where control over morphology, composition and crystallinity is essential.

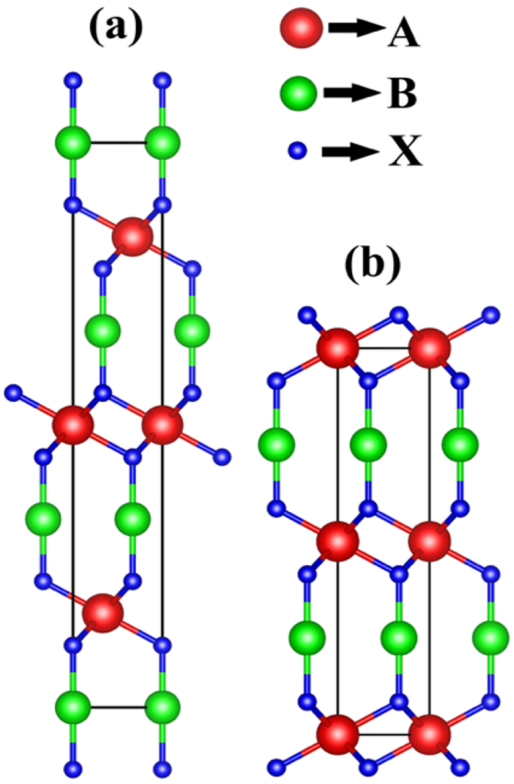

Figure 1. Crystal structure of Delafossite material a) 3R - $R\bar{3}m$ space group; b) 2H - $P6_3/mmc$ space group. (made with VESTA)

4. Electronic properties

Delafossite materials application in optoelectronic devices is assessed through their electronic properties, analysed by calculating the energy band structure and both the total and partial density of states using various methods. Cu-based delafossite oxides $CuMO_2$ (M= Al, Sc and Y) show an indirect band gap nature, with a band gap trend of $CuYO_2$ > $CuScO_2$ > $CuAlO_2$. The valence band maximum (VBM) is generally comprised of M-d and O-2p states, which results in $CuScO_2$ having the largest VBM among the three Delafossites and $CuAlO_2$ the lowest which has no d electrons (see ***Figure*** 2)[30]. Calculated fundamental direct band gaps at Γ of silver delafossite $AgMO_2$ (M=Al, Ga and In) using density functional Linear Muffin Tin Orbitals (LMTO) method also shows Al > Ga > In. While, the direct band gap calculation at M shows In > Al > Ga, with Ga slightly smaller than Al due to the Ga-4s state having lower energy than the Al-3s state[8]. The calculated electronic structure of β -$NaFeO_2$

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structured $CuMO_2$ (M=Al, Ga, In, Sc, Y, La) showed a band gap trend for group 13 and group 3 series as Al > Ga < In and Sc > Y < La respectively) using density functional theory (DFT)[9], which is similar to the those of direct band gap at M of silver Delafossites.

Report on substitutional doping of $CuFeO_2$ shows changes in the indirect band gap nature. N_O, S_O, Ag_{Cu}, and Mn_{Fe} doping slightly decrease the band gap, Zn_{Cu}, Ru_{Fe}, and Mg_{Fe} dopants show a more noticeable decrease while Ni_{Cu}, Mg_{Cu}, and Co_{Fe} dopants increase the band gap. The most remarkable one is F_O doping which shifted the band gap to direct from indirect with the band gap value increasing from 1.56 eV up to 2.20 eV. Substitution of O with N and F dopants, Cu with Ni, Zn and Mg as well as Fe with Co, Ru and Mg alter the band edge positions, enhancing the photocatalytic activity and suppressing recombination[22].

Among the Delafossite nitrides, two compounds namely, $CuVN_2$ and $AuVN_2$, were reported to be metallic with band gap values of 0.00 eV while compounds like $AgVN_2$, $AuTaN_2$, and $AuNbN_2$ had band gaps below 0.7eV were narrow-gap semiconductors, and $CuTaN_2$, $CuNbN_2$, $AgTaN_2$, and $AgNbN_2$, are shown to be semiconductors having band gaps ranging from 1.0-1.7eV[14]. The energy band gap values of different delafossite materials are shown in ***Table 2***.

The density of states (DOS) is divided into three regions; lower energy band (VB_{low}), valence band maximum (VBM), and conduction band (CB). Analysis of the DOS shows that the VBM of $CuFeO_2$ is mainly constituted by the hybridization of O-2p and Cu-3d states and the CB is dominated by Fe-3d states[22]. For delafossite $CuMO_2$ (M=Al, Sc and Y), the VBM is dominated by Cu-3d orbitals, the VB_{low} is composed of O-2p and the conduction bands mainly constituted by 3-d states of M cations except for $CuAlO_2$ where the Cu-3d and O-2p states are dominant (see ***Figure 2***)[30]. Further, there also exists a report on $CuAlO_2$ where the VBM is constituted by hybridized bonding of Cu-3d and O-2p states with the CB mostly dominated by antibonding of Al-2s and p and O-2p states[13]. For β -$NaFeO_2$ structured $CuMO_2$ (M=Al, Ga, In, Sc, Y, La) the VBM are predominantly composed of mixture Cu-3d and O-2p states and the CB by M-s states[9].

Materials	Energy band gap values (eV)		References
$AgNbN_2$	1.48		[14]
$AgTaN_2$	1.62		[14]
$AgVN_2$	0.28		[14]
$AuNbN_2$	0.57		[14]
$AuTaN_2$	0.69		[14]
$AuVN_2$	0.00		[14]
$CuAlO_2$	2.54		[13]
$CuAlO_2$	2.227, 1.962, 2.279		[30]
$CuFeO_2$	1.56		[22]
$CuScO_2$	2.391, 2.37, 2.388		[30]
$CuYO_2$	2.664, 2.694, 2.838		[30]
$CuNbN_2$	1.05		[14]
$CuTaN_2$	1.38		[14]
$CuVN_2$	0.00		[14]

Table 3. Calculated band gap values of different delafossite materials

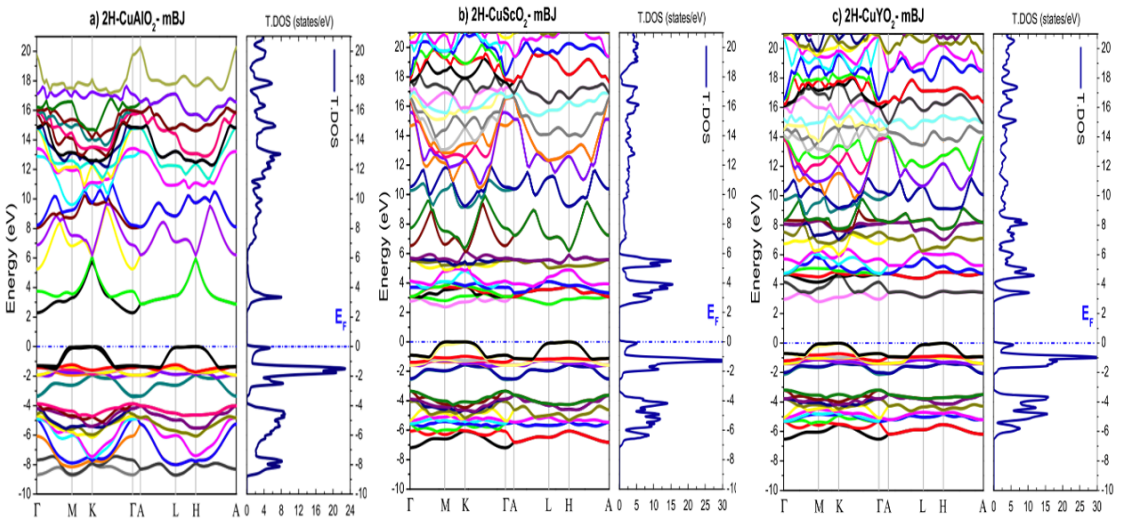

Figure 2. Electronic band structure and total density of states for a) CuAlO2, b) CuScO2 and c) CuYO2 within mBJ approximation. Reprinted from[30] with permission from Elsevier.

5. Optical properties

Optical properties are essential fundamental physical properties for optoelectronic materials. This paper reviews the optical absorption, optical conductivity and its importance in solar cells of different types of delafossite compounds reported by researchers. Copper and silver-based Delafossites having the same B cations show similar optical absorption[8]. As the group 13 B cations increase, the decreasing onset energy of a band-gap transition which is parity-forbidden leads to significant visible light absorption along with an increase in the energy of the calculated optical band gap. Szymanski *et al.* focused on the absorption onset of delafossite nitrides resulting in five of the materials ($CuTaN_2$, $CuNbN_2$, $AgTaN_2$, $AgNbN_2$, and $AuNbN_2$) having strong absorption onset ranging from 0.88-1.75eV which is suitable for solar cells[14].

Extrinsic point defects show new absorption peaks in the UV and visible region of $CuFeO_2$[22]. Doping with elements having higher electronegativity and smaller atomic radius decreases the absorption rate while elements with lower electronegativity and larger atomic radius increase the absorption rate. Zhao *et al.* studied intrinsic point defects and their effect on $CuAlO_2$ absorption spectrum[32]. Depending on the wavelength range, the intrinsic point defects have effects on the optical properties of $CuAlO_2$ material. The effect of intrinsic point defect in the UV is negligible while in the visible-NIR

region, new absorption peaks are produced. Therefore, imperfections in the crystal structure can introduce different optical characteristics for $CuAlO_2$ while preserving their essential optical characteristics.

The absorption coefficient is a crucial optical parameter that describes the amount of light that can be seen when it passes through a material. The longitudinal and parallel components in the absorption coefficient of light for 2H-$CuMO_2$ (M=Al, Sc and Y) demonstrated by Hadjab *et al.*[8] reported the first prominent peak arising at 20.91 eV for $CuAlO_2$, 9.81 eV for $CuScO_2$ and 12.34 eV for $CuYO_2$. The absorption edge for the α^{xx} component began at 2.15 eV, 1.98 eV and 2.1 eV, and for α^{zz} component 3.29, 2.24 and 2.92 eV for 2H-$CuAlO_2$, 2H-$CuScO_2$ and 2 H-$CuYO_2$, respectively. Som *et al*[13] reported the first significant peak arises at ~ 5 eV for $CuAlO_2$, and for perpendicular component absorption edge starting at 2.9 eV while for parallel component the edge starts at 4 eV.

The optical conductivity curves calculated within TB-mBJ approximation by Hadjab *et al.* for Cu-based Delafossites of B-site cation Al, Sc and Y are depicted in ***Figure 3***, with peaks observed at 14.68 eV, 9.619 eV and 11.932eV for the α^{xx} component, while for the α^{zz} component, it was observed at 14.408 eV, 9.319 eV and 8.857eV for Al, Sc and Y, respectively[30].

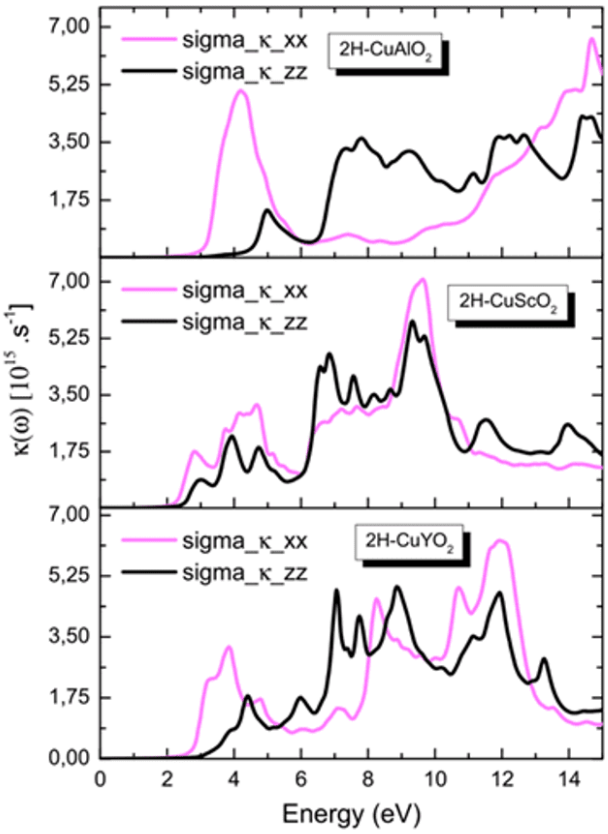

Figure 3. Conductivity of a) CuAlO2, b) CuScO2 and c) CuYO2 within mBJ approximation. Reprinted from[30] with permission from Elsevier.

6. Delafossite materials for solar cell applications

In 2012, Yu *et al.* reported delafossite $CuGaO_2$ nanoplates with a remarkably high saturation voltage of 464 mV for p-DSSCs[15]. The thermodynamic stability of these nanoplates is through 350 ℃. Fabrication of the solar cell was achieved by using P1 dye and I^-/I^-_3 electrolyte or $Co^{3+/2+}$ (dtb-bpy) electrolyte. To estimate the maximum open circuit voltage (V_{oc}), a measurement of the relationship between V_{oc} and the illumination intensity was carried out. The saturation V_{oc} was found to be 243 mV with I^-/I^-_3 electrolyte whereas 464 mV was recorded when using $Co^{3+/2+}$ (dtb-bpy) electrolyte, which is a 100% increase compared to NiO-DSSCs with similar conditions. Under 1 Sun AM 1.5 illumination, the V_{oc} for $CuGaO_2$ solar cells is 180 mV with I^-/I^-_3 electrolyte and 354 mV when $Co^{3+/2+}$ (dtb-bpy) electrolyte was used. Low current densities in $CuGaO_2$ cells is the main limitations. By measuring the

dye adsorption isotherms, the particle size of $CuGaO_2$ being large caused low dye loading which in turn results in limited light harvesting efficiency and current density. Further work on decreasing the nanoplates size is required to increase the dye loading, and thus increase the current density.

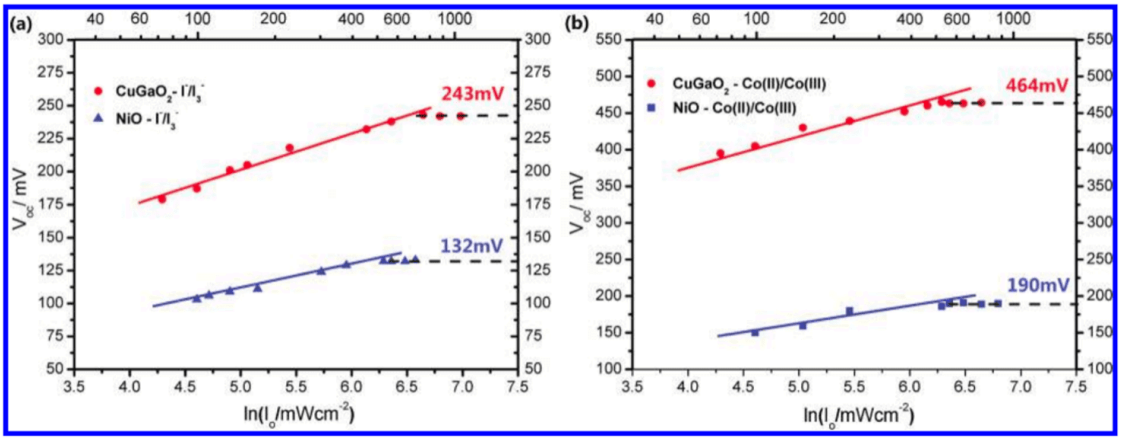

Figure 4. Voc and light intensity relations of: (a) CuGaO2-DSSC and NiO-DSSC with I3-/I- electrolyte; (b) CuGaO2-DSSC and NiO- DSSC with Co3+/2+(dtb-bpy) electrolyte.

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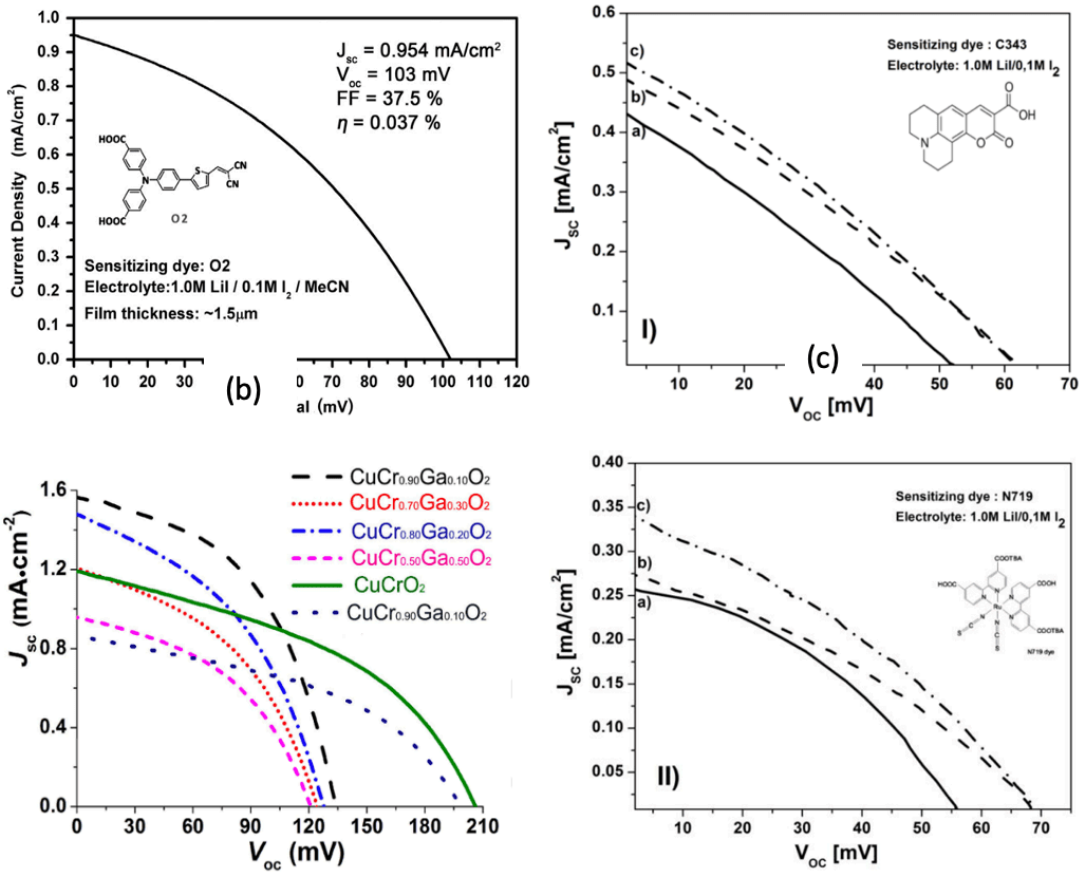

Figure 5. Photocurrent–voltage (J–V) curve of a) $CuAlO_2$ based p-type DSSCs using O_2 dye (Reprinted from[17] with permission from Elsevier) b) $CuCr_{1-x}Ga_xO_2$ (x=0, 0.10, 0.20, 0.30, 0.50.) photocathode. (Reprinted from[20] with permission from Elsevier) c) $CuCrO_2$, $CuCr_{0.95}Al_{0.05}O_2$, and $CuCr_{0.95}Mg_{0.05}O_2$ based p-type DSSCs with C343 (I) dye and N719 (II) dye. (Reprinted from[21] with permission from Elsevier).

In 2014, Ahmed *et al.* reported the preparation of delafossite $CuAlO_2$ nanoparticles with controlled oxygen partial pressure (pO2) of 105 atm and 775 °C[17]. The solar cell was fabricated using O2 dye as a sensitizer and I^-/I_3^-electrolyte. The short circuit current (J_{sc}) was found to be 0.954 $mAcm^{-2}$ which is higher than most delafossite compounds reported. The V_{oc} and saturated V_{oc} were reported to be 103 mV and 155 mV respectively, which is higher than NiO-based p-DSSCs but lower than delafossite CuMO2-based p-DSSCs. The site defects of Copper and oxygen non-stoichiometry attributed to the

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low photovoltage in $CuAlO_2$ nanomaterials. Therefore, using different routes to enhance the quality of the material should also improve the photovoltage of $CuAlO_2$ nanomaterials.

In 2015, Xiong *et al.* reported the hydrothermal synthesis of $CuCr_{1-x}Ga_xO_2$ (x = 0.10, 0.20, 0.30, 0.40 and 0.50) nanocrystals and used them in p-DSSCs as photocathodes, fabricated with P1 dye and I^-/I_3^- electrolyte[20]. After the incorporation of the materials in p-DSSCs, the solar cells were tested under AM 1.5 illumination. The J_{sc} decreased from 1.56 mA cm^{-2} to 0.96 mA cm^{-2} and the V_{OC} decreased from 205 mV to 198 mV while Ga rose from 0.10 to 0.50 with a thickness of 2.7 - 2.9 μ m. However, introducing a thicker electrode film (2.8 μ m) increase the J_{sc} to 1.56 mA/cm^2 while decreasing the V_{OC} to 134 V for $CuCr_{0.90}Ga_{0.10}O_2$. With a thickness of 1.5 μ m, $CuCr_{0.90}Ga_{0.10}O_2$ based solar cell shows the highest PCE of 0.10%. The author concluded that the performance of $CuCr_{0.90}Ga_{0.10}O_2$ based solar cells, as compared to $CuCrO_2$ was not high enough. In 2016, Daniel *et al.* reported the fabrication of (Al, Mg)-doped $CuCrO_2$ based p-DSSCs with an improved J_{sc} value[21]. In their work, Mg^{2+} and Al^{3+} doped nanocrystalline $CuCrO_2$ were synthesized through hydrothermal reaction. The specific surface area (SSA) measured by the Brunauer-Emmett-Teller (BET) method were 107 m^2 g^{-1}, 110 m^2 g^{-1} and 122 m^2 g^{-1} for $CuCrO_2$, $CuCr_{0.95}Al_{0.05}O_2$ and $CuCr_{0.95}Mg_{0.05}$ O_2 respectively, which was reported to be the biggest ever reported for delafossite materials in DSSCs applications. The solar cells were fabricated with Coumarin C343 and Ruthenium N719 dyes using I^-/I_3^-electrolyte. The J_{sc} was in the range of 0.44 – 0.52 mA/Cm^2 with Coumarin C343 dye and 0.26 – 0.34 mA/cm2 for Ruthenium N719 dye when doped with $Al_{0.05}$ and $Mg_{0.05}$ respectively. The V_{oc} was 52 mV, 62 mV and 62 mV for $CuCrO_2$, $CuCr_{0.95}Al_{0.05}O_2$ and $CuCr_{0.95}Mg_{0.05}O_2$ respectively when Coumarin C343 dye is used. For Ruthenium N719 dye the V_{oc} was found to be 56 mV $CuCrO_2$, 68.5 mV and 69 mV $CuCr_{0.95}Al_{0.05}O_2$ and $CuCr_{0.95}Mg_{0.05}$ O_2 respectively. The J_{sc} notably increase when doping because of the small particle width which results in a higher specific area.

In 2016, Keerthi *et al* reported heterojunction between n-copper indium oxide (CIO) and p-silicon for application in solar cells fabricated as a sandwich structure with a layer of n-CIO on p-Si with silver electrodes on the top and bottom[33]. The n-CIO and p-Si heterojunction shows a good ideality factor of 1.5V in the range of 0 to 4V and a threshold voltage of ~ 0.35 ± 0.05 V. When exposed to UV the V_{oc} ~ 0.05-0.07 V and 0.25 V when exposed to visible radiations. The work function evaluated was ~4.1 eV and 4.8 eV, and the electron affinity was ~ 3.8 eV and 4 eV for n-CIO and p-Si respectively. The PV effect, which can be attributed to the carrier generation and separation at the junction, suggests that a

potential junction can be formed for power production to utilize photons in the entire Vis-UV range using a layer of CIO with suitable thickness over Si.

In 2023, Prasad *et al.* theoretically analyzed the optoelectronic characteristics of $CuFeO_2$ or CFO to examine the photovoltaic performance[1]. Their work investigated various buffer counterparts that are compatible with CFO absorbers for making efficient p-n^+ junctions. Out of the metal oxides considered, ZnO, CdO and MoO_3 were explored owing to their ideal material parameters. The CFO/ZnO shows the best efficiency, with a spectrum loss of 59.6% and an absorber bandgap of 1.5eV. The CFO/ZnO/ITO device performance shows V_{OC} = 1.14 eV, J_{SC} = 27 mA/cm2, fill factor = 88% and efficiency=28.06%.

Compound	Year	Application	Parameters		Efficiency	Ref.
			J_{sc} (mV)	V_{oc} (mA cm^{-2})		
$CuGaO_2$	2012	$CuGaO_2$ nanoplates on p-DSSCs	-	357	-	[15]
$CuAlO_2$	2014	$CuAlO_2$ nanoparticles as a photocathode in p-type DSSCs	0.954	-	0.037%	[17]
	2019	Absorber layer for solar cell (Theoretical)	76.2	1.95	14.8%	[13]
$CuCrO_2$	2015	p-DSSCs based on $CuCrO_2$ with Al and Mg doping	0.52	69	-	[21]
	2016	p-DSSCs based on CuCrO2 with Ga doping	134	1.56	0.10%	[20]
$CuCoO_2$	2023	$CuCoO_2$/ZnO heterojunction as photoelectrodes for p-DSSCs	14.56	-	6.27%	[19]
$CuFeO_2$	2023	$CuFeO_2$/ZnO heterojunction for solar cell absorber (Theoretical)	27	1.14	28.06%	[1]

Table 4. Different delafossite-based solar cells with their efficiency and solar cell parameters.

In 2023, Roudgar-Amoli *et al.* reported a successful development of heterostructures between

delafossite $CuCoO_2$ and ZnO for enhancing the photovoltaic performance of DSSCs[19]. By hydrothermal reaction, the $CuCoO_2$ nanoparticles were synthesized and the ZnO particles using zeolitic imidazolate framework-8 (ZIF-8). By combining the materials, the $CuCoO_2$/ ZnO composites were produced with different mole ratios of $CuCoO_2$ to ZnO (0.05, 0.1, 0.15, 0.2): 1. The composites were used as photoelectrodes in DSSCs to study the effect of $CuCoO_2$ nanoparticles on the cell characteristics of the ZnO photoanodes in DSSCs. The PV data of $CuCoO_2$/ ZnO (0.1: 1) reveals that J_{sc} = 14.56 mA cm^{-2}, V_{oc} = 687.84 mV, and fill factor (FF) = 62.67% along with the highest PCE of 6.27% which was higher than ZnO alone (3.05%), therefore showing promise in photoanode for DSSCs.

7. Conclusion

In conclusion, this paper discussed the unique structural, electronic and optical properties of delafossite materials. Delafossite represents a wide range of electrical conductivities, such as insulating, metallic or semiconductor properties. Some Delafossites also showed p-type conductivity as well as transparency, making them attractive for optoelectronic devices. In addition, their structure can accommodate numerous B cations, allowing for tunable physical and chemical properties. From the preceding overview, it is clear that Delafossites show promising use in future solar cell technology. However, more effort and work are still needed to successfully manufacture solar cells using Delafossites as absorber material. Theoretical efficiency reaching as high as 28% has been witnessed when constructing a heterojunction with metal oxide. In addition, their performance as photocathode in p-DSSCs compared to metal oxides which are typically used shows good potential based on their photovoltaic parameters. Nevertheless, their efficiencies still need improvement, and this can be achieved by choosing the right conditions for fabrication and synthesis methods. Synthesis of delafossite structure to achieve pure-phase often requires precise conditions, resulting in manufacturing costs and reducing scalability. Due to their wide band gaps, absorption efficiency is also limited. Therefore, understanding their structure and properties to an extent is required to fabricate a solar cell successfully under the right conditions. It is clear from this report that delafossite materials could be a promising candidate for an absorber material in solar cells and could potentially be the solution for pressing global challenges in energy.

Statements and Declarations

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Conflicts of Interest

The authors have no conflict to declare.

Authors Contributions

- **H. Laltlanmawii:** the first author helps in the visualisation, conceptualisation, validation, writing and editing of the final review.
- **L. Celestine:** assist in writing a review article, literature survey, discussion, conceptualization, methodology and editing drafts.
- **R. Zosiamliana:** helps in the visualisation, formal analysis, conceptualisation, validation, and editing of the final draft.
- **S. Bhattarai:** formal analysis, visualisation, conceptualisation, validation, and editing of the final draft.
- **Z. Pachuau:** formal analysis, visualisation, conceptualisation, validation, and editing of the final draft.
- **D. P. Rai:** supervision, formal analysis, conceptualisation, methodology, validation, and editing of the final draft.

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Declarations

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