



# **Metal-Organic Frameworks Based Multifunctional Materials for Solar Cells: A Review**

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Abstract: Developing low-cost and stable materials for converting solar energy into electricity is vital in meeting the world's energy demand. Metal-organic frameworks (MOFs) have gained attention for solar cells due to their natural porous architectures and tunable chemical structures. They are built by high-symmetry metal clusters as secondary building units and organic carboxylate/azolate ligands as linkers. This review commences with an exploration of the synthetic methods of MOFs. Moreover, we discuss the various roles of MOFs, including photoanodes and counter electrodes in dye-sensitized solar cells and interfacial layers and charge carriers in perovskite solar cells. Additionally, studies involving the application of MOFs for OSC were additionally presented. Ultimately, burdensome tasks and possible directions for advancing MOFs-based nanomaterials are provided for solar cells.

Keywords: MOFs; hydrothermal method; sol-gel; porous materials; solar cells; photoanodes

# 1. Introduction

In recent years, melting ice, drought, and flooding have increased significantly. This is a direct result of global warming, attributed to the increased greenhouse gases released from using conventional fossil fuels [1–10]. Therefore, there needs to be a shift from fossil fuel to renewable energy to meet the increasing demands of power without causing much environmental contamination [11–20]. Among renewable energy sources, solar energy is considered an ideal solution due to zero  $CO_2$  emission and abundant resources [21–26]. Nonetheless, problems of solar cells are expensive, and restricted scale. Solar cells based on silicon are the most widely used for converting solar energy to electricity to satisfy human energy demands. Until now, Si-based materials displayed the highest performance for converting solar energy into electricity [27–31]. However, solar cell-based Si materials are ineffective with inside sunlight due to their unsuitable band gap. As a result, various types of solar cells involving dye-sensitized solar cells (DSSC), perovskite solar cells (PSC), and organic solar cells (OSC) have been explored with a large number of publications in recent years (Figure 1) [32–34].

Regarding DSSC, TiO<sub>2</sub> was identified as a typical photoanode material, whereas Ptbased materials are the most effective counter electrodes (CE). However, the fast excitons recombination of TiO<sub>2</sub> and the high cost of Pt have driven scientists to explore the novelty alternatives in solar cell applications. Furthermore, stability is an issue of concern for PSC and OSC researchers due to the instability of organic components. As a result, ultra-stable materials and integrated methodologies for increasing the long-term stability of PSC and OSC must be investigated [35-37].

The terminology metal-organic frameworks (MOFs) was first known in 1995 by Yaghi, which defined the structure construction from metal nodes along with organic linkers, which have high-symmetry properties. For instance, HKUST-1 was constructed by symmetry units, including a copper paddle wheel ( $-Cu_2(COO)_4$ ) along with benzene-1,3,5-



Citation: Do, H.H.; Kim, S.Y. Metal-Organic Frameworks Based Multifunctional Materials for Solar Cells: A Review. *Symmetry* **2023**, *15*, 1830. https://doi.org/10.3390/ sym15101830

Academic Editor: Sergei D. Odintsov

Received: 25 August 2023 Revised: 18 September 2023 Accepted: 22 September 2023 Published: 27 September 2023



**Copyright:** © 2023 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (https:// creativecommons.org/licenses/by/ 4.0/). tricarboxylic acid ( $H_3BTC$ ). MOFs have a crystal, porous framework structure, making them promising candidates in various applications such as gas adsorption, catalysis, and sensors [38–43]. In particular, MOFs containing unsaturated metal sites and Lewis basis sites were evaluated as promising materials for gas storage, such as  $CH_4$ ,  $CO_2$ , and  $H_2$  [44]. Moreover, the pore size of MOFs can be tunable, which is favorable for gas selectivity adsorption [45]. Additionally, the well-distribution of metal nodes indicated uniformly exposed active sites for catalytic application. On the other hand, enormous MOFs have recently been widely applied for photovoltaic applications with various functions in DSSC, PSC, and OSC [46–50]. As mentioned above, MOF structures were built from metal nodes and organic components, leading to bandgap (Eg) along with semiconducting features that could be adjusted by chemical composition change. Generally, the optical absorption ability of materials is identified by their Eg. Consequently, the preparation of a MOF with an appropriate Eg that is capable of adsorbing light in the spectrum of sunlight is an essential requirement. Several theoretical works indicated that organic components of MOFs will determine light absorption, whereas experimental studies revealed that the electron transport process takes place through metal site-linkers. These outcomes implied that MOFs could act as photoactive materials for photovoltaic applications. In particular, MOF-5 is the first structure in the MOF family used as active material in solar cell applications [51]. Also, MOFs were used as photoanode, counter electrode (CE), interfacial layers, and charger carriers in DSSC and PSC.



**Figure 1.** Number of publications resulting from the search of "solar cells" on Web of Science, accessed on 12 September 2023.

Although there are several kinds of literature about MOFs for solar cells, the finding of efficient and ultra-stable MOFs for solar cells is urgent and significant in minimizing the influence of  $CO_2$  emission. This review helps the researchers have a comprehensive view of the recent use of MOFs in solar cell applications. To begin, this literature discusses the general aspects of MOF production, such as the hydrothermal approach, solvothermal procedure, and sol-gel. Second, several DSSC responsibilities, including photoanodes and counter electrodes (CE), were shown utilizing MOFs. Third, using MOFs as interfacial layers (IL) and charge carriers in PSC were explored. Furthermore, several works related to the usage of MOFs for OSC also was introduced. Finally, present obstacles and prospects for the advancement of MOFs for solar cells are discussed.

#### 2. Synthetic Methods of MOFs

#### 2.1. Hydrothermal Technique

The hydrothermal process is a typical method for producing MOFs and materials developed from them for solar cells. Various sizes and structures of MOFs were created by varying the temperature, reaction duration, and pressure [52]. Despite the effectiveness of

obtaining MOFs, it was plagued by low yield and expansiveness. Furthermore, the reaction pathway of MOFs and their derived materials remains to be discovered.

#### 2.2. Solvothermal Method

The solvothermal technique is generally acknowledged as an effective method for synthesizing MOFs and their composites by virtue of its high yield and facial control. The solvent is vital in the solvothermal reaction process. Until now, the most often employed organic solvents for MOF fabrication are N, N-dimethylformamide, ethanol, and methanol. These organic solvents might shift MOFs' structure and size for specific applications. However, organic solvents' toxicity and environmental unfriendliness limit their widespread use. Furthermore, organic solvents are difficult to decontaminate and recycle. As a result, developing safe and ecologically acceptable solvents for the solvothermal process is critical [53].

#### 2.3. Sol-Gel

Recently, the sol-gel approach has been frequently used to produce inorganic nanomaterials. The synthesis procedure causes ion co-precipitation, which results in the generation of the desirable structures. This approach is more effective than the hydrothermal process for synthesizing MOFs. MOFs with variable sizes and shapes might be created by optimizing experimental parameters such as reaction temperature, duration, etc. Furthermore, MOFs might be employed as a precursor to create derivatives with outstanding properties [54].

# 2.4. Other Methods

Besides the hydrothermal technique, solvothermal process, and sol-gel methods, MOFs could be prepared by other strategies involving the electrochemical technique, microwave, and ultrasound methods [55–57].

#### 3. Fundamentals of Solar Cells

Solar cells are electronic devices for converting the sun's energy directly into electricity. Generally, a solar cell comprises a semiconductor with a photovoltaic effect once illuminated. In terms of DSSC, the mechanism of the photovoltaic device includes three steps: light adsorption, charge production, and charge transport. Notably, the first process is the light adsorption of the dye molecule to change the excited state (dye\*), after which this dye provides electrons for the conduction band of the semiconductor, accompanied by the oxidation process of dye\*. Then, the injected electrons will move to the photoanode before transferring to CE through an external circuit, as shown in Figure 2a [58]. In terms of PSC, this device generally includes five parts: FTO (Fluorine-doped Tin Oxide) glass as a conductive substrate, an electron transfer layer (ETL), a hole transfer layer (HTL), a perovskite layer, along with a metal electrode. PSC's operation may be broken down into three steps: light adsorption and production of excitons, electron-hole separation, and charge transfer process. In particular, the perovskite layer will absorb solar energy to create electrons in the conduction band and holes in the valance band. The electrons then move to ETL before being transported to the anode, whereas the holes flow to HTL before being transferred to the cathode (Figure 2b) [59]. The process includes four steps for OSC's working principle: light adsorption/electron-hole pairs production, charge diffusion, charge dissociation, and charge transport to the electrodes, as shown in Figure 2c [60]. In particular, when a p-type material absorbed solar energy, electrons will be excited from the highest occupied molecular orbital (HOMO) to the lowest unoccupied molecular orbital (LUMO). Then these electrons will move to the LUMO of the acceptor before transferring into the cathode. Simultaneously, holes will move to the anode of the OSC device. Overall, the power conversion efficiency  $(\eta)$  is linked to three parameters: the open-circuit voltage (Voc), short circuit current density (Jsc), and fill factor (FF) following the formula  $\eta = \text{Voc} \times \text{Jsc} \times \text{FF} \times \text{P}_{\text{input}}.$ 



**Figure 2.** (a) Working principle of a DSSC. Reproduced with permission [58]. Copyright 2019, American Chemical Society. (b) Graphic illustration of the production of electron-hole pairs and carrier transport in a PSC. (c) The operational mechanism of an OSC: 1 Light adsorption/electron-hole pairs, 2 Charge diffusion, 3 Charge dissociation, 4 Charge transport. Reproduced with permission [60]. Copyright 2017, Elsevier B.V.

# 4. MOFs for Dye-Sensitized Solar Cells

### 4.1. MOFs as Photoanodes

Over the past decades, DSSC have gained considerable interests of scientists around the world because of their low-price, facial preparation, and high  $\eta$ . A typical DSSC is constructed from a photoanode, a CE, and a redox solution.  $TiO_2$  was evaluated as a conventional photoanode material. But, the fast excitons recombination of  $TiO_2$  has driven researchers to find the novelty photoanode in solar cell applications. On the one hand, MOFs could be utilized as photosensitizers for the conversion of sunlight into electricity. For example, Lee et al. conducted hole doping on various structures, including Co-BDC (BDC = benzenedicarboxylate) and Co-NDC (NDC = 2,6-naphthalendicarboxylic acid) for DSSCs [61]. The results revealed that I<sub>2</sub>-doped Co-based MOFs as photoanodes displayed a potential performance for energy conversion. Notably, I<sub>2</sub>-doped Co-NDC/TiO<sub>2</sub> gave an efficiency of 1.12%, whereas this quantity is 0.96% for  $I_2$ -doped Co-NDC/TiO<sub>2</sub>. The improved performance was attributed to the well-interaction between I<sub>2</sub> and  $\pi$ -electrons of linkers. Spoerke et al. found that porphyrin-based MOFs could be efficient photosensitizers for DSSC. Notably, the authors utilized a pillared porphyrin framework (PPF) as an active component in solar cells, as shown in Figure 3 [62]. Although this device gave a low solar conversion efficiency, it opened a promising direction for the advancement of MOFs for photovoltaic applications. On the other hand, MOFs were utilized as interfacial modifiers. For instance, ZIF-8 was formed on the photoanode's  $TiO_2$  surface, which suppresses the electron-hole pair recombination, resulting in a much higher open-circuit voltage (Voc) than the pure DSSC [63]. Moreover, the cell efficiency was increased from 5.11% to 5.34% with the assistance of the ZIF-8 layer at the ideal growth time. Gu et al. also combined ZIF-8 with TiO<sub>2</sub> to improve DSSC performance from 7.75% to 9.42%, attributed to effectively prohibiting electron-hole pairs recombination from ZIF-8 [64]. He et al. used reduced graphene oxide (RGO) with ZIF-8 and UiO-66 to improve DSSC efficiency through improved charge transfer [65]. Notably, ZIF-8-RGO/TiO<sub>2</sub> as a photoanode gave an energy conversion efficiency ( $\eta$ ) of 7.33%, whereas this value is 7.67% for UiO-66-RGO/TiO<sub>2</sub>. Recently, He et al. mixed a 3D structure of graphene-based material with ZIF-8 to accelerate DSSC performance [66]. In particular, an optimal sample of ZIF-8/3DGN/TiO<sub>2</sub> displayed  $\eta$  of 8.77%, ascribed to the synergistic effect of efficient charge transfer and good conductivity from 3DGN. Besides ZIF-8, Cu-, Ni-, and Co-based MOF are also used to fabricate photoanode in DSSCs. For instance, Ramasubbu et al. fabricated a TiO2-Ni-MOF hybrid structure as an efficient photoanode for DSSC utilization [48]. In particular, this material displayed a 30% larger performance than bare  $TiO_2$  as a photoanode. The result

could be explained by the fact that Ni-MOF plays a vital role in changing optical properties and prohibiting excitons recombination. Kumar et al. prepared and evaluated the solar cell efficiency of various compounds such as Cu-MOF/TiO<sub>2</sub>, Ni-MOF/TiO<sub>2</sub> and TiO<sub>2</sub> [67]. The authors found that the diffusion time and charge transfer resistance of Ni-MOF/TiO<sub>2</sub> are the smallest among investigated materials, which were attributed to the highest energy conversion efficiency.



**Figure 3.** (**a**) Graphic illustration of PPF-4 and its application in DSSC, (**b**) SEM image of PPF-4 architecture, (**c**) the schematic diagram of energy for prediction of band gaps, (**d**) Current density-voltage plots of various devices under AM 1.5 conditions. Reproduced with permission [62]. Copyright 2017, American Chemical Society.

### 4.2. MOFs as Counter Electrodes

The counter electrodes (CE) play vital roles in the construction of photovoltaic devices and in determining efficiency. The CE is created from depositing an electrocatalyst on the conductive template. Herein, Pt is generally utilized as electrocatalyst. Although Pt-based thin layers are the best CE for DSSC, high cost leads to an increase in the cost of solar cells. MOFs with a well-distribution of metal active sites were appreciated as promising CE in DSSC. For instance, Chen et al. blended MOF-525 with a conductive polymer, followed by coating on the carbon cloth to form an efficient CE in DSSC, as shown in Figure 4 [68]. This device displayed a high cell performance of 8.91%, comparable with Pt CE-based solar cells. The effectiveness of using MOFs for CEs has been exemplified in a study by Zhao et al. [69]. The authors found that using ZIF-8 for fabrication CE brings higher power conversion efficiency than without MOF in DSSC. Yang et al. mixed a Cu-based MOF with poly(3,4-ethylenedioxythiophene), followed by depositing on the fluorine-doped tin oxide (ITO) to create a CE for DSSCs [70]. This cell displayed a higher performance of 9.45% and remarkable stability, attributed to the abundant catalytic sites of -Cu-S- phases and good film attachment on ITO. Tian et al. utilized Zn-TCPP nanolayers to efficiently advocate for embedding Pt nanoparticles to generate promising CE for DSSC [71]. In particular, DSSC with Zn-TCPP-Pt as a CE provided a solar cell performance of 5.48%. Overall, the

usage of MOFs as CE is still limited in DSSC by virtue of their poor conductivity. Therefore, enormous works have been reported on using MOFs as sacrificial agents for the fabrication of hybrid structures, which are efficient CE in DSSC.



**Figure 4.** (a) Graphic illustration of carbon cloth (CC), (b) graphic illustration of MOF-525/s-PT architecture on CC, (c) FE-SEM image of MOF-525/s-PT-3, (d) Incident PCE plots of various counter electrodes. Reprinted with permission [68]. Copyright 2017, Elsevier B.V.

# 5. MOFs for Perovskite Solar Cells

#### 5.1. MOFs as Interfacial Layers (IL)

PSCs have been proven as potential candidates for replacing inorganic solar cell by virtue of excellent optical adsorption, inexpensiveness, and fast charge transfer. Recently, works related to the enhancement of PSC's long-term durability have been implemented through a strategy of compositional engineering. Notably, by using inorganic ions to substitute unstable organic components, stability of PSC could be substantially improved. Also, interfacial engineering is an effective strategy to enhance stability of PSC. Recently, MOFs with high stability were employed as IL in PSC to improve the particle size and perovskite crystallinity and hinder electron-hole recombination, leading to increased solar cell efficiency. For instance, Shen et al. inserted ZIF-8 IL between the PSC application's mesoporous TiO<sub>2</sub> and perovskite component [72]. This strategy improved the solar cell efficiency from 14.75% (without ZIF-8) to 16.99% (with ZIF-8), attributed to the improved crystal quality and efficient suppression of exciton recombination. Ahmadian-Yazdi et al. used ZIF-8 as an interfacial modifier in PSC [73]. To confirm the ability of charge extraction, Photoluminescence (PL) was analyzed with various samples. The outcome revealed that c-TiO<sub>2</sub>/ZIF-8-10/perovskite displayed the smallest intensity of PL, implying the most effec-

tive charge extraction. As a result, this material exhibited the highest solar cell performance of 16.8%. Recently, Jin et al. utilized ZIF-8 as a host material to confine methylammonium chloride (MACl) to form an effective IL between  $SnO_2$  and the perovskite layer, as shown in Figure 5 [74]. This strategy brings several beneficial effects for PSC. First, oxygen vacancies of  $SnO_2$  were significantly decreased. Second, the new bonds were created from interaction ZIF-8 with unsaturated  $Pb^{2+}$ ,  $I^-$ , and  $Br^-$ . Furthermore, the MACl component would supply the ions to decline the Pb vacancies in perovskite material. As a result, the MACl@ZIF-8-based solar cell gave a high performance of 22.10%, open novelty direction in using MOF in PSC.



**Figure 5.** (a) Graphic representation of the preparation of MACl@ZIF-8, (b) Graphic representation of the defect passivation mechanism. Reproduced with permission [74]. Copyright 2023, The Royal Society of Chemistry.

#### 5.2. MOFs as Charge Transfer Layers

MOFs have been identified as promising materials for charge transporting in PSC. On the one hand, MOFs have been applied to improve electron transfer in PSC. For instance, Ryu et al. mixed a Ti-based MOF with commercial carbon material (PCBM) to create an electron transfer layer (ETL), as shown in Figure 6a [75]. This approach not only improves charge transport but also prevents the recombination of excitons. As a result, the rigid nTi-MOF/PCBM device exhibits a solar cell efficiency of 18.94%, whereas its flexible device has a performance of 17.43% (Figure 6b,c). Nguyen et al. used a metal doping strategy on TiO<sub>2</sub> derived from Ti-based MOF to produce an efficient ETL in PSC [76]. Notably, an optimized sample of Co-doped TiO<sub>2</sub> displayed a higher solar cell performance than a commercial TiO<sub>2</sub> PSC device, attributed to the enhanced optical absorption and electron transport by co-doping. The effectiveness of using MOF as an ETL has been reported in the literature by Andrade et al. [77]. The author found that a PSC efficiency of 5.9% was recorded on NH<sub>2</sub>-MIL-125 (Ti), whereas a lower performance of 4.1% was observed on NH<sub>2</sub>-MIL-101 (Fe). These outcomes were attributed to the influence of porosity and roughness of materials.

On the other hand, MOFs are also used in hole transfer layers (HTL) of PSC by mixing with Spiro-OMeTAD to improve conductivity, durability, and oxidation performance. For instance, Li et al. used In-based MOF for doping Spiro-OMeTAD to improve the oxidation process and electrical conducting of HTL [78]. This approach helped to increase

electron transfer and prevent exciton recombination of PSC. Thus, solar cell efficiency was accelerated. Notably, an efficiency of 17.0% was recorded on PSC with In-based MOF doping, whereas this quantity is 14.1% for PSC without MOF in HTL. The effectiveness of MOF doping in HTL has been reported in the literature by Wang et al. [79]. The authors used a Zn-based MOF to accelerate the conductivity of HTL in PSC. Besides, carbonyl groups of Zn-based MOF bind with Pb(II) ions, leading to improved solar cell performance significantly.



**Figure 6.** (a) Graphic illustration of PSC device with nTi-MOF/PCBM as an electron transfer layer, (b) Current density-voltage plots of the rigid nTi-MOF/PCBM device, (c) Current density-voltage plots of the flexible nTi-MOF/PCBM device. Reproduced with permission [75]. Copyright 2018, American Chemical Society.

# 6. MOFs for Organic Solar Cells

OSC are a potential new energy conversion device that has significant prospects to deliver excellent  $\eta$  by utilizing inexpensive, adjustable conductive polymers or organic molecules. Moreover, these materials could be applied for industrial applications, implying that large-scale preparation is achievable. However, the stability of OSC is a headache problem for scientists. Therefore various strategies were conducted to improve  $\eta$  as well as stability of OSC devices. Interfacial engineering was identified as a primary strategy for increasing power conversion efficiency. The interfacial layers in OSCs could take various roles, involving shifting the energetic barrier at the metal/photoactive material interface, providing contact selectivity, hindering chemical or photophysical interaction between the photocurrent. Compared to the rising uses in DSSC and PSC, MOFs have yet to be fully investigated in OSCs due to their low semiconducting characteristics. Up to now, only a few works related to MOFs for OSC application. For example, Xing et al. utilized polyethylenimine ethoxylate (PEIE) to exfoliate Te-based MOF bulk to nanolayers,

which was applied for interfacial layers in OSC [80]. This strategy accelerated the power conversion efficiency from 9.91% (ZnO/PEIE as an electron extraction layer (EEL) to 10.39%, which was attributed to the passivity of defective ZnO and improved conductivity (Figure 7). Additionally, the effectiveness of using MOFs for OSC has been exemplified in a work by Sasitharan et al. [81]. The author mixed three components, including Zn-based MOF nanolayers, poly(3-hexylthiophene-2,5-diyl) (P3HT), and [6,6]-PhenylC61-butyric acid methyl ester (PCBM) to create an active material layer in OSC device. This approach improved the power conversion efficiency from 2.67% (without MOF) to 5.2% (with MOF). This result could be explained by the fact that Zn-based MOF plays a vital role in forming P3HT and avoids the expansion of PCBM. The performances of MOFs for solar cell applications are summarized in Table 1.



**Figure 7.** (a) Graphic illustration of the fabrication of MOF nanolayers, (b) The solar cell structure and current density-voltage plots of the device with ZnO (black line) and MOF-PEIE (red line) as EEL. Reprinted with permission [80]. Copyright 2018, Elsevier B.V.

Solar Cell Types	MOF-Based Materials	Jsc (mA cm $^{-2}$ )	Voc (V)	FF	η (%)	Ref.
DSSC	I <sub>2</sub> @ Co-NDC/TiO <sub>2</sub>	2.56	0.63	0.63	1.12	[61]
	$ZIF-8/TiO_2$	10.28	0.753	0.69	5.34	[63]
	$ZIF-8/TiO_2$	14.39	0.897	0.73	9.42	[64]
	UiO-66-RGO/TiO <sub>2</sub>	18.6	0.678	0.608	7.67	[65]
	ZIF-8/3DGN/TiO <sub>2</sub>	20.9	0.681	0.616	8.77	[66]
	TiO <sub>2</sub> -Ni-MOF	27.32	0.624	0.516	8.846	[48]
	Cu-MOF/TiO <sub>2</sub>	1.70	0.32	0.236	0.13	[67]
	MOF-525/s-PT	16.14	0.80	0.70	8.91	[68]
	ZIF-8/PEDOT:PSS	11.46	0.852	0.70	7.56	[69]
	Cu-MOF/PEDOT	16.36	0.777	0.65	8.26	[70]
	Zn-TCPP-Pt	12.95	0.69	0.61	5.48	[71]
PSC	mp-TiO <sub>2</sub> /ZIF-8	22.82	1.02	0.73	16.99	[72]
	c-TiO <sub>2</sub> /ZIF-8-10	21.8	1.23	0.59	16.8	[73]
	MACl@ZIF-8	24.07	1.16	0.791	22.10	[74]
	nTi-MOF/PCBM	23.18	1.082	0.755	18.94	[75]
	Co-doped TiO <sub>2</sub>	24.078	1.027	0.64949	15.75	[76]
	NH2-MIL-125 (Ti)	19.10	0.64	0.48	5.9	[77]
	In-based MOF	24.3	1.0	0.70	17.0	[78]
	Zn-CBOB	23.17	1.135	0.784	20.64	[79]
OSC	ZnO/MOF-PEIE	17.09	0.86	0.7069	10.39	[80]
	P3HT-Zn <sub>2</sub> (ZnTCPP)-PCBM	10.8	0.69	0.69	5.2	[81]

Table 1. Performance of MOFs for solar cells application.

# 7. Conclusions and Outlook

In summary, MOFs have emerged as a new topic in solar applications, which introduced tremendous theoretical and experimental works to improve the photovoltaic capabilities of MOFs. In particular, MOFs could be utilized as counter electrodes or photoanodes for DSSC with potential efficiency. Moreover, interface modifiers and charge transport components could be made from MOFs for PSC. Additionally, several works related to the usage of MOFs for OSC could bring a novelty direction in photovoltaic applications. Although uses of MOFs in various functions of solar cells have advanced quickly in recent years, fundamental difficulties to accelerate solar cell efficacy are as follows:

- (1) The durability of solar cells is a critical factor in evaluating industrial application possibilities. Future research should periodically examine the applications of MOFs in PSCs under extreme conditions, e.g., high humidity.
- (2) Poor electron conductivity is one of the most significant barriers to MOF utilization in solar cells. This might be enhanced by rationally designing and manufacturing novelty kinds of MOFs. Combination MOFs with highly conductive materials or the development of conductive MOFs provide possible solutions for increasing the electrical conductivity of MOFs, allowing for their use in solar cells.
- (3) Metal compounds originating from MOFs are a novel selection that can potentially increase solar cell efficiency. Although these compounds lose the natural features of MOFs, their charge transport behavior may be enhanced. Furthermore, these materials often preserve adequate porosity and have a large surface area, implying a wide range of solar applications.
- (4) A thorough knowledge of the links between MOFs' architectures, characteristics, and solar cell efficiency is required. This may allow for the development of more expected MOFs for photovoltaic utilization. Further research into the uses of 2-dimensional MOFs could provide potential results in solar cells.
- (5) The growth of MOFs on a conductive substrate is a challenging task by virtue of the lack of chemical linking. Therefore, finding a new process to prepare MOF thin films on a conductive substrate is necessary.
- (6) The conduction mechanism of MOF materials is a controversial problem. Therefore, insight studies combining simulation works and experimental studies need to be conducted to explore relationships between structures and power conversion efficiency, as well as a better knowledge of how MOFs operate in photovoltaic devices.

Aside from existing obstacles, MOFs-based materials for solar cells offer substantial prospects due to the diversification of MOFs. Based on composition engineering, Eg of MOFs could be adjusted to optimal values in order to achieve maximum power conversion efficiency. Also, usage of MOF for OSC devices is still limited due to their optical properties. Therefore, the development of photoluminescence MOFs could bring potential results in solar cell applications. Additionally, using contemporary computer techniques to determine the optimum type of MOFs for solar cells might save a significant amount of time and cost in experimental studies. Moreover, the outstanding conductivity of conductive MOFs and the amazing stability of MOF derivatives have yielded promising results in photovoltaic applications.

**Author Contributions:** Writing—original draft preparation, H.H.D.; editing, S.Y.K. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Data Availability Statement: All the data are contained within manuscript.

Conflicts of Interest: The authors declare no conflict of interest.

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