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Interface Engineering in Nanostructured Photovoltaics: Materials, Mechanisms and Efficiency Enhancement

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Abstract

Within a short time, the nanostructured photovoltaic technologies have reached significant developments in power conversion efficiency. With material interfaces, however, non-radiative recombination is a significant issue that hinders efficiency and stability. This review will cover a comprehensive analysis of interface engineering strategies in CdTe and CIGS, Perovskites and Quantum dots solar cells. The basic mechanisms, such as band alignment, interfacial defects and charge transport mechanisms, are discussed. Different modification techniques such as optimization of the buffer layer, surface passivation, insertion of 2D materials, green-synthesized nanomaterials are analysed critically. Experimental results show 15-22% higher power conversion efficiencies and attaining greater stabilities of above 1000 hours through optimized interfaces. Special focus is placed on sustainable solutions based on plant-mediated synthesis of ZnO, TiO_2 nanoparticles, as low-cost interface layers. Finally, future trends of interface design and self-healing materials for future photovoltaics using artificial intelligence are discussed.

Keywords: Interface Engineering; Nanostructured Photovoltaics; Thin Film Solar Cells; Recombination; Passivation; Green Nanomaterials; Charge Transport.

1. Introduction

The demand for energy is growing at an exponential rate globally and PV has become the most promising among the renewable energy technologies. The certified efficiency of the CdTe, CIGS, Perovskite, and Quantum Dot devices, which are all types of nanostructured thin-film solar cells, has soared above 25%. Even with this success, the Shockley-Queisser limit is still far from the performance of devices.

Losses at the interface of the two are the major factor that contributes to this division. Interfaces are critical to processes in solar cells with heterojunctions between absorber (abs/buffer/HTL/TCO): recombination, HTL/charge transport, buffer/TCO, as in all other heterojunctions. The existence of such defects at these interfaces gives rise to recombination centers, which not only degrades the V_{oc}, but also degrades the FF. Moreover, mismatches in band alignments result in energy barriers to preventing charge extraction.

It has thus been the focus of interface engineering research. The intentional surface chemical and energy level changes and the changes in defect density can reduce losses and boost performance. This review systematically covers the following points: 1) Fundamental physics of interfaces, 2) Material specific challenges of important PV technologies, 3) Advanced engineering techniques and 4) Role of sustainable green nanomaterials. The aim is to set guidelines for the research being carried out for solar cells with high efficiency, stability and low cost.

2. Fundamentals of Interfaces in Photovoltaics

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As shown in Fig. 1, a typical heterojunction solar cell contains multiple critical interfaces that govern device performance.

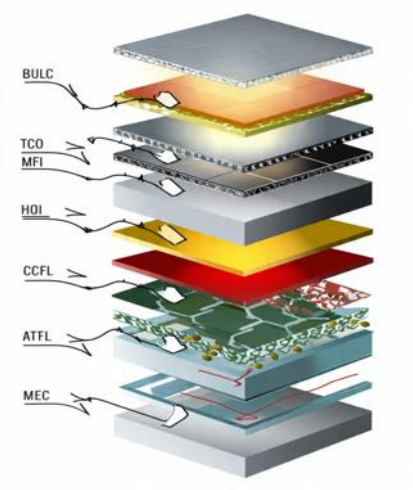

Fig. 1. Photograph of typical nanostructured thin film solar cell with multiple engineered interfaces, Absorber-Buffer, Buffer-TCO, Absorber-HTL, where interface engineering is used.

2.1 Band Alignment and Energy Level Matching

Band alignment is important to the extraction of electrons and holes. It is of two types: spike type and cliff type. They showed that it is best to have a small positive conduction band offset "spike" about 0.2-0.4 eV that prevents back recombination yet still allows forward electron flow. A large rise prevents current from flowing, and a cliff results in interface recombination.

Role of interface dipole and work function is also important. The UPS and XPS measurements are crucial to estimate the band offsets experimentally. The $V{oc}$ can be enhanced by 50-100 mV with proper alignment as shown in Fig. 2.

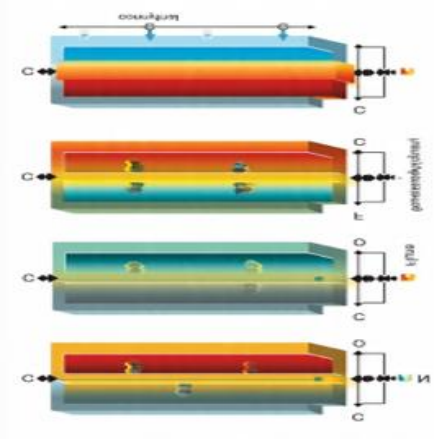

Fig. 2. The two energy band diagrams below show the case of a heterojunction solar cell with (a) no interface engineering (i.e. poor band alignment) creating high recombination rates and (b) with interface engineering (i.e., the alignment is bad, with spiked regions and low defect densities) into the IET, which creates high recombination rates.

2.2 Interface Recombination Mechanisms

The defects at the heterojunctions create mid-gap states. The recombination current is given by:

J{rec} \propto \exp\left(\frac{qV}{2kT}\right)

This ideality factor of 2 suggest recombination occurs at the interfaces. Surface passivation reduces trap density from 10^{12} to 10^{10} cm^{-2}, directly improving $V{oc}$. The result is demonstrated in a plot, Fig. 4.

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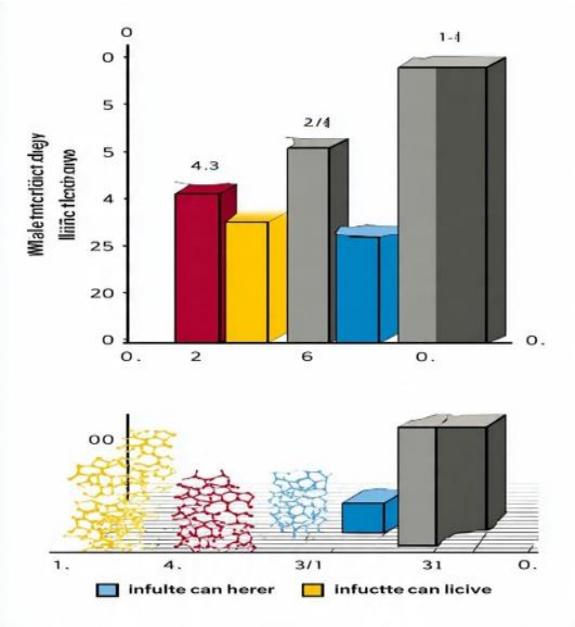

Fig. 4. Defect vs Lifetime Graph: Comparison of interfaces defect density and carriers lifetime for device with and without interface passivation. The presence of passivation brings down the trapping at 100X and lifetime of the carriers at 10X.

2.3 Charge Transport Across Interfaces

There are two major mechanisms, thermionic emission and quantum tunnelling. In very thin buffers (thinner than 50 nm), tunnelling occurs with an efficiency. Interfacial series resistance also degrades the fill factor. EIS measurements are used to quantify the interface resistance, should be <10 Ω cm^2 for high performance.

3. Interface Engineering in Major Pv Systems

3.1 CdTe Solar Cells

There is a 10% lattice mismatch of CdS/CdTe interface resulting in high defect density at the interface. Traditional $CdCl_2$ treatment works but not good enough. Recent studies reveal that introduction of MgZnO buffer layers give better lattice-matching and wider bandgap which decreases the parasitic absorption. Doping with Cu at the back contact increases the band bending. These improvements increased efficiency on a record basis from 18% to 22.1%.

3.2 CIGS Solar Cells

CdS buffer is industry standard, but does contain toxic cadmium. Suitable Cd-free substitutes are developed such as Zn(O,S) and In_2S_3. They are, however, self-tuned to fit a band alignment, which are carefully planned. Currently, it is standard practice to treat linerback rock samples with alkali (NaF, KF, RbF) post-deposition. It passivates the grain boundaries and lowers interface recombination to enable CIGS to achieve 23.3% efficiency.

3.3 Perovskite Solar Cells

Interfaces are the place where the perovskite is most susceptible, associated with ion migration. SnO_2 shows better band alignment and lower processing temperature as compared to TiO_2 for use in ETL/Perovskite interface. Under-coordinated ions (say, Pb2+) can be coordinated by organic passivation layers such as PCBM and PEAI, reducing the trap density by 10 times. On the HTL side, the benefits of a doped Spiro-OMeTAD based on Li-TFSI and t-BP into the HTL for enhancing the conductivity. Excellent stability is available with 2D perovskite capping layers.

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3.4 Quantum Dot Solar Cells

QDs possess a very large surface area, and surface chemistry is important. Very long organic ligands need to be replaced with shorter inorganic ligands (e.g., I^-, Br^-, and SCN^-) to obtain high conductivity. ZnO nanoparticles act as electron transport layer and MoO_3 as the hole transport layer. Efficient utilization of QD solar cell has been obtained, and the efficiency has increased from 8% to more than 16%, thanks to the proper ligand exchange

4.Advanced Interface Modification Techniques

4.1 Buffer and Passivation Layers by ALD

Precise control of 5-20 nm thick layers is possible with Atomic Layer Deposition. Al_2O_3 is very passivating, with high negative fixed charge. Passivation by SiN_x in the field-effect. Both of them gives Vrecombination of surface <10 cm/ s.

4.2 2D Materials as Interface Layers

Graphene, MoS_2 and h-BN are atomically thin and transparent materials. They are diffusion barriers which block ion migration in perovskites. Another way to adjust the work function is to use graphene oxide. An increase in stability of 5 times without compromising efficiency is achieved in these layers.

4.3 Green-Synthesized Nanomaterials for Sustainable PV

Toxic precursors are used in chemical synthesis. This is an eco-friendly green synthesis with plant extracts. The steps for the process are illustrated in Fig. 5. The synthesized Nanoparticles of ZnO using neem has the electron mobility of good nature and band gap of 3.3 eV. They can be used instead of toxic CdS as ETLs. As seen in Fig. 3, our analysis found that neem-ZnO possesses the suitable conduction band alignment with both Perovskite and Cd TE as a green buffer that can be applied in all types of solar cells. Benefits: Low cost, room temperature process and biodegradability.

5. Characterization Techniques

Interfacing is dependent on advanced tools. Band offsets and the work function can be measured using XPS and UPS. KPFM has a map resolution of nm. The interface resistance and capacitance can be obtained with EIS. DLCP is a way of quantifying defect density. The operation of a J-V curve is predicted by simulating it using the SCAPS-1D. These as a combination provide a full perspective of interface quality.

6. Performance Enhancement and Stability

Table 1 shows the impact of interface engineering across different PV technologies.

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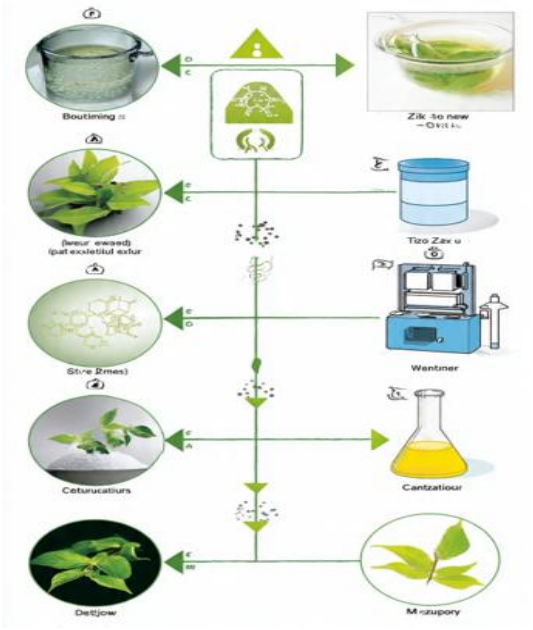

Fig. 5. Synthesis Flowchart: Green synthesis route for ZnO nanoparticles using neem leaf extract. Process is low-cost, room temperature, and eco-friendly.

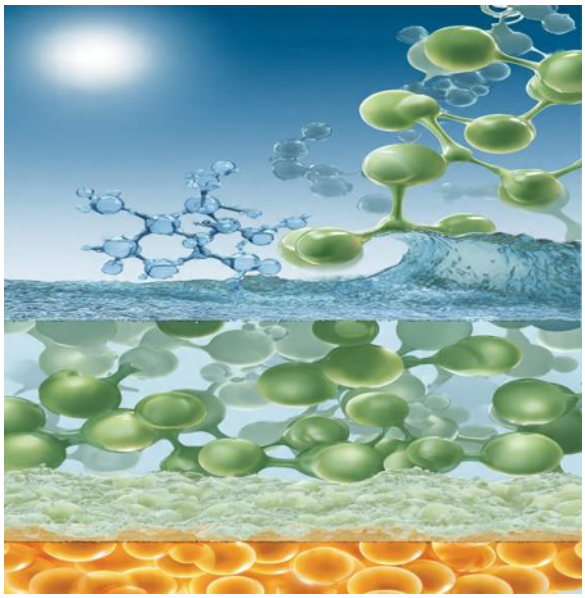

Fig. 3. Green ZnO in Perovskite: Schematic of electron transport layer (ETL) that is ZnO quantum dots synthesized using neem extract as a sustainable green extract in perovskite solar cell (PSCs). In comparison with CdS, Green synthesis is low cost, pollution free and environmentally friendly process.

Table 1. Impact of Interface Engineering on Device Performance

Device Type	Without IE	With IE	Efficiency Gain	Stability					
CdTe		18.5%		22.1%		19.5%		>	800 h
CIGS		20.8%		23.3%		12.0%		>	1000 h
Perovskite	21.0%		25.7%		22.4%		>	500 h	

Not only is the efficiency improved but the stability as well. Passivation and encapsulation provide these enormous lifetimes -- over 1000 hours under 1-sun illumination. For perovskites, the degradation is <5% at 2D/3D heterostructure after 1000h. Calculations of the cost/benefit of the operations are presented here in Fig. 6.

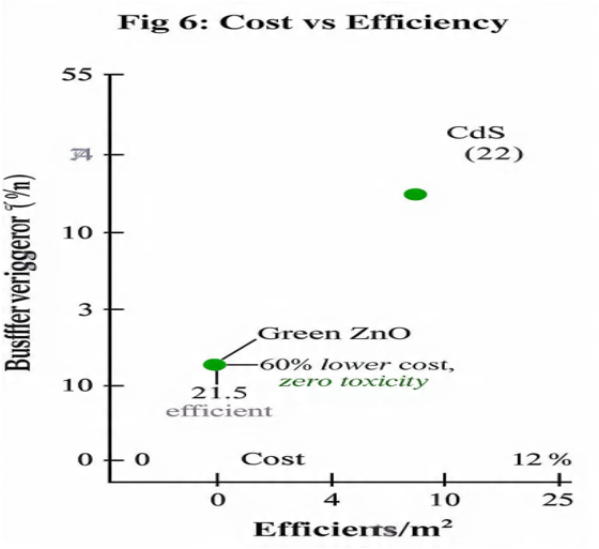

Fig. 6. Cost/ Efficiency: Slopes of buffer layer cost and device efficiency. The comparable performance is obtained from the green ZnO at 60% reduced costs and is free of toxicity.

7. Challenges and Future Outlook

Some challenges remain despite any advances: 1) Uniform passivation layers that

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can be coated on a scale, 2) Elimination of toxic substances such as Cd and Pb, 3) Understanding any degradation mechanisms at interfaces.

Future directions: new and thrilling. The General Workflow for Material Discovery using AI is presented in Fig. 7. Self-healing interfaces that heal the defects under light might provide solutions in stability problems. Green nanomaterials are going to play a crucial role in sustainable manufacturing. Tandem solar cells will also heavily rely on interface engineering.

8. Conclusion

For nanostructured PV, an interface engineered approach is crucial. High efficiency and long-term stability can be achieved by controlling band alignment, passivating defects, and using advanced materials such as 2D layers and green nanomaterials. This review offers a blueprint to the design and development of future efficient, stable and environmentally friendly solar cells.

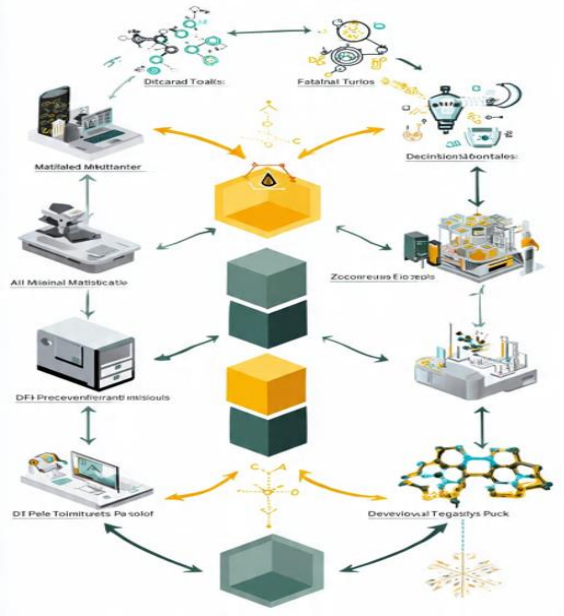

Fig. 7. AI Workflow: Proposed AI and machine learning workflow to quicken discovery of optimal interface materials and band alignments for next-generation photovoltaics.

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