Si Heterojunction Solar Cells: A Simulation Study of the Design Issues

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Abstract—Silicon heterojunction solar cells having semiconducting oxide-selective contacts can revolutionize the photovoltaic industry with the promise of low cost and high efficiency. In this paper, we have identified the potential design issues of silicon heterojunction cell using simulation. This paper compares two possible electron-selective oxides (TiO$_2$ and ZnO) and two possible hole-selective oxides (CuAlO$_2$ and NiO). The Fermi level in the oxide at the oxide/metal interface is pinned by the metal (its workfunction and eventual interface dipoles). We considered this effect, which determines the effective workfunction of the metal contact as opposed to the actual metal workfunction. Our simulation suggests that Fermi level pinning has significant impact on the device performance. We also considered different interface passivation effects and oxide dopings in our simulation. The simulation suggests that high doping in oxides is beneficial to counter balance the effect of poor surface passivation. This paper provides an extensive understanding of the design of Si to counter balance the effect of poor surface passivation. Our simulation suggests that Fermi level pinning has significant impact on the device performance. We also considered different interface passivation effects and oxide dopings in our simulation.

Index Terms—CuAlO$_2$, design optimization, fermi level pinning, interface passivation, NiO, selective contacts, Si heterojunction cell, TiO$_2$, ZnO.

I. INTRODUCTION

SELECTIVE contact is the key component in high-efficiency solar cell. Historically, a diffused p-n junction provided carrier selective contact. In this scheme, a low-doped (n or p) absorber is doped p$^+$ and n$^+$ on each side, respectively, along with metal contacts. The carrier selectivity is achieved through an asymmetry of carrier concentration types at the contacts from high doping. Fig. 1(a) shows a typical band diagram of such a structure, where the band bending from the doping asymmetry is responsible for the carrier separation and extraction. However, at operating condition, this structure cannot provide a high barrier to the dark current resulting from the carrier injection at forward bias. That is why, the record efficiency (∼25%) of a p-n homojunction Si solar cell [1] is still significantly below the limiting efficiency of 29.43% [2]. Moreover, fabricating a p-n homojunction device with dopant diffusion is a high-temperature process and is one of the sources of high-cost and high-energy payback time [3].

Simulation results suggest that band engineered heterojunctions having high band offset for one type of carrier and low for the other carrier type provides better carrier selectivity than homojunctions [4], [5]. Fig. 1(b) shows the energy band diagram of a conceptual Si solar cell, where both the electron- and hole-selective contacts are made by heterojunctions. Contact selectivity also depends on the passivation quality of the contacts otherwise the minority carriers would recombine at the contacts resulting in high dark current. The heterojunctions of a-Si and c-Si have shown great promise due to excellent passivation quality provided by a-Si. Introduced in 1992 by Sanyo [6] as HIT cell, it holds the current record of cell efficiency of 25.6% [7]. The bandgap of a-Si is such that it still absorbs sunlight in the visible spectrum resulting in a loss of short-circuit current [8]. Therefore, semiconducting metal oxides with asymmetric band offsets to Si can be viable candidates for designing selective contacts in heterojunction solar cells. These oxides replace highly doped emitter and back surface field (BSF) in a homojunction cell resulting in a low-temperature fabrication process. Our previous work shows NiO and TiO$_2$ to be excellent candidates for hole-selective and electron-selective contacts, respectively [4]. Numerous implementations of such devices have been reported in the literature [9]–[15], in which, TiO$_2$ [9] and LiF$_x$ [13] are used as an electron-selective contact and MoO$_x$ [11]–[13], PEDOT:PSS [10] and WO$_x$ [14], [15] as a hole-selective contact. Some of the materials (LiF$_x$ and MoO$_x$) implemented...
do not have a band offset that is suitable as a selective contact. The only way these materials work is by creating a defect band near the valence or the conduction band of Si [16].

Nonidealties in these oxides and oxide/Si interface are a bottleneck in implementing heterojunction solar cells. Most importantly, Fermi level pinning at the metal/oxide interface, which creates a Schottky barrier, needs to be considered properly. The built-in potential of a homojunction cell is determined by the Fermi level difference between the highly doped emitter and the BSF. Also the highly doped Si makes the contact resistance not a significant roadblock in designing Si homojunction cells. For oxide/Si heterojunctions, doping of the oxide and Fermi level pinning both will be important factors in determining barriers for both minority and majority carriers. The effect of nonideal transparent conducting oxide (TCO) workfunction on silicon heterojunction cell has been studied previously [20]. However, a small band offset at the majority carrier side poses more stringent design requirement for choosing the right metal workfunction and oxide doping. Therefore, proper design optimization taking Fermi level pinning into account is necessary. We have partially presented our study of selective contact optimization in [21]. In this paper, we will extend our previous work in understanding the optimization of selective contact, considering Fermi level pinning and interface passivation. Besides understanding the design constraints, this paper will provide a reasonable metric for evaluating different materials for carrier selective properties. However, various materials properties and process-related issues as well as degradation effects are not covered by the idealized approach presented in this simulation study. The contact optimization work presented here is based on the simulation study done using AFORS-HET simulation software [22]. The details of this simulation are explained in the Appendix.

II. METAL OXIDES FOR SELECTIVE CONTACTS

Fig. 2 shows the energy band alignment of different oxides and semiconductors [17]–[19].

The Appendix.

The simulation study done using AFORS-HET simulation software [22]. The details of this simulation are explained in

A. Simulation Framework

Fig. 3 shows the device structure simulated in this paper. Electron-selective contacts and hole-selective contacts are studied separately with respect to p and n Si, respectively, so that the heterojunction becomes the carrier separating junction.

for NiO and CuAlO₂, making these suitable for hole-selective contact or electron blocking layer. Moreover, TiO₂ and ZnO are n-type semiconductors, where both extrinsic and intrinsic doping through oxygen vacancy is possible [23]. ZnO has been shown to dope heavily with aluminum. On the other hand, NiO and CuAlO₂ are p-type semiconductors, where both extrinsic and intrinsic doping through cation vacancy is possible. All of these four materials have been studied as window layer or TCO for photovoltaics [24]–[27] due to their optical transparency in the visible spectrum and distinct semiconducting properties. In this paper, we will investigate these materials from selective contact point of view because of their band alignment with Si along with the aforementioned properties.

II. METAL OXIDES FOR SELECTIVE CONTACTS

Fig. 2 shows the energy band alignment of different oxides and semiconductors with respect to Si and other semiconductors. From Fig. 2, we can see that TiO₂ and ZnO have low conduction-band offset, ΔEC, and high valence-band offset, ΔEV with respect to Si, making these suitable for electron-selective contact or hole blocking layer. The opposite is true for NiO and CuAlO₂, making these suitable for hole-selective contact or electron blocking layer. Moreover, TiO₂ and ZnO are n-type semiconductors, where both extrinsic and intrinsic doping through oxygen vacancy is possible [23]. ZnO has been shown to dope heavily with aluminum. On the other hand, NiO and CuAlO₂ are p-type semiconductors, where both extrinsic and intrinsic doping through cation vacancy is possible. All of these four materials have been studied as window layer or TCO for photovoltaics [24]–[27] due to their optical transparency in the visible spectrum and distinct semiconducting properties. In this paper, we will investigate these materials from selective contact point of view because of their band alignment with Si along with the aforementioned properties.

A. Simulation Framework

Fig. 3 shows the device structure simulated in this paper. The 1-D Poisson equation is solved coupled with the current continuity equation. The standard AM1.5G spectrum is used to calculate photogenerated carriers, given the experimentally extracted absorption coefficient of Si. The oxides were simulated as wide bandgap semiconductors with the parameters taken from the published literature and are assumed not to absorb any photons. The nonideal surface passivation is simulated assuming a constant defect distribution along the bandgap of the oxide overlapping with that of the Si. Direct tunneling through the 5-nm oxide is ignored. This is justified due to the large thickness.

To evaluate the oxides as contacts forming carrier separating junctions, two separate device structures are considered for the electron-selective and the hole-selective contacts. In practical implementation, usually these oxides are used along with some TCOs (e.g., ITO, Ag nanowire, and so on) to allow sufficient lateral conduction. In this situation, the metal contact is made with the oxide through the TCO. Therefore, it might seem that the results presented in this paper are not applicable when there is a TCO present between the metal and the oxide. However, the TCOs are also subject to Fermi level pinning and this study is applicable to the contact between TCO and carrier selective oxide. Moreover, in case when the junction is formed in the back of the solar cell, especially in all back contact solar cell, the TCOs are not required. In that situation, this paper is of great importance and could provide a guide for designing the contacts effectively. The effect of nonideal lateral conduction in the TCO is an addition to the series resistance to the light I–V response. We have ignored it deliberately, in order to study the effect of Fermi level pinning properly because it
also causes an addition of series resistance and sometimes introduce extraction barrier to the carrier being extracted out of the contact.

III. FERMI LEVEL PINNING

Ideally, barrier height seen by the carriers (electrons/holes) from the band bending at an Metal Semiconductor (MS) junction is determined by the metal workfunction, \( \phi_M \), and the semiconductor workfunction, \( \phi_S \), determined by the semiconductor doping. However, metal-induced gap states (MIGS) are created by the electron wave function in metal, penetrating into the bandgap of the semiconductor [28]. This causes a dipole charge to be formed at the interface. In equilibrium, metal Fermi level (\( E_{FM} \)) moves close to the charge neutrality level (\( E_{CNL} \)) of the semiconductor, a point where the MIGS switch their characteristics from donorlike to acceptorlike in order to minimize the overall dipole charge. This causes the barrier height for a particular MS junction less sensitive to the metal workfunction, a phenomenon known as Fermi level pinning. How strongly \( E_{FM} \) will be pinned toward \( E_{CNL} \) is determined by the empirical parameter pinning factor (\( S \)) defined as [29]

\[
S = \frac{\partial \phi_B}{\partial \phi_M} = \frac{1}{1 + 0.1(\epsilon_\infty - 1)}.
\]

Here, \( \epsilon_\infty \) is the high-frequency dielectric constant of the semiconductor, and \( \phi_B \) is the barrier height at the MS interface. Effective metal workfunction, \( \phi_{M,\text{eff}} \), of a pinned MS junction is, therefore, given by

\[
\phi_{M,\text{eff}} = S\phi_M + (1 - S)\phi_{CNL}
\]

where \( \phi_{CNL} \) is the position of the charge neutrality level with respect to the vacuum.

A. Electron-Selective Contacts

Previously reported values of \( \phi_{CNL} \) and \( S \) [23] for the studied semiconducting oxides are used to calculate \( \phi_{M,\text{eff}} \) of different contact metals for the heterojunction solar cell and are shown in Fig. 4. The Fermi level pinning at the metal/oxide interface leads to an effective metal workfunction, i.e., the \( \phi_{M,\text{eff}} \) is a joint property of the metal in contact with the oxide, not the property of the oxide alone. Corresponding schematic band alignment of oxide and Si is shown to the right of each plot of effective metal workfunction to provide a visualization of the effective barrier that will be formed for different types of metals. The effect of workfunction on the ideal device performance (perfect surface passivation) for different oxide dopings is shown in Fig. 5. First thing to note here is that the maximum \( V_{OC} \) is 660 meV. However, a-Si passivated solar cells show \( V_{OC} \) greater than 700 meV [7]. This discrepancy is because of using a doped Si homojunction as the BSF. Doped a-Si readily achieves very high dopant concentration. We have assumed a doping of \( 1 \times 10^{19} \) cm\(^{-3} \) for the BSF in our simulation. If the doping of \( 1 \times 10^{20} \) cm\(^{-3} \) is assumed for the BSF instead, the \( V_{OC} \) is greater than 700 meV according to our simulation. Nevertheless, if we observe Figs. 4 and 5 together, we would find some constraint for each oxide. Fig. 4(a) reveals that the lowest \( \phi_{M,\text{eff}} \) that we can expect from TiO\(_2\) is 4.5 eV for the commonly used metal aluminum. Around that \( \phi_{M,\text{eff}} \), the device performance (Fig. 5) is degraded because of the high barrier seen by electrons. Comparatively, ZnO can provide much lower \( \phi_{M,\text{eff}} \) [\( \sim 4.1 \) eV in Fig. 4(b)], which ensures the best device performance for a range of doping in ZnO. Higher effective barrier adds to the overall series resistance of the device degrading the fill factor (\% FF). ZnO can provide lower effective barrier to electrons
than TiO$_2$, because the charge neutrality level lies much closer to the conduction band in ZnO, and it has a higher pinning factor ($S = 0.58$) than TiO$_2$ ($S = 0.24$) that gives it more control to change the barrier height by changing $\phi_M$. It is also observed that devices having low oxide doping suffer the most. This can be attributed to the fact that Schottky barrier thickness increases as the doping is reduced. Moreover, higher doping in the oxide causes the charge to screen the effect of metal Fermi level pinning. This means that the effect of nonideal metal Fermi level diminishes with higher doping in the oxide, where the oxide Fermi level determines the built-in potential. Since the barrier thickness is narrow in highly doped oxide, whatever barrier that is formed between the oxide and the metal has an insignificant effect.

### B. Hole-Selective Contacts

Fig. 4(c) and (d) shows $\phi_{M,\text{eff}}$ achievable for the hole-selective contacts CuAlO$_2$ and NiO. If we look at the band offset diagram, we can see that the comparison here is not that straightforward. The reason is that NiO has a positive valence band offset (VBO) with Si (valence band of NiO lies lower than that of Si) whereas CuAlO$_2$ has a negative VBO (valence band of CuAlO$_2$ lies higher than that of Si). The literature also suggests a range of NiO bandgap [30], which makes it difficult to pinpoint a single value to use in simulation. This positive VBO in NiO creates an additional extraction barrier for the hole. However, the presence of no additional barrier from the VBO in CuAlO$_2$ does not help much because its $E_{\text{CNL}}$ lies farther away from the valence band resulting in the highest $\phi_{M,\text{eff}}$ to be around 4.7 eV. This causes a high barrier for holes and around that value the performance starts to degrade. For NiO, the pinning situation is much better as it can ensure a high $\phi_{M,\text{eff}}$ $\sim 5$ eV in Fig. 4(d). However, the additional barrier caused by the positive VBO affects carrier extraction. Nevertheless, we have assumed a conservative value of VBO between NiO and Si. In practice, the bandgap of NiO can be engineered by varying the deposition condition [31] resulting in the tuning of VBO.

### IV. Effect of Interface Defects

Interface trap states, $D_{\text{it}}$, play a significant role in determining the effectiveness of the selective contacts. Fig. 1(b) shows the band diagram of a double heterojunction cell with the directions of different current components. The high band offset is supposed to suppress the injected dark current. However, if that interface has a high density of $D_{\text{it}}$ in the midgap region, instead of getting reflected at the high band offset barrier, the minority carrier recombines at the interface. The recombination current flows in the direction opposite to that of the photocurrent, resulting in increased dark current. As a result VOC drops, since it depends on the ratio of the photocurrent and the dark current. In effect, poor surface passivation can defeat the whole purpose of using band engineered oxide heterojunction as the selective contacts, because it will provide an additional path for the dark current to flow. In this section, we will determine the effect of interface passivation and explore its interaction with other design constraints.

#### A. Quantifying Interface Passivation

AFORS-HET allows us to define the $D_{\text{it}}$ distribution and its density. We assume a constant $D_{\text{it}}$ distribution along the bandgap of Si. The character of $D_{\text{it}}$ switches from donor type to acceptor type at the $E_{\text{CNL}}$ of Si as we move from valence band toward conduction band. We varied the total $D_{\text{it}}$ density from $1 \times 10^{10}$ cm$^{-2}$ to $1 \times 10^{13}$ cm$^{-2}$. This corresponds to the surface lifetime, $\tau_s$, of 1 ms to 1 $\mu$s. The bulk lifetime, $\tau_b$, is assumed to be 10 ms, which is very common for an Float Zone (FZ) wafer. So, at $\tau_s = 1$ ms, the overall lifetime is dominated by both the bulk and surface passivation. At $\tau_s = 1$ $\mu$s, the overall lifetime is completely dominated by the surface passivation. The detailed explanation of the interface passivation modeling and how the lifetime is calculated are given in the Appendix.

#### B. Electron-Selective Contact

Fig. 6 compares the light $I-V$ response for the electron-selective contacts for different $\phi_{M,\text{eff}}$ values,
interface passivations ($\tau_i$), and oxide dopings. Fig. 6 suggests that high doping can compensate some of the drastic effects of poor interface passivation. This can be explained by Fig. 7, which shows the difference between Fermi level and the valence band edge at the interface in thermodynamic equilibrium ($\phi_{inv,n}$) in dark condition. The thermodynamic equilibrium signifies the device condition after junction formation with no external excitation (light or bias). This metric corresponds to the overall band bending of the junction due to the asymmetry of carriers in the heterojunction.

From the device physics point of view, $V_{OC}$ represents a point where the band bending is such that the forward injection current (source of dark current) is equal to the photocurrent (flowing in opposite direction). Higher band bending at the thermodynamic equilibrium causes the $V_{OC}$ point to occur at higher voltage. It has recently been shown that the carrier separation at the selective contacts, and hence, the $V_{OC}$ is governed by the conductivity difference for holes and electrons at the contacts [5]. Band bending at the thermodynamic equilibrium determines the conductivity near the contact region. Therefore, $\phi_{inv,n}$ effectively determines the overall performance of the device. From Fig. 7, we can see that high oxide doping increases $\phi_{inv,n}$ and makes it insensitive to $\phi_{M,eff}$ for ZnO. For TiO$_2$, $\phi_{inv,n}$ decreases with $\phi_{M,eff}$. This is because TiO$_2$ has a very high relative dielectric constant (~86) compared with ZnO (~7). So high doping does not screen the electric field, resulting in band bending dependent on metal workfunction. This effect is also manifested in Fig. 6, where we see that $V_{OC}$ in TiO$_2$ cell is more sensitive to metal workfunction than that in ZnO even at high doping.

We see a distinct kink and overall S-shaped $I-V$ in low-doped oxide for high $\phi_{M,eff}$. The two main causes of this S-shape are the presence of a barrier for majority carrier extraction and the charge stored in $D_{it}$ given by the following equation:

$$Q_{it} = \varepsilon_0 \varepsilon_{r}^{oxide} \frac{\partial \phi(x)}{\partial x} \bigg|_{x_{it}^{oxide}} - \varepsilon_0 \varepsilon_{r}^{Si} \frac{\partial \phi(x)}{\partial x} \bigg|_{x_{it}^{Si}}.$$  \hspace{1cm} (3)

Here, $\varepsilon_{r}^{oxide}$ and $\varepsilon_{r}^{Si}$ represent the relative dielectric constant of oxide and Si, respectively. Also, $x_{it}^{oxide}$ and $x_{it}^{Si}$ denotes the oxide/Si interface from the oxide side and the Si side, respectively, to account for the discontinuity of the electric field at the interface. $Q_{it}$ is plotted as a function of voltage for different oxide dopings and surface passivations in Fig. 8. From Fig. 8, we can get a comparative picture between TiO$_2$ and ZnO based on their stark difference in dielectric constant. High-$k$ TiO$_2$ changes the $Q_{it}$ distribution rapidly as a function of gate voltage. Especially for a high $\phi_{M,eff}$ at low oxide doping, the Fermi level at the interface moves as the voltage changes. This changes the amount and the type of charge stored in $D_{it}$. The voltage where this occurs shows up as a kink in the $I-V$ characteristics. For high doping in oxide, change in voltage is screened by the dopant charge and the Fermi level at the interface remains constant, and hence, the $Q_{it}$ remains constant. Therefore, at high oxide doping, we do not see a significant kink in the $I-V$ characteristics. For a high-$k$ oxide like TiO$_2$, the voltage change at the metal terminal can still have an effect on the Fermi level at the interface. This can affect the cell performance based on the interface passivation. If the interface passivation quality is good, the effect of nonideal (high for electron-selective contact) metal workfunction needs to be kept as low as possible. In that case, both low-$k$ dielectric and high doping are beneficial. We can see this clearly by comparing Fig. 6(a) and (b) for both TiO$_2$ and ZnO. If the interface passivation quality is poor, it can be compensated by choosing a combination of metal workfunction, dielectric constant, and doping of the oxide in such a way that the $Q_{it}$ crossover does not appear in the voltage range of interest. Only charge stored in the interface defect states cannot completely explain the S-shape seen in Fig. 6. When $\phi_{M,eff}$ increases, Schottky barrier height at the contact increases, resulting in an increased barrier for majority carrier extraction. These nonextracted majority carriers recombine at the interface causing S-shaped $I-V$. The S-shape disappears when the oxide doping increases, which reduces the space charge region and enhances the internal electrical field.

C. Hole-Selective Contact

Fig. 9 compares $I-V$ response under illumination for hole-selective contacts for different $\phi_{M,eff}$ values, $\tau_s$ values, and oxide dopings. There is a 0.23-eV VBO between
NiO and Si [32]. Therefore, holes in Si see a barrier of 0.23 eV when extracted. This poses a strict limit on the allowable $\phi_{M,\text{eff}}$. Since we have not taken tunneling into account, the simulation convergence becomes an issue when $\phi_{M,\text{eff}}$ becomes too low. CuAlO$_2$ on the other hand has a slight negative band offset ($\sim-0.12$ eV) with Si [Fig. 4(c)]. This makes the carrier extraction from Si to CuAlO$_2$ easier than NiO. However, doping in oxides still plays a significant role specifically for low workfunction metals. This is because in CuAlO$_2$ $E_{\text{CNL}}$ lies far away from the valence band edge, and it is hard to reduce the barrier between metal and oxide. Even a high workfunction metal Pt pins 0.3 eV away from the valence band edge.

Only the band offset consideration should not dictate the choice of a contact material (oxide and metal). This also depends on pinning and doping of the oxide. The most important point here is the drastic reduction of $V_{OC}$ when the interface passivation is poor in CuAlO$_2$/Si interface even at a high doping. In order to explain this, we look in Fig. 10, which shows the difference between the Fermi level and conduction band edge at the interface in equilibrium ($\phi_{\text{inv},p}$). Fig. 10 represents the extent of inversion at the interface when the heterojunction is formed. From Fig. 10, we observe that for CuAlO$_2$, $\phi_{\text{inv},p}$ decreases significantly when the surface passivation becomes poor [Fig. 10(a) red solid and dotted lines] for highly doped oxide. No reduction is seen for NiO. This is due to the small positive VBO between NiO and Si, which cause a triangular well for holes to accumulate at the equilibrium. Because of these accumulated holes, the band bending remains high irrespective of the interface passivation. Therefore, a slight positive band offset might be useful depending on whether the oxide can be doped and the Fermi level pinning is such that very low barrier height is possible from the metal side. However, such an offset should be carefully engineered as the accumulated majority carrier account for a possible S-shaped $I-V$ characteristics. Also, doping in these oxides induces trap levels near the band edge, resulting in an increase in trap-assisted tunnelling, which can improve the contact selectivity. Previous simulation suggests that high doping in oxide can provide additional band bending, resulting in a reduction in the tunnel barrier thickness [33]. Therefore, our simulation not including tunneling is a conservative estimate of the device performance.

Fig. 11 shows $Q_{\text{it}}$ as a function of voltage for different dopings, interface passivations, and $\phi_{M,\text{eff}}$ values.
Fig. 11 suggests that kink in the $I-V$ response to light for low $\phi_{M,\text{eff}}$ can be explained using the crossover of $Q_{\text{It}}$. The voltage where the crossover occurs corresponds to the voltage where kink appears. For low-doped oxide with good surface passivation, this crossover occurs in the usable voltage range and is visible. For poor surface passivation, this crossover occurs outside of the voltage range between short circuit and open circuit. Hence, the kink is not visible. However, the usual shape of $I-V$ response is altered and a slight S-shape is seen. For high oxide doping, S-shape is not visible as the Fermi level at the interface between oxide and semiconductor changes only slightly as a function of voltage.

V. CONCLUSION

In this paper, a thorough understanding of the design and optimization of heterojunction solar cells using semiconducting oxides as selective contact is presented. Our simulations suggest that the surface passivation and metal/oxide barrier height play important roles in determining the performance of such devices. However, proper design considering the aspects of selective contacts is the key to replace highly doped emitter and the BSF used in traditional Si homojunction cell. Specifically the following hold.

1) Besides band offset, the Fermi level pinning properties of the oxides need to be taken into account, requiring $E_{\text{CNL}}$ to lie close to one of the band edges, and it should have relatively high pinning factor.

2) High-$k$ oxides allow the electric field at the oxide/Si interface to be influenced by the metal workfunction more than the low-$k$ oxides. So high-$k$ oxides are affected by the nonideal metal workfunction more than the low-$k$ oxides.

3) High doping in oxides is beneficial to counter balance the effect of poor surface passivation. Low doping can cause S-shaped $I-V$ for nonideal metal workfunction.

4) The ideal band offset for the majority carrier is supposed to be zero. However, if it is negative, it can provide low barrier to carrier extraction but impacts $V_{\text{OC}}$. If it is positive, it can provide some barrier to the carrier flow, but it can cause higher inversion at the interface, resulting in high $V_{\text{OC}}$. The exact value of the band offset that is tolerable is determined by the effective metal workfunction, doping of the oxide, and the relative improvement in $V_{\text{OC}}$.

APPENDIX

SIMULATION DETAILS

We utilized the software package AFORS-HET 2.4.1 (Automat FOR Simulation of Heterostructures) in order to simulate the Si heterojunction solar cells [22]. In AFORS-HET, The 1-D Poisson equation and the carrier continuity equations are solved within the optical carrier generation determined by the Beer–Lambert law. We simulated four one-sided Si heterojunction solar cells; in two of them 5-nm-thick, p-doped NiO and CuAlO$_2$ were used as the hole-selective contacts while 0.2-$\mu$m, highly n-doped Si was utilized as the electron-selective contact for a 250-$\mu$m-thick, n-doped Si absorber (Fig. 3). In the other two solar cells, 5-nm-thick, n-doped ZnO and TiO$_2$ were utilized as the electron-selective contacts, while 0.2-$\mu$m, highly p-doped Si was used as the hole-selective contact for a 250-$\mu$m-thick, p-doped Si absorber (Fig. 3). No optical losses were considered, so that all the incident sunlight is captured. However, the Si absorber is considered to absorb the spectra based on its absorption coefficient at a certain wavelength. At the bottom contact, $\phi_M$ is assumed such that it behaves as an ohmic contact. The top contact is where the Fermi level pinning of metal on oxide is considered, and $\phi_{M,\text{eff}}$ is set as a simulation parameter, which determined the boundary condition. AFORS-HET allows us to define the interface trap defect distribution and its density. The details of how trap distribution is defined and how it is related to the surface and bulk lifetimes can be found in [22]. Finally, Table I shows the essential material parameters of the four oxides used in this simulation.

### REFERENCES


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