MECHANICAL ENGINEERING | RESEARCH ARTICLE

The influences of the front work function and intrinsic bilayer \((i_1, i_2)\) on p-i-n based amorphous silicon solar cell’s performances: A numerical study

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Abstract: In this study, the front work function \(WF_{ITO}\) and absorber layer bandgap's influences on two solar cells structure performances, namely ITO/(p)a-Si:H/(i)\(\alpha\)-Si:H/(n)a-Si:H/metal (single intrinsic, \(S_{inv}\)) structure and ITO/(p)a-Si:H/(i)\(\alpha\)-Si:H/(i)\(\alpha\)-Si:H/(n)a-Si:H/metal (double intrinsic, \(D_{int}\)) structure, fabricated using RF-PECVD method were simulated, using AFORS-HET (Automated FOR Simulation of hetEROstructures) software. Based on these simulations, the work functions (WF\(_{ITO}\)) value ought to range from 4.9 to 5.7 eV, in order to determine the optimum WF\(_{ITO}\) for high solar cell efficiency, confirmed with the J-V dark characteristic, the band diagram in thermodynamics equilibrium, build-in electric field distribution, trapped holes density, as well as the quantum efficiency. The simulation results showed the \(D_{int}\) structure's external parameters (e.g., \(V_{OC}, J_{SC}, FF, E_{H}\)) are higher, compared to the \(S_{int}\) structure. Furthermore, the absorber \((i_1\) and \(i_2)\) layers bandgap is optimized in an effort to

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PUBLIC INTEREST STATEMENT

Hydrogenated amorphous silicon-based solar cells (\(\alpha\)-Si:H) have several advantages to be developed as inexpensive, non-toxic, and environmentally friendly solar cells. In this study, optimization efforts were carried out to increase the conversion efficiency through simulation of the \((p-i-n)\alpha\)-Si:H structure solar cells fabricated using RF-PECVD realized by our research group. Modification of the work function at the ITO/(p) \(\alpha\)-Si:H interface and the addition of intrinsic layers with different band gap values resulted in a new structure \((p-i_1, i_2-n)\alpha\)-Si:H which has been shown to increase the conversion efficiency, both based on experimental and simulation results. Furthermore, the simulation results are compared with the simulation results of other similar thin-film solar cells. The results showed that the structural modification using the work function value at the appropriate ITO/(p)\(\alpha\)-Si:H interface and the addition of an intrinsic layer on the \((p-i-n)\alpha\)-Si:H structure resulted in higher \(V_{OC}\) values and good conversion efficiency. The proposed structure of the \((p-i_1-i_2-n)\) solar cells provides a reference for further development in solar cells technology.
improve the $D_{int}$ solar cell’s performance. According to the results, the $D_{int}$ structure had a 10.76 % maximum efficiency ($V_{OC} = 969.8$ mV, $J_{SC} = 16.03$ mA/cm$^2$, and $FF = 70$ %), using $WF_{ITO}$, $I_1$ layer bandgap, and $I_2$ layer bandgap of 5.7 eV, 1.82 eV, and 1.86 eV, respectively.

**Subjects:** Renewable Energy; Clean Tech; Semiconductors

**Keywords:** $WF_{ITO}$; RF-PECVD; AFORS-HET; a-Si:H; bandgap; absorber layers

**1. Introduction**

Hydrogenated amorphous silicon (a-Si:H) is a semiconducting material explored in the last three decades, due to its potential application in thin-film solar cell development. Green et al., 2021, reported a-Si:H single-junction based solar cells have a low efficiency of about 10.2% (Green et al., 2021), due to several limitations, including parasitic optical absorption in doped layers, defects at p/i and i/n interfaces, lower optical absorption in the absorber layer, and limited light trapping within the cells (Shin et al., 2017). Therefore, one of the main issues to increase the a-Si: H solar cell's efficiency is to improve the quality a-Si:H layers. The intrinsic layers (i-a-Si:H) must have good electrical transport, in order to sustain photogeneration for holes and electrons to exit the device before recombination. In addition, this layer must have a suitable ability to absorb light and consequently, generate more electron-hole (e-h) pairs (Son et al., 2018). According to a previous study, adding an active layer with a different bandgap in the p-i-n layer with an optimum thickness in order to maintain material quality improved the solar cell's efficiency from 5.61 % (p-i-n type) to 8.86 % (p-i1-i2-n type; Prayogi et al., 2021). The TCO's work function also strongly influences the cell's performance (Belfar, 2015). Thus, quality TCO/(p)a-Si:H contact, as well as Ohmic contact, is achievable through increased TCO work function, in order to minimized the band offset, and consequently, reduce the device's electron injection barrier height (Y. S. Park et al., 2013).

The energy band offset between semiconductor and TCO ought to be minimized, in order to improve ohmic contact. Therefore, inserted transparent conductive oxides (for instance, Indium Tin Oxide, ITO) with high conductivity (a > 10$^3$ S/cm), good transparency in the visible range (T > 90 %), and higher work function values are required for the higher possibility to carrier injection into TCO/(p) a-Si:H interface. For thin film solar cells, a work function of TCO associated with carrier injection into TCO/(p) window interface which influences plays a dominant role in the device parameters such as $V_{OC}$ and $FF$ (Oh et al., 2012; Rached & Mostefaoui, 2008). The deposition of ITO films on Corning 1737 substrate, using RF-Magnetron Sputtering method improved ITO work function from 4.67 to 5.66 eV, by the $O_2$ plasma treatment and an almost stable resistivity (J. Park et al., 2013). Meanwhile, the electrical and optical characteristics of the ITO films are improved by doping the films with high permittivity materials (Zr, ZrO$_2$), and this results in high mobility and work functions due to the excellent surface (Hussain et al., 2014; Khokhar et al., 2020; Zhang, 2010). Furthermore, optical losses in TCO were reduced without compromising with $R_i$ and recombination loss, using ITO/SiO$_2$ stacks, to produce the short circuit current density ($J_{sc}$) > 41.3 mA/cm$^2$, with a 100 $\Omega$ sheet resistance, while ITO/SiO$_2$/SiO$_2$ produced a 42 mA/cm$^2$ $J_{sc}$, with a 300 $\Omega$ sheet resistance (Herasimenka et al., 2016). Cruz et al., also reported the effect of various TCO (ITO, ZnO:Al, I0:H) as rear-junction of the silicon heterojunction solar cells, through experiments and simulation (Cruz et al., 2019).

In this study, the effect of changes in work function ($WF_{ITO}$) of the ITO/p-layer interface, on the single intrinsic layer, $S_{int}$ (p-i-n type) and double intrinsic layer, $D_{int}$ (p-i1-i2-n type) solar cell performances were simulated using AFORS-HET software. The band diagrams, J-V characteristics, electrical field distribution, trapped holes density, and quantum efficiency were also simulated, to further understand the solar cells’ high performances. In addition, the optimum absorber layer bandgaps’ influence in improving the $D_{int}$ structure’s optical and electrical output was investigated.
2. Simulation methods

2.1. Physical model

This study used well-practiced AFORS-HET to accurately evaluate the effect of numerous parameters on the solar cell’s performances. This software solves the 1-D Poisson’s equation and the continuity equation for electrons as well as holes, using Shockley–Read–Hall (SRH) recombination statistics. Also, e−h pair generation in the absorber layer is estimated with the Beer–Lambert absorption equation, using the optical model in AFORS-HET. The detailed equation used in AFORS-HET is expressed in (Stangl, 2010).

\[
\frac{\varepsilon_0 \varepsilon_r (x) \partial^2 \phi (x, t)}{q} \frac{\partial \phi (x, t)}{\partial x} = p(x, t) - n(x, t) + N_D (x) - N_A (x) + \sum_{\text{trap}} \rho_{\text{trap}} (x, t)
\]

(1)

\[
\frac{\partial J_n (x, t)}{\partial x} - \frac{1}{q} \left( \frac{\partial J_p (x, t)}{\partial x} \right) = G_n (x, t) + R_n (x, t) - \frac{\partial n (x, t)}{\partial t}
\]

(2)

\[
+ \frac{1}{q} \left( \frac{\partial J_p (x, t)}{\partial x} \right) = G_p (x, t) - R_p (x, t) - \frac{\partial p (x, t)}{\partial t}
\]

(3)

where \( \varepsilon_0 \varepsilon_r \) is the absolute dielectric constant, \( \phi (x, t) \) is the electric potential, \( q \) is the electron charge, \( n(x, t) \) and \( p(x, t) \) are electrons and holes densities, \( N_D (x) \) and \( N_A (x) \) are the doping densities (donor and acceptor) at the fixed position \( x \), \( \rho_{\text{trap}} \) is the defect density of charge defect specifying the number of traps at any energy position \( E \) within band gap (the defect type can be empty or occupied with a single or double electron), \( G(x, t) \) denotes the generation rate for carriers, \( R(x, t) \) is the recombination rate, respectively.

Furthermore, localized state density describing layers a-Si:H is expressed as exponential band tail defect states (Urbach tails) and Gaussian mid-gap states (dangling bond) is expressed in (Stangl, 2010).

\[
N_{\text{trap}} (E) = N_{\text{trap}}^{C, \text{tail}} \exp \left( \frac{E_C - E}{E_{C, \text{trap}}} \right)
\]

(4)

\[
N_{\text{trap}} (E) = N_{\text{trap}}^{V, \text{tail}} \exp \left( - \frac{E_C - E}{E_{V, \text{trap}}} \right)
\]

(5)

\[
N_{\text{trap}} (E) = \frac{N_{\text{db}}}{\sigma_{\text{trap}}^2} \exp \left( - \frac{1}{2} \left( \frac{E - E_{\text{db}}}{\sigma_{\text{db}}^2} \right)^2 \right)
\]

(6)

where \( N_{\text{trap}}^{C, \text{tail}} \) and \( N_{\text{trap}}^{V, \text{tail}} \) are the tail state density per energy range at the conduction and valence bands, \( E_{C, \text{trap}} \) and \( E_{V, \text{trap}} \) are characteristic decay energy (Urbach energy) of the conduction and valence bands, \( E_V \) and \( E_C \) are the valence and conduction band energies, \( N_{\text{db}} \) is total dangling bond state density, \( E_{\text{db}} \) is specific energy of Gaussian dangling bond peak, and \( \sigma_{\text{db}} \) is standard deviation of the Gaussian dangling bond distribution.
2.2. Devices structures and input parameters

In this study, the S_int and D_int hydrogenated amorphous silicon solar cell structures were fabricated by our research group, fabricated using RF-PECVD reactor realized in our research group.

![Figure 1. Prototypes of p-i-n and p-i1-i2-n based amorphous silicon solar cell's fabricated using RF-PECVD reactor realized in our research group.](image)

![Figure 2. Schematic of (a) single intrinsic (S_int) structure, (b) double intrinsic (D_int) structure, (c-e) the DOS for different types of the α-Si:H produced by AFORS-HET simulator. D-like and A-like declares donor like and acceptor like Gaussian mid-gap states, VB-tail and CB-tail declares valence band and conduction band, respectively.](image)

In this study, the S_int and D_int hydrogenated amorphous silicon solar cell structures were fabricated by our research group, fabricated using RF-PECVD reactor (MVSystechn Inc., USA), as shown in Figure 1. Meanwhile, Figure 2(a-e) shows the simulation details, ITO/(p)α-Si:H(15 nm)/(i)α-Si:H(600 nm)/(n) α-Si:H(25 nm)/metal (S_int), and ITO/(p)α-Si:H(15 nm)/(i1)α-Si:H(300 nm)/(i2)α-Si:H(300 nm)/(n)α-Si:H (25 nm)/metal (D_int). Meanwhile, the solar cell’s second structure was fabricated with the (i)α-Si:H split into two parts, (i1)α-Si:H (300 nm and Eg = 1.70 eV) as well as (i2)α-Si:H (300 nm and Eg = 1.85 eV). The structure detailed fabrication was carried out as described by (Prayogi et al., 2021). Figure 2(c-e) shows the (p)α-Si:H (i)α-Si:H, and (n)α-Si:H layers’ gap states distribution, described as exponential band tail defect states and Gaussian mid-gap states (dangling bond states).

The effects of WFITO at ITO/(p)α-Si:H interface on the S_int and D_int solar cell devices’ performances were observed numerically using AFORS-HET, however, this was not studied by Prayogi, et al. In addition, the absorber (i1,i2) layers’ bandgap was optimized for improved D_int solar cell performance.
performance. The radiation AM1.5 G spectrum with 100 mW/cm² power density was used as illuminating source, while the operational temperature was 300 K. Meanwhile, for parameters input simulation, the surface recombination velocity ($S_d$) of the front as well as back contact was assumed to be both $1.0 \times 10^7$ cm/s. The barrier height at front contact $\psi_{p0}$ (ITO/(p)-Si:H layer) was taken to the calculation by changing the $WF_{ITO}$, while the barrier height at back contact $\psi_{b0}$ ((n) a-Si:H layer/metal) was kept constant 0.2 eV. Also, the front contact was assumed to reflect (RF) 10 % of the incident light, while the back counterpart was assumed to be 0 or no back reflector (RB). The p-window and n layers’ mobility bandgap were set to be 2.0 eV and 2.2 eV, respectively, while the absorber layers ($i_1$ and $i_2$) counterpart ranged from 1.7 to 1.86 eV. Table 1 shows the typical parameters used in the simulations in more detail, as described in previous studies (Belfar, 2015; Hernández-Como & Morales-Acevedo, 2010; Prayogi et al., 2021).

3. Simulation results and discussion

3.1. Influences of $WF_{ITO}$ on the performances of the solar cells

In this simulation, the ITO work function’s values were varied between 4.9 to 5.7 eV, according to experimental results deposited by RF sputtering, depending on deposition conditions (Kim et al., 2009; Klein et al., 2010; Y. S. Park et al., 2013). Figure 3 illustrates the $S_{int}$ and $D_{int}$ solar cells simulated electrical parameters as a function of $WF_{ITO}$ using AFORS-HET, in order to determine the optimum $WF_{ITO}$ for high solar cell efficiency. According to Figure 3(a), the $V_{OC}$ values increased with increase in $WF_{ITO}$ from 4.9 to 5.3 eV for both structures, due to shift of the front contact barrier $\psi_{b0}$ (reduction in the band bending), with a direct influence on increasing built-in potential, $V_{bi}$, as shown in expression (Belfar, 2015; Jensen et al., 2002).

$$V_{bi} = WF_{ITO} - \chi_{e|x=0} - \psi_{bl}$$ (7)

$$V_{OC} = \left\{ V_{bi} - nKT \ln \left( \frac{qN_vS_r}{J_{SC}} \right) \right\}$$ (8)

where $\chi_{e|x=0}$ is the electron affinity of p-window layer, $\psi_{bl}$ is the barrier height at back contact, $n$ is diode ideality factor, $KT$ is the thermal energy, $N_v$ is the effective density of states in the valence band, $S_r$ is the interface recombination velocity. From eq. (7)-(8), it is clear that the $V_{bi}$ has a larger value when $WF_{ITO}$ is higher and the $V_{OC}$ increases with the built-in potential. However, when $WF_{ITO}$ = 5.7 eV, the built-in potential $V_{bi}$ = 1.7 eV which is enough to effectively separate the carriers and provides the strong electrical field, resulting in a high value of $V_{OC}$.

Figure 3(b) shows the current density values $J_{SC}$ for both structures were observed to increase with change in $WF_{ITO}$, consequently, improving photogenerated hole passage from the p-window to ITO layer. According to Figure 3(c), as the $WF_{ITO}$ increases, the two structures' FF values also increased, due to migration of holes from the p-window layer to the ITO interface, with reduction in the surface band bending the hole injection barrier (Oh et al., 2012). Meanwhile, Figure 3(d) shows the $S_{int}$ and $D_{int}$ structure’s maximum efficiency is about 6.73 % ($V_{OC} = 839.4$ mV, $J_{SC} = 14.78$ mA/cm², and FF = 54.25 %) and 9.21% ($V_{OC} = 858.1$ mV, $J_{SC} = 16.07$ mA/cm², and FF = 66.80 %), respectively, at $WF_{ITO}$ = 5.7 eV. Low FF values from the simulation result is following with the experimental results reported by (Park et al., 2012). This is presumably for both structures, due to the imperfect joint formation mechanism creating defect conditions at the ITO/p-window layer interface.

As previously mentioned, the $D_{int}$ solar cell structure has a better performance, compared to the $S_{int}$ solar cell structure, and is therefore to be the focus of the discussion. The correlation between the behavior of solar cells in the dark and the $WF_{ITO}$ value will be analyzed to test the quality of the solar cells with electrical parameters in the dark (dark parameters), namely the reverse saturation current, $J_0$. Figure 4 shows the J-V characteristics under dark for typical $WF_{ITO}$ of 4.9 eV, 5.3 eV, and 5.7 eV,
Table 1. Parameters input for simulation of the solar cells using AFORS-HET

| Parameters                                      | (p)α-Si:H | (i)α-Si:H | (i)α-Si:H | (n)α-Si:H |
|------------------------------------------------|-----------|-----------|-----------|-----------|
| Layer (nm)                                      | 15        | 100–500   | 100–500   | 25        |
| Dielectric constant                            | 11.9      | 11.9      | 11.9      | 11.9      |
| Electron affinity (eV)                          | 3.8       | 3.80      | 3.80      | 3.80      |
| Bandgap (eV)                                    | 2.0       | 1.70–1.86 | 1.70–1.86 | 2.2       |
| Effective cond. band density (cm⁻³)             | 2.5 × 10²⁰| 2.5 × 10²⁰| 2.5 × 10²⁰| 2.5 × 10²⁰|
| Effective val. band density (cm⁻³)              | 2.5 × 10²⁰| 2.5 × 10²⁰| 2.5 × 10²⁰| 2.5 × 10²⁰|
| Acceptor concentration, Na (cm⁻³)               | 3.0 × 10¹⁸| 0         | 0         | 0         |
| Donor concentration, Nd (cm⁻³)                  | 0         | 0         | 0         | 1.0 × 10¹⁹|
| Electron (hole) mobility (cm²V⁻¹s⁻¹)            | 10 (1)    | 20 (2)    | 20 (2)    | 10 (1)    |
| Thermal velocity of electron (hole) (cms⁻¹)     | 1.0 × 10⁷ | 1.0 × 10⁷ | 1.0 × 10⁷ | 1.0 × 10⁷ |
| Defect density at conduction (valence) band edge (cm⁻³eV⁻¹) | 6.67 × 10⁻⁰⁶(6.67 x 10⁻⁰⁶) | 2.33 × 10⁻¹⁴(2.33 x 10⁻¹⁴) | 2.0 × 10⁻¹⁴(2.0 x 10⁻¹⁴) | 2.0 × 10⁻¹⁴(2.0 x 10⁻¹⁴) |
| Urbach energy for conduction (valence) band tail (eV) | 0.03(0.06) | 0.03(0.06) | 0.03(0.06) | 0.03(0.06) |
| Capture cross-section σp (αp) for conduction band tail (cm²) | 1.0 × 10⁻¹⁷(1.0 x 10⁻¹⁷) | 1.0 × 10⁻¹⁷(1.0 x 10⁻¹⁷) | 1.0 × 10⁻¹⁷(1.0 x 10⁻¹⁷) | 1.0 × 10⁻¹⁷(1.0 x 10⁻¹⁷) |
| Capture cross-section σv (αv) for valence band tail (cm²) | 1.0 × 10⁻¹⁵(1.0 x 10⁻¹⁵) | 1.0 × 10⁻¹⁵(1.0 x 10⁻¹⁵) | 1.0 × 10⁻¹⁵(1.0 x 10⁻¹⁵) | 1.0 × 10⁻¹⁵(1.0 x 10⁻¹⁵) |
| Gaussian density of states (cm⁻³)                | 8.0 × 10¹⁷ | 8.0 × 10¹⁵ | 8.0 × 10¹⁵ | 8.0 × 10¹⁷ |
| Gaussian peak energy for donor/acceptor (eV)    | 1.22(0.70) | 1.22(0.70) | 1.22(0.70) | 1.22(0.70) |
| Standard deviation of Gaussian for donor (acceptor) (eV) | 0.23(0.23) | 0.23(0.23) | 0.23(0.23) | 0.23(0.23) |
| Capture cross-section σp (αp) for donor-like Gaussian states (cm²) | 1.0 × 10⁻¹⁴(1.0 x 10⁻¹⁴) | 1.0 × 10⁻¹⁴(1.0 x 10⁻¹⁴) | 1.0 × 10⁻¹⁴(1.0 x 10⁻¹⁴) | 1.0 × 10⁻¹⁴(1.0 x 10⁻¹⁴) |
| Capture cross-section σv (αv) for acceptor-like Gaussian states (cm²) | 1.0 × 10⁻¹⁴(1.0 x 10⁻¹⁴) | 1.0 × 10⁻¹⁴(1.0 x 10⁻¹⁴) | 1.0 × 10⁻¹⁴(1.0 x 10⁻¹⁴) | 1.0 × 10⁻¹⁴(1.0 x 10⁻¹⁴) |
applied to D\textsubscript{int} structure. In reverse bias, the $J_0$ is not typically dependent on the $WF\textsubscript{ITO}$ and the $J_0$ values at $V_{app} = -1000$ mV were about $5.39 \times 10^{-8}$ mA/cm$^2$ ($WF\textsubscript{ITO} = 4.9$ eV), $5.29 \times 10^{-8}$ mA/cm$^2$ ($WF\textsubscript{ITO} = 5.3$ eV), and $5.26 \times 10^{-8}$ mA/cm$^2$ ($WF\textsubscript{ITO} = 5.7$ eV), respectively. Conversely, the dark current’s value in forward bias is influenced by $WF\textsubscript{ITO}$. Figure 4 also shows the dark current is entirely controlled by recombination of e-h pairs through mid-gap states within the absorber layer ($V_R$ region), at low forward bias ($< 250$ mV). Meanwhile, for voltage inside the exponential region ($V_E$), the dark current is limited by the combination of diffusion and recombination. However, for the region between $V_R$ < $V$ < $V_E$ (250 < $V$ < 400 mV), the dark current trundles, terraces more slowly with voltage, and is fully controlled by electron diffusion around virtual cathode. This region is the space charge limited current (SCLC) in region $V$ > $V_{SC}$, as a function concentration of trapped electrons and holes (Sturiale et al., 2009). For forward bias $V$ > 400 mV, the forward dark current increases significantly and is controlled by hole injection at the ITO/p-window layer interface (Belfar, 2015).
A study by Prayogi et al., (2021) reported the fabrication of D_{int} solar cell with RF-PECVD, using SiH\textsubscript{4} (10 % concentration in H\textsubscript{2} gas), B\textsubscript{2}H\textsubscript{6} (10 % concentration in H\textsubscript{2} gas) for dopant source of the p-type layer, and PH\textsubscript{3} (10 % concentration in H\textsubscript{2} gas) for dopant source of the n-type layer gases mixture. The presence of hydrogen in a-Si:H film plays a role in filling localized states to degrade defect states. However, the excess hydrogen traced after filling localized states in the absorber layer tends to become an impurity. Consequently, the J_{SC} is reduced by the defects generated by hydrogen impurity (J. Park et al., 2013).

Figure 5 shows the D_{int}'s band diagram simulation generated using AFOSR-HET simulator for typical WF_{ITO}. An increase in WF_{ITO} requires an increase in the front contact barrier $\phi_{bo}$ and a significant decrease in the downward band bending $\phi_{hbo}$ emerges at the ITO/p-window layer leading to improvement of $V_{OC}$, as shown in Equations. (7)-(8). Simultaneously, the FF values were increased due to the migration of holes to the front contact ITO/p-window layer interface, as the hole injection barrier, $\phi_{hbo}$ was reduced (Oh et al., 2012). Table 2 shows the AFORS-HET simulation results from the D_{int} solar cell performances with different WF_{ITO}. The high WF_{ITO} of 5.7 eV produced a 9.21 % maximum efficiency in the D_{int} solar cell, due to the enhanced $V_{OC}$ and FF, as shown in expression (Bechane et al., 2021; Singh et al., 2012; Sultana et al., 2017).

$$V_{OC} = \frac{n k T}{q} \ln \left( \frac{J_{ph}}{J_0} + 1 \right)$$

(9)

$$FF = \frac{V_{OC} - \ln(V_{OC} + 0.72)}{V_{OC} + 1}$$

(10)

Figure 5. Simulated band diagram of the p-i$_2$-i$_2$-n solar cell generated by AFORS-HET for typical WF$_{ITO}$ = 4.9 eV, 5.3 eV, and 5.7 eV.

Table 2. AFORS-HET simulation results for the D_{int} solar cell performances with different the WF_{ITO}

| WF_{ITO} (eV) | V_{OC} (mV) | J_{SC} (mA/cm$^2$) | FF (%) | Eff (%) |
|--------------|-------------|---------------------|--------|--------|
| 4.9          | 529.1       | 13.69               | 39.7   | 2.88   |
| 5.3          | 854.5       | 14.70               | 56.6   | 7.11   |
| 5.7          | 858.1       | 16.07               | 66.8   | 9.21   |
where \( J_{ph}, J_0, q, V, n, kT, V_{OC} = \frac{aV_{OC}}{n^3} \) are the photogenerated current, the reverse saturation current, the elementary charge, the terminal voltage, the ideality factor, and thermal energy, the normalized \( V_{OC} \) and \( P_{in} \) is power density of light entering the cell, respectively. According to the Equations (9)-(11), the open circuit voltage \( V_{OC} \) terrace with the photogenerated current \( (J_{ph}) \). It is clear from Table 2, that maximum value of the \( V_{OC} \) and \( FF \) are 858.1 mV and 66.8 % for WF\textsubscript{ITO} = 5.7 eV. At the same time, the efficiency enhancement is due to increases in the \( V_{OC} \) and \( FF \) values.

However, the WF\textsubscript{ITO}’s influence on optical properties and photogenerated current were examined for light spectrum at 300–800 nm. The AFORS-HET simulated results of the p-i-n solar cell’s quantum efficiency indicate a WF\textsubscript{ITO} of 5.7 eV is able to improve in blue light response between 300 and 633 nm, with a maximum quantum efficiency of 94.3 % at 522 nm (Figure 6). The photogenerated current \( (J_{ph}) \) value can be written as (Belfar, 2015).

\[
J_{ph} = q \int \Phi(\lambda)(1 - R(\lambda))QE(\lambda) d\lambda
\]  

(12)

where \( \Phi(\lambda) \) is the photon flux incident on the solar cell at wavelength \( \lambda \), \( R(\lambda) \) is the reflection coefficient from the top surface; \( QE(\lambda) \) is the quantum efficiency. From eq. (12), it is obvious that with high value of WF\textsubscript{ITO}, \( QE(\lambda) \) and \( J_{ph} \) \( (J_{ph} \approx J_{SC}) \) of D\textsubscript{int} solar cell are significantly improved, as shown in Table 2.

Furthermore, the changes in \( \Phi_{hao} \) with WF\textsubscript{ITO} are due to alteration of the electric field at ITO/p-window layer interface, caused by different carrier concentrations, leading to a significant reduction in \( J_0 \), and consequently, improving the \( V_{OC} \). Based on Figure 7, an increase in WF\textsubscript{ITO} from 4.9 eV to 5.3 eV, results in a change in the electric field from \( +5.23 \times 10^5 \) to \( +2.51 \times 10^5 \) V cm\(^{-1}\) at ITO/p-window layer interface, and this impedes the photogenerated hole from reaching the front contact. Meanwhile, at a WF\textsubscript{ITO} of 5.7 eV, the electric field’s value shifted to negative \( (-3.89 \times 10^5 \) V cm\(^{-1}\)), thus, providing effective forces for holes transport to reach the front contact.

As mentioned above, reduction of the \( \Phi_{hao} \) associated with the barrier of the ITO/p-layer Schottky contact is lessened even to be negligible with high value ITO work function (WF\textsubscript{ITO}). Consequently, the quantity of photogenerated holes more collect at front contact as trapped holes density (Kumar & Ranjan, 2020). Figure 8 shows that the trapped holes concentration at ITO/
p-window layer increased to $1.14 \times 10^{19}$ cm$^{-3}$ for the highest WF$_{ITO}$ of 5.7 eV, as compared to $7.14 \times 10^{17}$ cm$^{-3}$ and $2.38 \times 10^{17}$ cm$^{-3}$ for lower WF$_{ITO}$ of 5.3 eV and 4.9 eV, respectively. However, for silicon thin film solar cells a change in the work function of ITO films (WF$_{TCO}$) is associated with a change of the front barrier height ($\phi_{b0}$) affects to the efficiency of carrier injection into TCO/(p) a-Si:H interface.

### 3.2. Optimization results of the a-Si:H absorber layers
According to Benigno and Darminto, p-i-n a-Si:H based solar fabrication using RF-PECVD technique, by varying the hydrogen dilution ($R = [H_2]/[SiH_4]$) = 0, 16, 36 for intrinsic (absorber) layers with 600 nm optimum thickness, inserted between p-type and n-type layers, has been conducted, and a 5.78% maximum efficiency was achieved (Benigno & Darminto, 2017). Prayogi et al., reported an effort to enhance the p-i-n solar cell's performance through modification by adding the intrinsic layer ($i_2$) with different hydrogen dilution to the original $S_{int}$ structure produced a $D_{int}$ solar cell structure with good optical properties, as well as an 8.61% maximum efficiency (Prayogi et al., 2021). The $i_1$-$i_2$ layers serial structure leads to a more excitonic (e-h pairs) state because the $i_1$ ($= 1.70$ eV) and $i_2$ ($= 1.85$ eV) layer bandgaps are different.

Figure 9(a-b) shows the optimized results of the $i_1$ and $i_2$ layer bandgap variations, in order to improve the p-i-n-n solar cell's performance. During the absorbers' optimization, the (p)a-Si:H and (n)a-Si:H layers bandgap values were taken to be 2.0 and 2.2 eV, respectively. Meanwhile, the (p)a-Si:H, ($i_1$)a-Si:H, ($i_2$)a-Si:H, and (n)a-Si:H films' thicknesses were 15 nm, 300 nm, 300 nm, and 25 nm, respectively. In this case, the WF$_{ITO}$ value as neutral contact at ITO/p-window layer was
also taken to be 5.7 eV. Based on Figure 9(a) shows the $V_{OC}$ values gradually increased from 858.1 to 1007 mV in the bandgap range of 1.70 to 1.86 eV, and this confirmed the p-i$_1$-i$_2$-n solar cell’s band diagram structures (Figure 10(a-c)). Furthermore, the bandgap offsets ($\Delta E_V$) emerges in each junction at valence band, due to the bandgap difference between the p-i$_1$, i$_1$-i$_2$, and i$_2$-n layers, and this offset (discontinuity) is able to increase the recombination rate and trapped hole density at those interfaces, consequently, leading to low $V_{OC}$ (Figure 10(a)). According to Figure 10(b,c), a change in the i$_1$ bandgap change to 1.78 eV and 1.84 eV, led to a decline in the $\Delta E_V$ within the p-i$_1$ and i$_1$-i$_2$ valence band, associated with high $V_{OC}$. However, with a change in the i$_2$ layer band gap 1.70 to 1.78 eV, the i$_1$ layer bandgap remained 1.82 eV, and the $V_{OC}$ values remained constant at 1004.4 mV, but slowly increased with changes in the i$_2$ layer bandgap (Figure 9(b)).

Based on Figure 9(a), the $J_{SC}$ values were discovered to be constant in the bandgap range of 1.70 to 1.74 eV, but were observed to drastically dwindle from 16.08 to 15.98 mA/cm$^2$, with a change in the i$_1$ bandgap from 1.74 to 1.86 eV, due to less generation of excitonic in absorber layers with increase in the i$_1$ bandgaps. Meanwhile, the i$_2$ bandgap (Eg-i$_2$ = 1.82 eV) change from 1.7 to 1.86 eV did not cause any significant change (Figure 9(b)). $V_{OC}$ increased with the i$_1$ layer bandgap, from 1.70 to 1.80 eV, as well with the variations of FF, from 66.80 % to 69.12 %. FF also slightly declines for the i$_1$ layer bandgap > 1.80 eV. Conversely, the reduction in FF from 70.27 % to 67.10 % was associated with changes in the i$_2$-layer bandgap from 1.70 to 1.82 eV. However, beyond 1.82 eV, FF was observed to gradually increase, with a rise in the i$_2$ layer bandgap. Figure 9(a-b) shows the p-i$_1$-i$_2$-n simulated conversion efficiency increases with changes of the i$_1$ and i$_2$ layer bandgaps. The optimized bandgap used based on simulation were 1.82 eV (i$_1$-layer) and 1.86 eV (i$_2$-layer), while the maximum conversion efficiency obtained was 10.76 %.

Figure 11 shows the quantum efficiency analyzed and calculated with change in the i$_1$, i$_2$ layer bandgaps, using optimized WFI of 5.7 eV, in order to obtain the D$_{int}$ solar cell’s outstanding performance. The photocurrent density, $J_{ph}$ ($J_{ph} = J_{SC}$) denotes the quantum efficiency as stated in (Yang et al., 2016).

$$J_{ph} = \int_{300nm}^{800nm} \frac{q}{hc} \phi_{AM1.5EQE(\lambda)} d\lambda$$  \hspace{1cm} (13)
Figure 10. Simulated band diagram of the D_{int} structure with different of the i_1 and i_2 bandgaps which valence band offsets were appeared at p/i_1, i_1/i_2, and i_2/n interfaces. (a) $E_{g-i_1} = 1.70 \text{ eV}$, $E_{g-i_2} = 1.86 \text{ eV}$, (b) $E_{g-i_1} = 1.78 \text{ eV}$, $E_{g-i_2} = 1.86 \text{ eV}$, (c) $E_{g-i_1} = 1.84 \text{ eV}$, $E_{g-i_2} = 1.86 \text{ eV}$.

(a) $E_{v1} = 1.70 \text{ eV}$, $E_{v2} = 1.86 \text{ eV}$, $\Phi_{p} = 1.90 \text{ eV}$, $\Phi_{h} = 0.1 \text{ eV}$, $\Phi_{bL} = 0.200 \text{ eV}$, $\Delta E_{v1} = 0.300 \text{ eV}$, $\Delta E_{v2} = 0.160 \text{ eV}$.

(b) $E_{v1} = 1.78 \text{ eV}$, $E_{v2} = 1.86 \text{ eV}$, $\Phi_{p} = 1.90 \text{ eV}$, $\Phi_{h} = 0.1 \text{ eV}$, $\Phi_{bL} = 0.200 \text{ eV}$, $\Delta E_{v1} = 0.220 \text{ eV}$, $\Delta E_{v2} = 0.080 \text{ eV}$.

(c) $E_{v1} = 1.84 \text{ eV}$, $E_{v2} = 1.86 \text{ eV}$, $\Phi_{p} = 1.90 \text{ eV}$, $\Phi_{h} = 0.1 \text{ eV}$, $\Phi_{bL} = 0.200 \text{ eV}$, $\Delta E_{v1} = 0.160 \text{ eV}$, $\Delta E_{v2} = 0.020 \text{ eV}$.
Where, \( q, \lambda, h, c, \phi_{AM1.5}, \) and \( EQE \) are the unit charges, wavelength of light absorbed by \( D_{int} \) solar cell, Planck’s constant, speed of light in vacuum, the solar spectral irradiance under 1.5 G air mass, and the external quantum efficiency, respectively. As previously mentioned, with change in the \( i_1 \) layer bandgaps (1.70 eV, 1.78 eV, 1.84 eV), and a constant \( i_2 \) layer bandgap of 1.86 eV, there is a possibility of improving the quantum efficiency in the spectrum wavelength range from 300–550 nm, due to the additional electric field and reduced dangling bond density, consequently, more excitonic generated are separated at p/i interface, leading to higher \( J_{SC} \), (Figure 9(a); Hao et al., 2019).

Figure 12 shows the simulated optimized \( D_{int} \) solar cell’s J-V characteristic. The \( V_{OC}, J_{SC}, FF, \) and \( E_{ff} \) are possibly enhanced with the higher work function of 4.9–5.7 eV and \( (i_1)_a\text{-Si:H} \) and \( (i_2)_a\text{-Si:H} \) layer bandgaps from 1.70 to 1.86 eV. Table 3 shows the comparison results with other simulation results for the p-i-1-2-n solar cell structure.

4. Conclusion
In Summary, the ITO/(p)_a-Si:H/(i)_a-Si:H/(n)_a-Si:H/metal (\( S_{int} \)) and ITO/(p)_a-Si:H/(i_1)_a-Si:H/(i_2)_a-Si:H/(n) \( a\text{-Si:H/metal (D}_{int} \))’s performances were successfully investigated, using AFORS-HET software. The front work function \( WF_{ITO} \) on performances of the \( S_{int} \) and \( D_{int} \) solar cells was first simulated. Through simulation, the \( WF_{ITO} \) value was varied from 4.9 to 5.7 eV, in order to determine the optimum \( WF_{ITO} \) for high solar cell efficiency, confirmed with the J-V dark characteristic, the band diagram in
Table 3. Comparison of several simulation results of the p-i-n solar cell structures

| Sources                | Structures                  | $V_{OC}$ (mV) | $J_{SC}$ (mA/cm$^2$) | FF (%) | $E_{ff}$ (%) | Simulator |
|------------------------|-----------------------------|--------------|----------------------|--------|--------------|-----------|
| This work              | (p)α-Si:H/(i)$_2$ α-Si:H/(n)α-Si:H | 969.8        | 16.03                | 70.0   | 10.76        | AFORS-HET |
| (Belfar, 2015)         | (p)nc-Si:H/(p) nc-Si:H/(i) α-Si:H/(n)α-Si:H | 936.0        | 13.96                | 71.4   | 9.35         | AMPS-1D   |
| (Ahmad et al., 2017)   | (p)α-SiO:H/(i)$_2$ α-Si:H/(n)α-Si:H | 905.0        | 12.98                | 72.0   | 8.41         | TCAD      |
| (Abega et al., 2021)   | (p)α-SiO$_x$-H/(i)$_2$ α-Si:H/(i)α-Si:H | 905.0        | 16.55                | 76.0   | 10.58        | SCAPS     |
| (Hamdani et al., 2022) | (p)α-SiO$_x$-H/(i)$_2$ α-Si:H/(n)μc-Si:H | 925.5        | 12.64                | 72.8   | 8.52         | AFORS-HET |

thermodynamics equilibrium, build-in electric field distribution, trapped holes density, and the quantum efficiency. At WF$_{ITO}$ = 5.7 eV, the $S_{int}$ and $D_{int}$ solar cells had a maximum efficiency of about 6.73 % ($V_{OC} = 839.4$ mV, $J_{SC} = 14.78$ mA/cm$^2$, and $FF = 54.25$ %) and 9.21 % ($V_{OC} = 858.1$ mV, $J_{SC} = 16.07$ mA/cm$^2$, and $FF = 66.80$ %), respectively. Furthermore, in an effort to enhance the $D_{int}$ solar cell's electrical and optical properties, the $i_1$-$i_2$ layer bandgaps' serial structures were optimized to created more excitonic states in the absorber layers, and consequently, improve the cell's performance. The $D_{int}$ solar cell was discovered to have a maximum efficiency of 10.76 % ($V_{OC} = 969.8$ mV, $J_{SC} = 16.03$ mA/cm$^2$, and $FF = 70$ %), with WF$_{ITO}$, $i_1$ layer bandgap, and $i_2$ layer bandgap of 5.7 eV, 1.82 eV, and 1.86 eV, respectively. Subsequently, the simulation results were compared with other relevant thin film solar cell simulation results. It can be seen that the structure with adding an intrinsic layer to the p-i-n structure solar cell produces a higher $V_{OC}$ and good conversion efficiency.

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