

# An optimized structure for CdTe Solar Cells

Yunfei Chen<sup>1</sup>, Peng Shou<sup>2</sup>, Xuehai Tan<sup>1</sup>, Cao Xin<sup>3</sup>, Bastian Siepchen<sup>4</sup>, Ganhua Fu<sup>5</sup>, Alan E. Delahoyl<sup>1</sup>, Ken K. Chin<sup>1</sup>

<sup>1</sup>Department of Physics and CNBM New Energy Materials Research Center, New Jersey Institute of Technology, Newark, NJ 07102, USA

<sup>2</sup>China Triumph International Engineering Co., Ltd, Shanghai, P.R. China 200063

<sup>3</sup>Bengbu Design & Research Institute for Glass Industry,

<sup>4</sup>CTF SOLAR GmbH, 01109 Dresden, Germany

<sup>5</sup>AVANCIS GmbH, 81739 Munich, Germany

\*TEL: 9734954666 Email: yc289@njit.edu

**Abstract** — In the last five years, the world record of CdTe thin film solar cell conversion efficiency has been increased from 16.5% to 21.0%. Most noticeable and dramatic efficiency improvement has been originated from the elimination of blue loss by using wider band gap n-window layer such as CdSO to replace the traditional n-CdS of band gap 2.4 eV. In this work, we use CdSO as the new n-window layer and systematic computer simulation is used to investigate the influence of the conduction band offset between CdSO and CdTe layer, the thickness and the doping concentration of CdSO layer on the efficiency of the solar cell. Finally, a new optimized CdTe solar cell with highest simulated efficiency is designed and the role of CdSO layer is clarified. Simulation results also suggest that the new structure can almost remove the blue loss.

**Index Terms** — CdTe solar cells, blue loss, n-window layer, conduction band offset, doping concentration.

## I. INTRODUCTION

CdTe solar cell is one of the three major branches of the thin film photovoltaic technology. From Shockley Queisser diagram, CdTe with a band gap of 1.45eV has the potential to yield a theoretical high efficiency.[1] A typical structure of CdTe solar cell can be glass superstrate/ TCO layer/ HRT layer/ CdS n-window layer/ CdTe absorber layer/ Cu back contact. There are some limiting factors for the current CdTe solar cells. One is the limited doping concentration of absorber material CdTe itself, usually cannot be higher than  $10^{15}\text{cm}^{-3}$ , which means loss of efficiency. It is difficult to solve because it is due to the property of the material itself. The other one is the blue loss caused in CdS n-window layer. CdS once is the most widely accepted n-window layer from decade years of experience. Due to its low carrier lifetime, it cannot contribute to the photovoltaic effect a lot and we do not want light to be absorbed in this layer. However with a relatively low band gap, the light with wavelength smaller than blue light will be absorbed in this layer which is called blue loss. This blue loss can reduce the efficiency of CdTe solar cell by 4-5 %. [2] Thus, Finding a new material with higher band gap as the n-window layer is a way to help improve the performance of CdTe solar cell. In the last five years, the world record of CdTe thin film solar cell conversion efficiency has been increased from 16.5% to 21.0%. Actually, the reason for this noticeable and dramatic efficiency improvement is mainly

originated from the elimination of blue loss by using wider band gap buffer-window layer to replace the traditional n-CdS.

Many attempts have been made to find proper new n-window layers. Recently, some researchers have already increased the band gap of CdS from 2.4eV to 3.2eV by oxygen incorporation, which results in  $\text{CdS}_{1-x}\text{O}_x$  [3, 4]. It will bring some interesting topics when the traditional CdS n-window material is replaced by CdSO.

First is the conduction band offset ( $\Delta E_C$ ) between n-window layer and absorber layer. A flat band diagram of a typical CdTe solar cell with traditional CdS material as n-window layer is shown Fig.1.  $\Delta E_C$  is defined as

$$\Delta E_C = E_{C_{n\text{-window}}} - E_{C_{\text{Absorber}}} \quad (1)$$

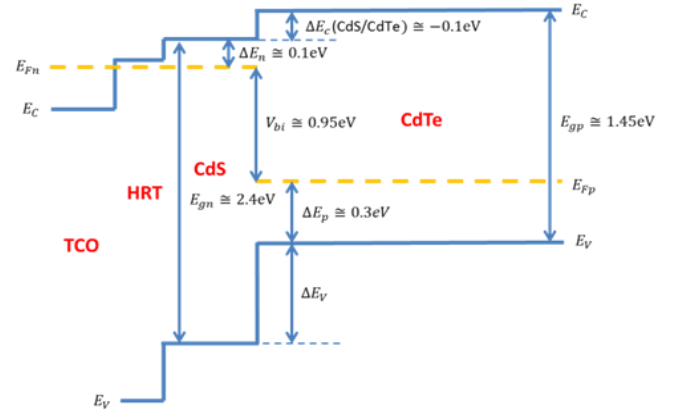


Fig.1. Flat band diagram of a typical CdTe solar cell

For this traditional CdTe solar cell,  $\Delta E_C$  is negative and is approximately equal to -0.1eV. And it is easy to find that the open-circuit voltage  $V_{OC}$  should be no bigger than built-in voltage  $V_{bi}$  which is approximately equal to 0.95eV calculated from the following equation.

$$V_{OC} \leq V_{bi} = \frac{1}{q} (E_{gp} + \Delta E_C - \Delta E_n - \Delta E_p) \quad (2)$$

All the symbols and their approximate values are shown in Fig.1.. When the new material is used, the value of  $\Delta E_C$  can be changed. A positive  $\Delta E_C$  may help increase the efficiency of CdTe solar cell. The efficiency of a solar ( $\eta$ ) is defined as

$$\eta = V_{OC} * J_{SC} * FF / P_{in} \quad (3)$$

Where  $J_{SC}$  is short-circuit current,  $FF$  is the fill factor and  $P_{in}$  is the input power. [5]

$J_{SC}$  is mainly limited by the band gap of CdTe which cannot be changed. However, the high limit of  $V_{OC}$  is increased when  $\Delta E_C$  is changed from negative to positive. In addition, from the following equation

$$V_{OC} = \frac{AKT}{q} \ln \left( \frac{J_{SC}}{J_0} \right) \quad (4)$$

Where  $A$  is the diode quality factor,  $\frac{KT}{q}$  is the thermal voltage,

$J_0$  is the saturation or dark current density. There are two models to express  $J_0$ , one is the Shockley Model, as CdTe solar cell is a minority carrier dominated solar cell. The expression for  $J_0$  can be given

$$J_0 \propto \sqrt{\frac{D_n n_i^2}{\tau_n N_A}} \quad (5)$$

Where  $D_n$  is the diffusion coefficient of electrons,  $\tau_n$  is the carrier lifetime of electrons,  $n_i$  is intrinsic concentration,  $N_A$  is the doping concentration of p-CdTe layer.

The other one is Shockley-Read-Hall Model. The expression for  $J_0$  can be given

$$J_0 \propto \frac{qn_i W}{\tau_n} \quad (6)$$

Where  $W$  is the width for the depletion region.

Compared with two equations, we can find that in both model  $J_0$  is inverse proportional to  $\tau_n$ . When  $\Delta E_C$  is changed from a negative value to a positive value, the possibility of the electrons to be trapped by a defect at the interface is reduced. Thus, the deep trap surface recombination rate is decreased and  $\tau_n$  for the electrons is increased. When  $\tau_n$  is increased,  $J_0$  is decreased and  $V_{OC}$  is also increased. So when  $\Delta E_C$  is changed from negative to positive, both the upper limit and the value of  $V_{OC}$  will increased. With  $J_{SC}$  and  $FF$  not being influenced a bit, the efficiency of the solar cell should be improved. However,  $\Delta E_C$  cannot be too big, because when  $\Delta E_C$  is too big, the electron will not have enough thermal energy to go through the 'spike' and thus the normal photocurrent will be influenced. [6] Therefore, there will be an exact value or range for the  $J_{SC}$  where the highest efficiency of the solar cell occurs.

The other interesting issue is the role of the new material CdSO. If we want it to be an n-window layer, then CdSO layer should be a little thicker and the doping concentration of it should be as high as possible. However, if we want it to be a buffer, then CdSO layer should be thinner and the doping concentration of it will no longer be that important. Thus, we have to use systemic computer simulation to find out the relationship between the efficiency of the solar cell and the thickness, doping concentration of CdSO layer.

With the proper conduction band offset between CdSO layer and CdTe layer, the best thickness and doping concentration being found, we then can make a design for CdTe solar cells and computer simulation will be used to prove that the blue loss is almost removed.

## II. METHOD

With different O2 partial pressure in the pure Ar ambient, Many CdSO samples with different content of incorporated oxygen have been deposited. We get the sample's absorption coefficient in terms of wavelength by doing UV-visible-NIR transmittance. The band gap of the sample is achieved through Tauc plot. Here, we choose a CdSO sample deposited under pure Ar and 5% O2, use its optical analysis result to do our simulation. The thickness of the sample is 70nm and the doping concentration of it is  $10^{16} \text{cm}^{-3}$ .

SCAPS (a Solar Cell Capacitance Simulator) is a one dimensional solar cell simulation program which is popular used in solar cell area. After set up the structure of a solar cell, we can do various simulations like J-V, QE on it using this software. [7]

We set up a solar cell with the following orders, back contact/p-CdTe / (Interface) /CdSO/TCO/front contact. The initial parameter of each part is included in Table 1.

To find out the influence of the conduction band offset between CdSO and CdTe. We just change the electron affinity ( $\chi$ ) of CdSO, because the value of  $\Delta E_C$  can be approximately achieved using the follow equation.

$$\Delta E_C = \chi_{CdTe} - \chi_{CdSO} \quad (7)$$

We run J-V simulation every time when  $\chi_{CdSO}$  is set at different values, record the simulation result, efficiency and open-circuit voltage, then the conduction band offset when the highest solar cell's efficiency occurs is investigated.

To find out the influence of the thickness and doping concentration of CdSO layer, we just do systematic simulations and record the simulation results when the thickness and doping concentration of CdSO is set at various values.  $\Delta E_C$  will be fixed at a certain number found from previous work. An efficiency vs doping concentration diagram will be drawn at different thicknesses. Then the thickness and doping concentration of CdSO with highest solar cell's efficiency is investigated. The role CdSO layer should be is consequently clarified.

## III. RESULTS

### A. The influence of conduction band offset

Fig.2. shows the simulated J-V responses of three solar cells with  $\Delta E_C$  equals to -0.1, 0.2, 0.4eV respectively. It is shown from the figure that when  $\Delta E_C$  is increased,  $J_{SC}$  almost remains same with  $V_{OC}$  increases dramatically, thus the efficiency of the solar cell also increases. However, when  $\Delta E_C$  is too big, then the J-V performance of the solar cell is not good any more as  $FF$  decreases significantly. Fig.3. and Fig.4. depict the open-circuit voltage and efficiency of several solar cells respectively with  $\Delta E_C$  being varies from -0.2eV to 0.4eV. Our simulation results show that: (i) when  $\Delta E_C$  changes from negative to positive e.g. from -0.2eV to 0.1eV, the solar cell's performance enhances dramatically mainly because of the significant increase of  $V_{OC}$ ; (ii) when  $\Delta E_C$  changes from 0.1eV to 0.3eV, the solar cell performance shows marginal

improvement as same as  $V_{OC}$  and optimum performance happens at this range with efficiency higher than 19.3%; (iii) when  $\Delta E_c$  is more positive such as 0.4eV, the solar cell performance instead degrades significantly although  $V_{OC}$  does not decrease. The result shows that a positive conduction band offset in the range of 0.1-0.3eV is highly preferred for CdTe solar cells, which is within our expectation.

*B. The influence of the doping concentration and thickness of the CdSO layer*

Fig.5. depicts the efficiency of several solar cells with various thickness and doping concentration.  $\Delta E_c$  is set at 0.2eV for each cells. The result shows that when the thickness of CdSO is small, under 10nm, the doping concentration of CdSO layer do not have much influence on the performance of the solar cell, so it can be treated as a buffer layer. However, when the thickness of CdSO layer continues increasing, the effect of the doping concentration of CdSO layer on the performance of the solar becomes more serious and the higher the doping concentration, the better the efficiency. It is shown from the figure that a CdSO layer with 50nm thickness and  $10^{18} \text{ cm}^{-3}$  doping concentration is a good choice for a high efficiency solar cell. It is probably because with a high doping concentration of CdSO layer,  $\Delta E_n$  can be very small and the open-circuit voltage of the solar cell can be very high.

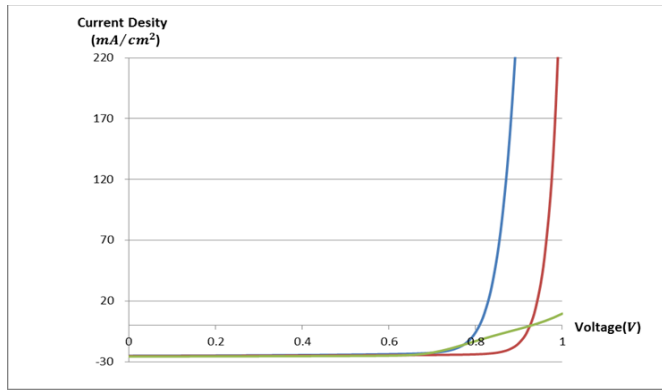


Fig.2. J-V curve of the solar cell at different conduction band offset. Red, blue, green lines indicate  $\Delta E_c$  is -0.1eV, 0.2eV, 0.4eV respectively.

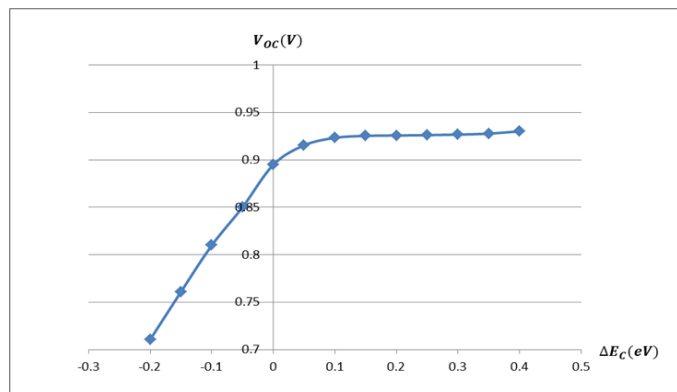


Fig.3. Simulated solar cells' open-circuit voltage as a function of conduction band offset.

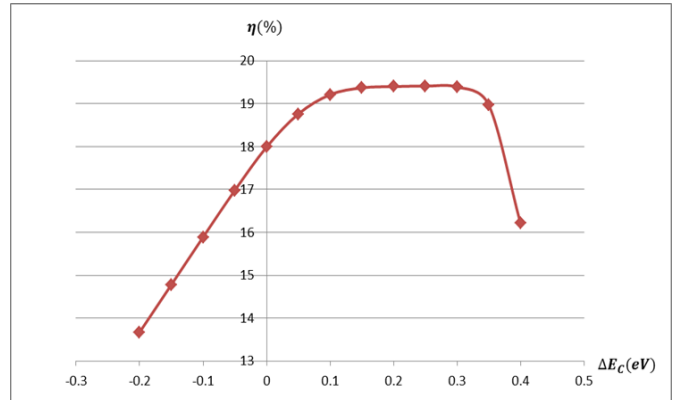


Fig.4. Simulated solar cells' efficiency as a function of conduction band offset.

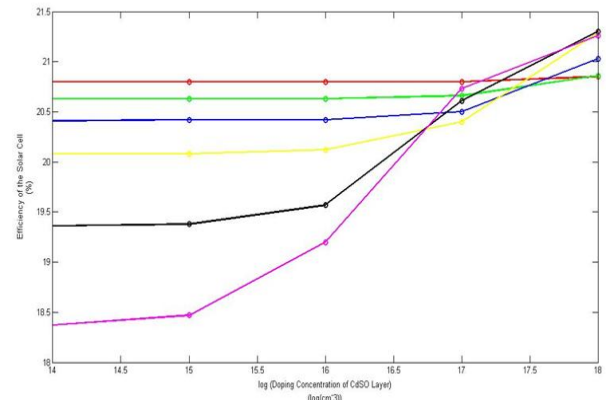


Fig.5. Simulated solar cells' efficiency as a function of the thickness and doping concentration of CdSO layer. Red, green, blue, yellow, black, pink line indicates the thickness of CdSO layer is 2nm, 5nm, 10nm, 20nm, 50nm, 100nm respectively.

*C. The new optimized structure of CdTe solar cell and the removal of blue loss*

From the previous results mentioned above, we propose a new optimized structure for CdTe solar cells with glass superstrate/ CdSO n-window layer/ CdTe absorber layer/ Cu back contact. The band gap of CdSO layer is 3.2eV and the doping concentration is  $10^{18} \text{ cm}^{-3}$ . The conduction band offset between CdSO layer and CdTe layer is 0.2eV. The flat band diagram of the new optimized structure is indicated in Fig.6. Fig.7 shows the simulated QE results of the new optimized CdTe solar cell together with the traditional CdTe solar cell. It is clear that the new structure can largely remove the blue loss as expected.

#### IV. CONCLUSION

The performance of the solar cell can be enhanced when the band gap of the n-window layer is increased because the blue loss is largely removed. CdSO is proved to be a good choice. The best efficiency is found when the conduction band offset between CdSO layer and CdTe layer is 0.1~0.3eV. The efficiency of the solar cell in terms with CdSO layer's thickness and doping concentration is clarified. Thus, a new optimized structure for CdTe solar cell is investigated, where CdSO layer's thickness is 50nm, its doping concentration is  $10^{18} \text{ cm}^{-3}$  and the conduction band offset between CdSO layer and CdTe layer is 0.2eV.

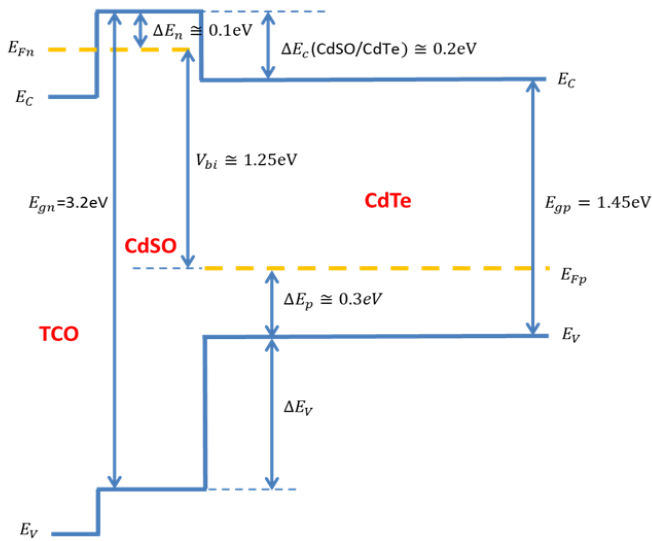


Fig.6. Flat band diagram of the new optimized CdTe solar cell

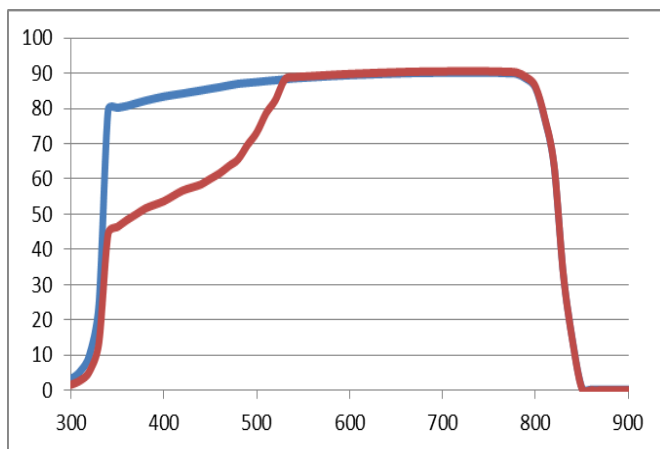


Fig.7. Simulated QE results of the new optimized and traditional CdTe solar cells. Red and blue lines indicate when the n-window layer is CdS and CdSO respectively

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#### REFERENCES

- [1] William Shockley and Hans J. Queisser. Detailed Balance Limit of Efficiency of p - n Junction Solar Cells. *Journal of Applied Physics* 32, 510 (1961); doi: 10.1063/1.1736034
- [2] James R. Sites. Quantification of losses in thin-film polycrystalline solar cells. *Solar Energy Materials & Solar Cells* 75 (2003) 243–251
- [3] Wu X, Dhare RG, Yan Y, Romero IJ, Zhang Y, Zhou J, DeHart C, Duba A, Perkins C, To B. High-efficiency polycrystalline CdTe thin-film solar cells with an oxygenated amorphous CdS(a-CdS:O) window layer. In *Photovoltaic Specialists Conference, 2002. Conference Record of the Twenty-Ninth IEEE*. IEEE: New Orleans, LA, 2003; 531-534. DOI:10.1109/PVSC.2002.1190619
- [4] Kephart Jason M., Geisthardt Russell M., and Sampath W. S. (2015), Optimization of CdTe thin-film solar cell efficiency using a sputtered, oxygenated CdS window layer, *Prog. Photovolt: Res. Appl.*, doi: 10.1002/pip.2578
- [5] Markus Gloeckler(2005). DEVICE PHYSICS OF Cu(In,Ga)Se2 THIN-FILM SOLAR CELLS (Doctoral dissertation). Retrieved from [http://physics.colostate.edu/groups/photovoltaic/PDFs/MGloeckler\\_Thesis.pdf](http://physics.colostate.edu/groups/photovoltaic/PDFs/MGloeckler_Thesis.pdf)
- [6] Sabaghi M, Majdabadi A, Marjani S, Khosroabadi S. Optimization of High-Efficiency CdS/CdTe Thin Film Solar Cell Using Step Doping Grading and Thickness of the Absorption Layer. *Orient J Chem* 2015;31(2).
- [7] G. Agostinelli, D.L. Bätzner, M. Burgelman, An Alternative model for V, G and T dependence of CdTe solar cells IV characteristics. In *Twenty-ninth IEEE Photovoltaic Specialists Conference*. (New Orleans, LA, 20-24 May 2002), 744-747, IEEE, New York (2002)
- [8] Kikuchi, A. (1997), Calculation of Misfit-Dislocation Density Generated by Lattice Mismatch at the NiSi<sub>2</sub>-Si Interface. *Phys. Status Solidi B*, 203: 79–86. doi: 10.1002/1521-3951(199709)203:1<79::AID-PSSB79>3.0.CO;2-A
- [9] Inoue Y, Hála M, Steigert A, Klenk R, Siebentritt S. Optimization of Buffer Layer/i-Layer Band Alignment. Manuscript submitted for publication

TABLE I  
THE PARAMETER OF EACH LAYER OF THE SOLAR CELL [4, 8, 9]

Layer	n-AZO	n-CdSO	n-CdS	Interface	p-CdTe
Thickness [nm]	500	70	70	-	2500
Band Gap [eV]	3.7	3.2	2.42	-	1.5
Electron Affinity [eV]	4.5	4.2	4.2	-	4.4
Relative Dielectric Permittivity	10	10	10	-	9.4
Density States of Conduction Band [cm <sup>-3</sup> ]	2.2×10 <sup>18</sup>	2.2×10 <sup>18</sup>	2.2×10 <sup>18</sup>	-	8.0×10 <sup>17</sup>
Density States of Valence Band [cm <sup>-3</sup> ]	1.8×10 <sup>19</sup>	1.8×10 <sup>19</sup>	1.8×10 <sup>19</sup>	-	1.8×10 <sup>19</sup>
Electron Mobility [cm <sup>2</sup> /V.s]	32	100	100	-	320
Hall Mobility [cm <sup>2</sup> /V.s]	30	25	25	-	40
Donor Concentration [cm <sup>-3</sup> ]	1.0×10 <sup>20</sup>	1.0×10 <sup>16</sup>	1.0×10 <sup>16</sup>	-	-
Acceptor Concentration [cm <sup>-3</sup> ]	-	-	-	-	1.0×10 <sup>15</sup>
Dopant energy level [eV]	-0.09	0.14	0.14	-	0.255
Defect Type	SA	SA	SA	N	SD
Electron Cross Section [cm <sup>-2</sup> ]	1.0×10 <sup>-15</sup>	1.0×10 <sup>-17</sup>	1.0×10 <sup>-17</sup>	1.0×10 <sup>-15</sup>	1.0×10 <sup>-13</sup>
Hole Cross Section [cm <sup>-2</sup> ]	1.0×10 <sup>-12</sup>	1.0×10 <sup>-12</sup>	1.0×10 <sup>-12</sup>	1.0×10 <sup>-15</sup>	1.0×10 <sup>-15</sup>
Defect Concentration [cm <sup>-2</sup> ]	1.0×10 <sup>16</sup>	3.0×10 <sup>15</sup>	3.0×10 <sup>15</sup>	1.0×10 <sup>14</sup>	2.0×10 <sup>13</sup>
Defect energy level [eV]	2.0	1.9	1.12	0.6	0.585

\* SA = single acceptor, N = Neutral, SD = single donor