Design and simulation of C2N based solar cell by SCAPS-1D software

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Abstract: Recently, a novel nitrogenated holey two-dimensional material, C2N, has been successfully synthesized via a simple wet-chemical reaction. Its merits have drawn much attention from the scientists. However, to the best of our knowledge, few reported works employed C2N as photovoltaic materials and the practical solar cells based on C2N have not been fabricated in lab. In this work, we carried out simulation using Scaps-1D to investigate the influences of different parameters on the C2N based solar cell. By varying the acceptor density, layer thickness, defect density of C2N and changing different N layers coupling with C2N, we found out that suitable acceptor density, around 10^{15} cm^{-3}, large layer thickness of C2N and low defect density were key factors to obtain high-performance solar cells. Small band offset also played an importance role in enhancing the performance of photovoltaic materials. With optimized parameters, C2N coupling with CdS as heterojunction can achieve an efficiency of over 17%. This work may provide valuable insights into future design of C2N based solar cells.

1. Introduction

Owing to the global warming, extensive fossil fuel consumption and environmental pollution, there is an increasing demand for more efficient and environmental-friendly photovoltaic materials. Plenty of materials have been investigated and developed, such as Si, CdTe, perovskite, etc, which have high photovoltaic efficiencies and successful commercial products [1–10]. However, these materials possess some disadvantages, which limit their further development. For example, the volatile organic components may induce thermal and chemical instability of perovskite solar cells. The manufacturing cost of CIGS and CdTe is high due to the use of rare material of Indium, Gallium or Tellurium.

Recently, C2N, a novel nitrogenated holey two-dimensional material, has been successfully synthesized via a simple wet-chemical reaction [11] (Mahmood et al 2015). Its unique structure and large surface to volume ration make it appealing to many fields, such as catalyst, batteries, sensors, hydrogen storage [12–20]. C2N is also a promising photovoltaic candidate owing to its suitable direct bandgap, high absorption coefficient, environmental-friendly composition and high thermal stability [21, 22]. However, few related works have been reported in this field till now. Hence, it is crucial to investigate the properties of C2N based solar cells to instruct future developments.

In this work, we aimed to study the effects of different parameters of C2N based solar cells by using SCAPS-1D software developed by Gent university, whose working principles are based on solving continuity equation of holes and electrons and the Poisson equation [23]. Such software was demonstrated a successful simulation technique in designing and studying various kinds of high-performance solar cells, such as perovskite, CIGS, CdTe, CZTS and so on [24–29]. Inspired by the structure of CIGS solar cells and highly tunable electronic properties. We designed a pn-heterostructure to perform our simulations. We first varied the acceptor density to...
determine the influence of acceptor density on C2N based solar cell. Then we investigated the effects of different thickness have on C2N based solar cells. After that, we studied the effects of deep-level defects originated in C2N. Finally, we selected 5 kinds of n-type materials to see effects of different n-type materials coupling with C2N. To the best of our knowledge, it is the first time that the parameters of C2N based solar cells are studied and optimized. Our study offers researchers valuable insights into designing C2N based solar cells and enhancing its performance C2N.

2. Methods

The simulation was carried out under irradiation by the global Air Mass (AM) 1.5G solar spectrum at room temperature (300 K). The absorption coefficient of C2N and N layer are obtained by the equation below [23]:

Figure 1. Schematic illustration of C2N based solar cells.

Figure 2. (a)–(d) Dependence of cell performance on acceptor density of C2N films. (e) I-V characteristics of C2N/ZnS solar cells with various acceptor density of C2N films. (f) External quantum efficiency with various acceptor density of C2N films. (g) Illustration of carrier distribution with acceptor density of C2N of 10^{15} (h) schematic band diagrams of various acceptor density of C2N films.
The solar cell is composed of FTO (front contact layer), n layer (ZnO CdS SnO2 ZnS In2S3) (window layer), C2N (absorption layer) and Au (back contact layer), as shown in figure 1. Most solar light passes through the FTO layer and N layer and be absorbed by C2N layer and contribute to the effective photocurrent. Simulation parameters are listed in table 1 [11, 21, 30–36]. The selection of all 5 types n-type materials, ZnO, CdS, In2S3, ZnS and SnO2, are based on previous published literatures [29, 37, 38]. Point defects in C2N materials, such as H interstitial in benzene rings, C substituted by N, which may provide deep states in the band gap of C2N, were also investigated in this study [38, 39].

### 3. Results and discussions

#### 3.1. Effects of C2N acceptor density on solar cell performance

From figures 2(a)–(d), we can observe that short-circuit current (\(J_{sc}\)) decreases and open-circuit voltage (\(V_{oc}\)) increases with increased acceptor density of C2N. Fill factor (FF) decreases and then increases slightly after the acceptor density if above \(10^{16}\) cm\(^{-3}\). As a result, the power conversion efficiency (PCE) also shows a ‘\(^{∧}\)’ type evolution. Furthermore, we studied the origination of the relationship between photovoltaic performance and acceptor density. The photogenerated minority carriers move to the depletion region of the heterojunction and are separated by built-in electrical field. The region with band bending represents the location and built-in field

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### Table 1. Basic materials parameters used in this simulation.

|          | SnO2 | ZnO | In2S3 | CdS | ZnS | C2N |
|----------|------|-----|-------|-----|-----|-----|
| Bandgap (eV) | 3.6  | 3.3 | 2     | 2.4 | 3.68| 1.81|
| Electron affinity (eV) | 4.55 | 4.55| 4.75  | 4.45| 4.3 | 4.42|
| Dielectric permittivity | 9    | 9   | 13.5  | 10  | 8.3 | 4.5 |
| CB effective density of states (cm\(^{-3}\)) | \(2.20 \times 10^{18}\) | \(3.10 \times 10^{18}\) | \(2.20 \times 10^{18}\) | \(1.30 \times 10^{18}\) | \(2.20 \times 10^{18}\) | \(10^{19}\) |
| VB effective density of states (cm\(^{-3}\)) | \(1.80 \times 10^{19}\) | \(1.80 \times 10^{19}\) | \(1.80 \times 10^{19}\) | \(9.10 \times 10^{19}\) | \(1.50 \times 10^{19}\) | \(10^{19}\) |
| Electron thermal velocity (cm s\(^{-1}\)) | \(10^{7}\) | \(2.40 \times 10^{7}\) | \(10^{7}\) | \(3.10 \times 10^{7}\) | \(10^{7}\) | \(10^{7}\) |
| Hole thermal velocity (cm s\(^{-1}\)) | \(10^{7}\) | \(1.3 \times 10^{7}\) | \(10^{7}\) | \(1.6 \times 10^{7}\) | \(10^{7}\) | \(10^{7}\) |
| Electron mobility (cm\(^{2}\) V\(^{-1}\) s\(^{-1}\)) | 100  | 100 | 100   | 72  | 165 | 13  |
| Hole mobility (cm\(^{2}\) V\(^{-1}\) s\(^{-1}\)) | 25   | 31  | 25    | 20  | 5   | 20.6|
| Shallow uniform donor density (cm\(^{-3}\)) | \(2 \times 10^{19}\) | \(10^{17}\) | \(10^{16}\) | \(1.1 \times 10^{18}\) | \(10^{17}\) | 0   |
| Shallow uniform acceptor density (cm\(^{-3}\)) | 0    | 0   | 10    | 0   | 0   | Variable |

\[
\alpha(h\nu) = (\alpha_0 + \beta h) \frac{E_g}{h\nu} \sqrt{\frac{h\nu}{E_g}} - 1
\]
of the heterojunction. As seen in figure 2(h), with the increase of acceptor density of C2N, the width of the depletion region is reduced while the band bending is increased, indicating a stronger built-in field [42]:

\[ V_D = \frac{qN_D(\varepsilon_N N_D + \varepsilon_p N_p)}{2\varepsilon_0 \varepsilon_D (N_D + N_D)^2} \]

\[ X_D = \frac{2\varepsilon_0 (N_A + N_D) V_D}{qN_D N_D} \]

On the one hand, reduced depletion region weakens the collection of carriers and leads to a decreased photocurrent. On the other hand, the increased band bending enhances built-in field and increase the photovoltage.

Lower acceptor density would increase the series resistance of the device, while higher acceptor density would decrease the shunt resistance of the device, which can both decrease the performance of solar cell. Therefore, an optimized acceptor density of C2N should be carried on around \(10^{15} \text{ cm}^{-3}\) according to our simulation.

3.2. Effects of C2N thickness on solar cell performance

Figures 3(a)–(d) shows the variation of device efficiency, fill factor, short-circuit current and open-circuit voltage with different C2N thickness. Among them, efficiency, short-circuit current, open-circuit voltage show a saturated behavior with increased thickness above 600 nm, while fill factor saturates with the thickness of >200 nm. Larger thickness of C2N contributes to better light-absorption as shown in quantum efficiency (QE) of figure 3(f) and consequently higher short-current and efficiency.

According to the Beer–Lambert law, owing to the high-absorption coefficient of C2N, above \(10^5 \text{ cm}^{-1}\), a few hundred nanometer film is capable of absorbing enough sunlight and lead to the saturation of photocurrent and device efficiency. An usual ‘M’ shape of FF is also noticed. This ‘M’ shape could be understood considering the diffusion length of holes in C2N. When the thickness of C2N is below 200 nm, the diffusion length is greater than the thickness of C2N. While with the increased of the thickness of C2N, the absorption increased, leading to a higher FF. When the thickness of C2N is in the range of 200 nm and 600 nm, the diffusion length is smaller than the thickness of C2N. Thus, recombination increases and resulting in the decrease of FF. When the thickness of C2N is above 600 nm. Because the diffusion length is much smaller than the thickness of C2N, the relatively small diffusion length has minor effect on the FF. Increased absorption caused by increased thickness of C2N plays a major role in the increasing of FF. Simultaneously, thicker absorption layer will increase the cost of device. Therefore, our simulation suggests an optimized thickness of 600 nm.

3.3. Effects of deep defects of C2N on solar cell performance

According to previous published literatures, there exist some kinds of deep-level defects in the band gap of C2N [39, 40]. Figure 4(h) shows the energy level of those deep-level defects. Including N substituted by C, interstitial
H in benzene. Since the deep-level defects often play an important role in the semiconductor device, we investigated their effects on the performance of solar cells. Owing to co-existent of different defects in C2N, we mainly focus the defect possessing the relatively small formation energy, that is interstitial H in benzene ring and N substituted by C, which means they may be the most common defects occurred in C2N and may have the largest impact on the solar cells. The parameters of this simulation are summarized in table 2. Figures 4(a)–(d) shows that efficiency, open-circuit voltage, short circuit current, fill factor all decrease with increased defect density of C2N. When the defect density of C2N is below $10^{15}$ cm$^{-3}$, all four kinds of device performances exhibit slight decrease. With the defect density above $10^{15}$ cm$^{-3}$, significant drops of efficiencies are observed in the simulation results. Generally, those deep-level defects mainly act as recombination centers. With the increase of defect density, the recombination rate in solar cells become increased, resulting in lower short-circuit current and open-circuit voltage. Increased defect density also leads to higher series resistance and poor fill factor. Above all, efficiency exhibits a significant drop when the defect density of C2N is larger than $10^{15}$ cm$^{-3}$. It is necessary to control the densities of deep-level defects in the real experiments.

### Table 2. Defect parameters used in this simulation.

| Defect type | Neutral |
|-------------|---------|
| energy level above E_v | 0.9 eV |
| capture cross section electron | $10^{-14}$ cm$^{-2}$ |
| capture cross section hole | $10^{-17}$ cm$^{-2}$ |

3.4. Effects of different n-type layer coupling with C$_2$N as solar cells

With optimized C$_2$N layer, we investigated the effects of different n-type layer coupling with C$_2$N on the performance of solar cells. We selected 5 kinds of n-type layer as window layer to form heterojunction with C$_2$N and the thickness of 5 n-type layers are set to 10 nm. The band alignments of all 5 types of heterojunction with different acceptor density of C$_2$N are shown in figure 5(g). For CdS/C$_2$N, ZnO/C$_2$N, SnO$_2$/C$_2$N and In$_2$S$_3$/C$_2$N heterojunctions, due to the large electron affinities, they form a kind of type-II heterojunction with a small band cliff at the interface, while the ZnS/C$_2$N is a kind of type-I heterojunction with a small band spike at the interface [41].

\[
\text{Band offset} = \chi e(C_2N) - \chi e(\text{N layer})
\]

The quantum efficiency shown in figure 5(f) indicates that C$_2$N coupling with different n layers have only minor effect on light absorption. This is because the small thickness as well as large bandgap of all n layers. From the optimum results of each heterojunction shown in figures 5(a)–(d). We can conclude that the CdS/C$_2$N is better than the other 4 types of heterojunctions. This can be understood by the fact that the electron affinity of CdS is very close to the C$_2$N, the band cliff is very small and allows an easy separation of photo-exited electrons.
and holes and transfer of electrons from C2N to CdS. As a result, CdS/C2N based solar cell possess the best performance among all 5 kinds of solar cells.

4. Conclusion

In this work, we investigated the effects of different parameters on the performance of C2N based solar cell using Scaps-1D. The optimized acceptor density of C2N was found to be around $10^{15} \text{cm}^{-3}$. Efficiency became saturated when the thickness reached 600 nm. When the thickness of C2N was above 1000 nm, the maximum efficiency could exceed 17%. When the deep-level defect density of C2N was lower than $10^{15} \text{cm}^{-3}$, there were only slight damages on the performance of C2N based solar cell. With the deep-level defect density above $10^{15} \text{cm}^{-3}$, sudden drop in efficiency, fill factor, open-circuit voltage and short-circuit current could be observed. Therefore, it was necessary to reduce the defect density to acquire high-performance solar cell. Finally, we selected 5 kinds of n-type semiconductor materials to investigate their influences to future researches in the field of C2N based solar cell. This work provides valuable insights to future researches in the field of C2N based solar cell and indicates that C2N could be a promising material for future photovoltaic devices.

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Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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