Solution-processed silicon/SnCl₂-treated Ti₃C₂T_x MXene Schottky junction solar cells

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ABSTRACT In this study, a novel photovoltaic cell based on the Ti₃C₂T_x MXene/n-type silicon (n-Si) Schottky junction is developed by a simple solution-processed method of drop-casting the Ti₃C₂T_x MXene ethanol suspension onto the surface of n-Si wafers and the subsequent natural drying in air. The demonstration device with a simple configuration of Ag (top electrode)/Ti₃C₂T_x/n-Si/In:Ga (back electrode) delivers a power conversion efficiency (PCE) of 5.70% with a short-circuit current density (J_{sc}) of 20.68 mA cm⁻², open-circuit voltage (V_{oc}) of 0.530 V and fill factor (FF) of 52.0% under AM 1.5G illumination. After treating the MXene layer with the SnCl₂ aqueous solution, an improved PCE to 6.95% (J_{sc} : 23.04 mA cm⁻²; V_{oc} : 0.536 V; FF: 56.2%) can be achieved because of the reduced light reflection, improved quality of junction and electrical contact, as well as the increased carrier lifetime/suppressed carrier recombination. Given the simple device configuration, facile preparation and huge potential for performance improvement, this work is believed to provide valuable exploration of developing novel solar cells.

Keywords: Ti₃C₂T_x MXene, silicon, solar cells, Schottky junction, drop-casting

INTRODUCTION

Thanks to the relatively high performance, excellent stability, non-toxicity, matured fabrication technology and abundant raw materials, crystalline silicon (c-Si) solar cells have been always dominating the photovoltaic market since they were commercialized [1–5]. Although their price has been substantially cut down in these years, large-scale deployment still necessitates further improvement of the performance-to-cost ratio for c-Si solar cells [6,7]. Considering the limited room for both increasing the power conversion efficiency (PCE) and reducing the price for c-Si wafers, simplifying the fabrication process and thus cutting the associated cost by exploring novel device configurations is one possible approach [2,8,9].

In recent years, Si-based Schottky junction/heterojunction solar cells have drawn increasing attention because of the simplified fabrication process and continuously improved performance with the development and application of appropriate materials [10]. To date, PEDOT:PSS [11–13], graphene, and some metal oxides such as molybdenum oxide [14–17], vanadium oxide [18–21], and tungsten oxide have been introduced to form Schottky

junction/heterojunction with c-Si [22–24], and the PCE of up to 23.5% has been reported [25], exhibiting the competitive performance with the traditional c-Si pn junction devices [26]. On the other hand, as one family of advanced two-dimensional (2D) materials, MXenes have gained extensive attention because of their similar properties to graphene including excellent electrical and optical properties [27–34]. Moreover, the work function (WF) of MXenes can be easily tuned in a broad range, e.g., from <2 eV to >6 eV for the Ti₃C₂T_x MXene by adjusting the surface-terminating groups [35–38], indicating the potential as a carrier-selective material [39,40]. In addition, abundant raw materials can be used to produce high-quality MXenes just by the cost-effective wet-etching method [41–45]. Although MXenes possess such advantages, there are few reports on the related Si-based Schottky junction solar cells [46–49].

In this study, we report the Ti₃C₂T_x MXene/n-Si (n type c-Si) Schottky junction solar cells fabricated by simply drop-casting Ti₃C₂T_x MXene ethanol suspension onto the surface of n-Si and the subsequent natural dry in air. The PCE of 5.70% with the short-circuit current density (J_{sc}) of 20.68 mA cm⁻², open-circuit voltage (V_{oc}) of 0.530 V and fill factor (FF) of 52.0% under AM 1.5G illumination is delivered for the demonstration device with a simple configuration of Ag (top electrode)/Ti₃C₂T_x/n-Si/In:Ga (back electrode). Further study indicates that treatment of the Ti₃C₂T_x MXene layer with the SnCl₂ aqueous solution can improve the junction performance, electrical contact quality and minority carrier lifetime, and meanwhile reduce carrier recombination and light reflection. As a result, the improved J_{sc} of 23.04 mA cm⁻², V_{oc} of 0.536 V and FF of 56.2% lead to the enhanced PCE to 6.95%.

EXPERIMENTAL SECTION

Materials

Titanium aluminum carbide (Ti₃AlC₂, 98%, 400 mesh) powder, lithium fluoride (LiF, 98.5%) powder, hydrochloric acid (HCl, 36%–38%), tin(II) chloride dehydrate (SnCl₂·2H₂O, 98%), lithium chloride (LiCl, 98.5%) and one-side polished n-type (100) Czochralski Si wafers (290 μm thickness, 0.05–0.1 Ω cm) were purchased from commercial suppliers.

Preparation of the Ti₃C₂T_x MXene nanosheets

One gram of Ti₃AlC₂ powder was put into the etchant containing 40 mL of HCl (12 mol L⁻¹) and 2 g of LiF, and the

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mixture was stirred continuously for 48 h at 40°C. Following that, the mixture was centrifuged at 3500 r min⁻¹ for 5 min, and the supernatant was discarded. The sediment was collected and then re-dispersed into deionized (DI) water. The above processes were repeated several times until the pH value of the supernatant was about 6, and then the collected sediment was re-dispersed into LiCl aqueous solution of 20 mg mL⁻¹, which was followed by stirring at room temperature for 12 h. The mixed solution was centrifuged repeatedly until a dark supernatant was present, and then the collected sediment was dispersed into ethanol, which was followed by ultrasonication in an ice-water bath and the subsequent centrifugation at 3500 r min⁻¹ each for 60 min to obtain the supernatant suspension containing the Ti₃C₂T_x MXene nanosheets. Finally, the suspension of ~2.0 mg mL⁻¹ Ti₃C₂T_x MXene nanosheets in ethanol was prepared for solar cell fabrication.

Fabrication of the solar cells

The n-Si wafer was first cut into pieces measuring 1 cm × 1 cm, and then ultrasonically cleaned in ethanol, acetone, isopropyl alcohol and DI water in sequence for 15 min each time. Subsequently, the n-Si pieces were immersed in the 5% diluted HF solution for 5 min to remove the native oxide layer, which was followed by rinsing with DI water and drying for solar cell fabrication. Then, the Ti₃C₂T_x MXene suspension in ethanol was drop-casted onto the n-Si pieces and naturally dried in air. Finally, the 150-nm-thick Ag comb (front) electrode (12% coverage) was deposited on the Ti₃C₂T_x MXene layer by thermal evaporation at the base vacuum of 5.0 × 10⁻⁴ Pa using the corresponding shadow mask and the In:Ga alloy paste was coated onto the Si backside to serve as the back electrode. For the case of treating Ti₃C₂T_x MXene with SnCl₂, the corresponding aqueous suspension was spin-coated onto the MXene layer and then naturally dried in air before deposition of the Ag electrode.

Characterization

The surface morphology of the samples was characterized by scanning electron microscopy (SEM, MIRA3, TESCAN) and atomic force microscopy (AFM, Multimode8-HR). The structural and compositional information was checked by X-ray diffraction (XRD, Malvern Panalytical Empyrean with Cu Kα radiation). The absorption spectra of the Ti₃C₂T_x MXene layer (on glass) were recorded by an ultraviolet/visible/near infrared (UV/VIS/NIR) spectrophotometer (Shimadzu UV-3600). The current density (*J*)-applied voltage (*V*) characteristic curves of the solar cells were measured using a Keithley 2400 precision source meter in the dark and at AM 1.5G illumination (100 mW cm⁻²). The sheet resistance of the Ti₃C₂T_x MXene layer was measured by a four-point probe (KDY-1). The electrochemical impedance spectroscopy (EIS) test was performed in a frequency range of 1–10⁶ Hz at an AC voltage with an amplitude of 10 mV using a CHI660E electrochemical workstation (at the bias of 0 V). The minority carrier lifetime (τ) was measured by the microwave photoconductivity decay method, and the diffusion length (*L_D*), light reflectance and external quantum efficiency (EQE) were characterized by the laser beam induced current method all using WT-2000 (SEMILAB).

RESULTS AND DISCUSSION

Fig. 1a shows the XRD patterns of the synthesized Ti₃C₂T_x

MXene powder, as well as the raw material, i.e., the Ti₃AlC₂ powder. The vanished peaks from Ti₃AlC₂, e.g., (104) around 38.8° and the shifted (002) peak to a small angle, i.e., from 9.5° to 6.5° indicate elimination of the Al layer in Ti₃AlC₂ and therefore the successful fabrication of the Ti₃C₂T_x MXene nanosheets with an enlarged interlayer spacing [50]. In the meantime, the AFM image shown in Fig. 1b indicates the single-layered MXene nanosheets with a thickness of about 1.5 nm [32,47]. Moreover, the SEM characterization of the Ti₃C₂T_x MXene drop-casted onto the Si wafer demonstrates the sheet structure, as exhibited in Fig. S1a, and the lateral size of the MXene nanosheets mainly falls in the range of 200 to 400 nm with an average value of ~323 nm (see the histogram in Fig. S1b) [51]. Fig. 1c, d exhibit the schematized device configuration and energy level alignment of the solar cells investigated in this study. When the Ti₃C₂T_x/n-Si Schottky junction is under illumination, the photon-generated carriers in and near the space-charge region would be separated by the built-in electric field across the junction [47]. The electrons diffuse to the In:Ga back electrode through n-Si, and meanwhile the holes transfer to the Ag front electrode through the Ti₃C₂T_x MXene layer, as schematized in Fig. 1d.

Furthermore, we investigated the impact of SnCl₂ treatment on the Ti₃C₂T_x MXene layer. As demonstrated by the SEM images shown in Fig. 2a, b, it is evident that the surface of the MXene layer becomes more wrinkled after SnCl₂ treatment, leading to the reduced reflection to the incident light, as verified by the comparison of the reflection mapping shown in Fig. S2. The XRD characterization of the SnCl₂-treated Ti₃C₂T_x MXene on indium tin oxide (ITO) glass indicates that there is no phase change for MXene and moreover are no other materials created by SnCl₂ treatment besides the peaks from MXene and ITO, as demonstrated by Fig. 2c. The shift of the (002) peak to a small angle, i.e., from 6.50° to 6.27°, indicates the enlarged interlayer spacing from 1.350 to 1.408 nm for the MXene layer after SnCl₂ treatment because of the interaction between the surface functional groups of MXene and Sn²⁺ ions [52]. In addition, we compared the absorption spectra of the Ti₃C₂T_x MXene layers before and after SnCl₂ treatment. As exhibited in Fig. 2d, only the typical peaks around 318 and 769 nm associated with the Ti₃C₂T_x MXene can be observed, confirming the results drawn from XRD characterization [47,53].

For the investigation of device performance, we first optimize the concentration and usage quantity of the MXene ethanol suspension to form a good junction with n-Si. As indicated by Fig. S3, 0.16 mg mL⁻¹ concentration and 40 μL usage quantity for the suspension, i.e., 6.4 μg cm⁻² MXene, are beneficial to delivering good performance for the corresponding devices. Based on the above optimization, the study related to SnCl₂-treatment was performed. Fig. 3a shows the illuminated *J-V* curves of the solar cells with the SnCl₂-treated MXene layers and the key parameters extracted from the *J-V* curves are summarized in Table 1. It is evident that for the solar cells with SnCl₂-treated MXene layers, *J_{sc}*, FF and *V_{oc}* are improved, thus leading to the enhanced PCE. For the case treated with the optimal quantity of 30 μL SnCl₂ aqueous solution, the PCE is increased by ~22.0%, i.e., from 5.70% for the control device without SnCl₂ treatment to 6.95%. To further understand the influence of the treatment to the MXene layers on device performance, the dark *J-V* curves were recorded in the voltage range of -0.7 to 0.7 V (see Fig. 3b). It can be seen that the 30 μL SnCl₂ solution-treated device delivers the best rectification characteristics and the

Figure 1 (a) XRD patterns of the $\text{Ti}_3\text{C}_2\text{T}_x$ MXene and Ti_3AlC_2 powder. (b) AFM image of the single-layered $\text{Ti}_3\text{C}_2\text{T}_x$ MXene. (c) Device configuration and (d) energy level alignment of the Ag (top electrode)/ $\text{Ti}_3\text{C}_2\text{T}_x$ /n-Si/In:Ga (back electrode) solar cells.

Figure 2 Top-view SEM images of the $\text{Ti}_3\text{C}_2\text{T}_x$ MXene layers on n-Si (a) before and (b) after SnCl_2 treatment. Comparison of (c) XRD patterns on ITO glass and (d) absorption spectra of the $\text{Ti}_3\text{C}_2\text{T}_x$ MXene layers before and after 30 μL SnCl_2 treatment. The inset of (c) shows the enlarged (002) peak of the $\text{Ti}_3\text{C}_2\text{T}_x$ MXene layer.

Figure 3 J - V curves of the solar cells with the treatment of the MXene layers by the SnCl_2 solution of varying quantities under (a) AM 1.5G illumination and (b) dark condition. (c) J_{sc} , (d) V_{oc} , (e) FF and (f) PCE of eight independent devices for each case with the MXene layers treated by the SnCl_2 solution of varying quantities. The control devices without the treatment by the SnCl_2 solution serve as the reference.

Table 1 Key device parameters extracted from the J - V curves in Fig. 3a

Device ^a	J_{sc}^{b} (mA cm^{-2})	V_{oc}^{b} (V)	FF ^b (%)	PCE ^b (%)
Control	20.68 (19.64 $\pm$ 1.11)	0.530 (0.519 $\pm$ 0.016)	52.0 (51.8 $\pm$ 2.6)	5.70 (4.95 $\pm$ 0.20)
10- SnCl_2	22.23 (20.74 $\pm$ 1.23)	0.542 (0.551 $\pm$ 0.025)	57.5 (54.8 $\pm$ 2.9)	6.94 (6.26 $\pm$ 0.33)
30- SnCl_2	23.04 (20.86 $\pm$ 0.57)	0.536 (0.554 $\pm$ 0.025)	56.2 (56.9 $\pm$ 1.5)	6.95 (6.58 $\pm$ 0.17)
50- SnCl_2	23.26 (22.32 $\pm$ 1.50)	0.539 (0.527 $\pm$ 0.011)	50.6 (49.3 $\pm$ 3.1)	6.33 (5.80 $\pm$ 0.33)

a) Data and statistics based on eight independent devices for each case; b) upper numbers denote values of the champion devices and the bottom numbers indicate the average values.

lowest reverse saturation current, which are closely correlated to the improved quality for the junction and electrical contacts.

Moreover, the ideality factor (n) and the reverse saturation

current density (J_0) were calculated for the 30 μL SnCl_2 solution-treated device based on its dark J - V curve following the equation of $J = J_0[\exp(eV/(nkT)) - 1]$, where e is the elemental charge, k is

the Boltzmann constant and T is the Kelvin temperature (for this study, the measurement of the dark J - V curves was performed at room temperature, and thus T of 298.16 K was adopted). The calculated n and J_0 are 3.37 and $7.25 \times 10^{-3} \text{ mA cm}^{-2}$ for the device with the treatment by the 30 μL SnCl_2 solution. As a comparison, the respective values are 4.70 and $7.57 \times 10^{-2} \text{ mA cm}^{-2}$ for the control device, thus indicating the improved junction quality and rectification characteristic for the SnCl_2 -treated device [54]. Moreover, measurement of the sheet resistance for the MXene layers indicates that the treatment by the 30 μL SnCl_2 solution can remarkably reduce the sheet resistance, i.e., from $\sim 1264 \Omega \text{ m}^{-1}$ for the case without the SnCl_2 treatment to $248 \Omega \text{ m}^{-1}$ (note: these two values are the average values based on eight independent measurements for each case), which thus contributes the improved FF for the corresponding solar cell [55].

Fig. 3c-f exhibit the distribution of J_{sc} , V_{oc} , FF, and PCE counted based on eight independent devices for each case. The change trend further confirms the positive contribution and reproducibility of the treatment to the MXene layers by the SnCl_2 solution to device performance, and moreover verifies the optimal quantity of the SnCl_2 solution, i.e., 30 μL .

To more deeply understand the improved performance for the devices with the treatment to the MXene layers by the SnCl_2 solution, more characterizations were conducted. Fig. 4a shows the EQE curves (vs. surface coverage), in which the horizontal coordinate indicates the surface coverage with the EQE value larger than the corresponding longitudinal coordinate, illuminated by the laser of 985 nm wavelength. Note that for the device with the treatment of the 30 μL SnCl_2 solution, the EQE is higher than that of the control device because of the reduced light reflection as above discussed. More EQE data at the wavelength

Figure 4 (a) EQE vs. surface coverage. (b) Nyquist plots in the frequency range of 1 to 1×10^6 Hz. Inset: the equivalent circuit. (c) Mapping of the minority carrier lifetime in the area of $1 \text{ cm} \times 1 \text{ cm}$. (d, e) L_D histograms with the corresponding surface coverage.

Table 2 Summary of some key electrical parameters

Device	R_s (Ω)	R_{rec} (k Ω)	τ_{min} (μ s)	τ_{max} (μ s)	τ_{ave} (μ s)
Control	9.89	36.19	19.5	30.8	27.3
30-SnCl ₂	4.78	42.10	23.0	406.3	59.0

of 405, 658 and 876 nm are summarized in Fig. S4, further confirming that the improved J_{sc} for the SnCl₂ solution-treated devices is from the enhanced light absorption and further from the reduced light reflection because of the wrinkled surface of the MXene layers (see Fig. 2b) [56].

EIS is an effective tool to reveal the carrier transport behaviors and recombination processes in solar cells [57]. Fig. 4b shows the Nyquist plots of the devices with and without the treatment of the 30 μ L SnCl₂ solution to the MXene layers in dark at the bias of 0 V over the frequency from 1 to 1×10^6 Hz and the equivalent circuit is exhibited in the inset. The radius of the semicircle represents the overall recombination resistance (R_{rec}), and the left intersect of the EIS curve with the Z' axis indicates the equivalent series resistance (R_s). Compared with the control device (see Table 2), the SnCl₂-treated device exhibits larger R_{rec} of 42.10 k Ω and smaller R_s of 4.78 Ω , indicating the improved quality for the junction and electrical contact, which thus contributes to the improved V_{oc} and FF.

Fig. 4c shows the mapping of the minority carrier lifetime, τ , for the cases of the MXene layers without (left) and with (right) the treatment of the 30 μ L SnCl₂ solution, and the key parameters are summarized in Table 2. It is evident that both the minimum and maximum minority carrier lifetimes are increased for the SnCl₂-treated case with an average τ of 59.0 μ s, much longer than the corresponding value of 27.3 μ s for the control case. Because these samples have the similar bulk lifetimes and wafer thicknesses, the prolonged τ together with the increased R_{rec} thus well indicates the suppressed recombination for carriers at the interface between the Ti₃C₂T_x MXene layer and n-Si substrate [58].

Diffusion length, L_D , is another key electrical parameter characterizing the carrier transport behavior [59]. L_D histograms with the corresponding surface coverage are shown in Fig. 4d, e and the related values are summarized in Table S1. Note that for the case with the MXene layer treated by the 30 μ L SnCl₂ solution (Fig. 4e), the increased L_D is achieved as compared with that of the control case (Fig. 4d). Moreover, after including the data of the cases treated by the 10 and 50 μ L SnCl₂ solutions (see Fig. S5), the case with the treatment by the 30 μ L SnCl₂ solution delivers the longest average L_D , thus (partially) supporting the corresponding best performance delivery as discussed above.

To comprehensively characterize the influence of the SnCl₂ treatment on device performance, stability test was conducted. Fig. S6 shows the time-dependent change of the normalized PCEs for the control and SnCl₂-treated devices. After 288-h exposure in air, the control and SnCl₂-treated devices maintained ~84.9% and 85.6% of the corresponding initial PCE, indicating that there is no obvious negative effect on the operation stability for the SnCl₂-treated device as compared with the control case.

CONCLUSIONS

In this study, we report a novel Schottky junction solar cell (configuration: Ag (top electrode)/Ti₃C₂T_x/n-Si/In:Ga (back

electrode)) prepared by simply drop-casting the Ti₃C₂T_x MXene ethanol suspension onto n-Si and the subsequent natural drying in air. Based on the first achieved PCE of 5.70% (J_{sc} : 20.68 mA cm⁻²; V_{oc} : 0.530 V; FF: 52.0%), the performance of the related solar cells can be elevated to 6.95% (J_{sc} : 23.04 mA cm⁻²; V_{oc} : 0.536 V; FF: 56.2%) by treating the MXene layer with the SnCl₂ solution. Further investigation indicates that the SnCl₂ treatment can wrinkle the MXene layer, thus leading to the reduced light reflection and further to the increased J_{sc} . Moreover, the SnCl₂ treatment can improve the quality of the junction and electrical contact, resulting in the improved V_{oc} and FF. In addition, it is proved that the passivation effect because of the SnCl₂ treatment can effectively suppress carrier recombination and then increase the minority carrier lifetime.

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Author contributions Yao X participated in the design of this study, conducted the experiments, performed data analysis and drafted the manuscript. Yin L participated in the part of the experiments and collected

important background information. Wang Y, Liu W and Xie C participated in the literature search, data acquisition and analysis, and manuscript preparation. Liu Q and Fu Y provided assistance for data acquisition and analysis. Li Y proposed the idea, supervised the research and revised the manuscript. Li J supervised the research and revised the manuscript. He D performed the manuscript review. All authors have read and approved the content of the manuscript.

Conflict of interest The authors declare that they have no conflict of interest.

Supplementary information Supporting data are available in the online version of the paper.

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溶液法制备硅/ SnCl_2 处理的 $\text{Ti}_3\text{C}_2\text{T}_x$ MXene肖特基结太阳能电池

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摘要 非掺杂异质结晶硅太阳能电池是目前光伏领域的一个研究热点. 本文通过简单的滴涂工艺, 并经自然干燥制备了一种基于 $\text{Ti}_3\text{C}_2\text{T}_x$ MXene/n-Si肖特基结的新型光伏电池. 此非掺杂异质结光伏电池在标准AM 1.5G模拟太阳光下短路电流密度为 20.68 mA cm^{-2} , 开路电压为 0.530 V , 填充因子为52.0%, 光电转换效率达到了5.70%. 新型 $\text{Ti}_3\text{C}_2\text{T}_x$ MXene/n-Si肖特基结光伏电池具有简单的器件结构和简便的制备工艺. 通过异质结界面改良, 二维材料性能改善等都可大幅提高其光电转换性能. 经 SnCl_2 水系溶液对MXene层进行处理后, 器件光电转换效率进一步提升至6.95% ($J_{sc} = 23.04 \text{ mA cm}^{-2}$, $V_{oc} = 0.536 \text{ V}$, $\text{FF} = 56.2\%$). 经处理后的MXene层, 可以有效减少光反射并提高光吸收. SnCl_2 水系溶液的处理, 还能进一步改善异质结质量及MXene层与顶电极的接触, 进而通过抑制载流子复合提高载流子寿命.