Supporting information

Air-Stable MXene/GaAs Heterojunction Solar Cells with a High Initial Efficiency of 9.69%

Zhijie Zhang,[a] Jing Lin,[a] Peiye Sun,[a] Qinghao Zeng,[a] Xi Deng,[ab] Youtian Mo,[a] Jiaying Chen,[a] Yulin Zheng,[a] Wenliang Wang,*[ab] and Guoqiang Li*[ab]

[a]*State Key Laboratory of Luminescent Materials and Devices, South China University of Technology, Guangzhou 510640, China.* E-mail: *wenliangwang@scut.edu.cn; msgli@scut.edu.cn*

[b]*Department of Electronic Materials, School of Materials Science and Engineering, South China University of Technology, Guangzhou 510640, China*

Figures:

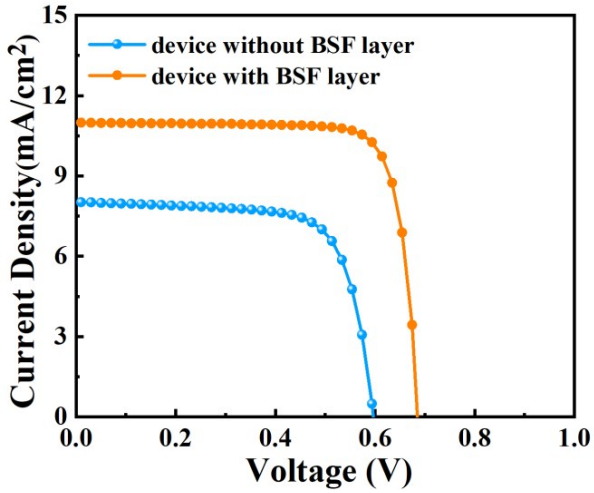


Figure S1. *J-V* curves of devices with and without InGaP BSF layer under AM 1.5 illumination. The concentration of $Ti_3C_2T_X$ colloidal solution used here is 0.05mg/mL.

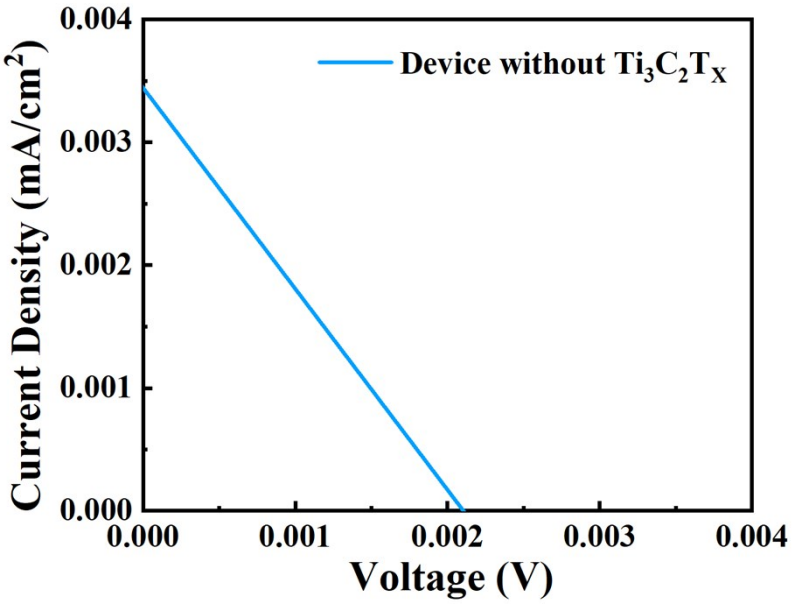


Figure S2. *J-V* curve of device without $Ti_3C_2T_X$ under AM 1.5 illumination.

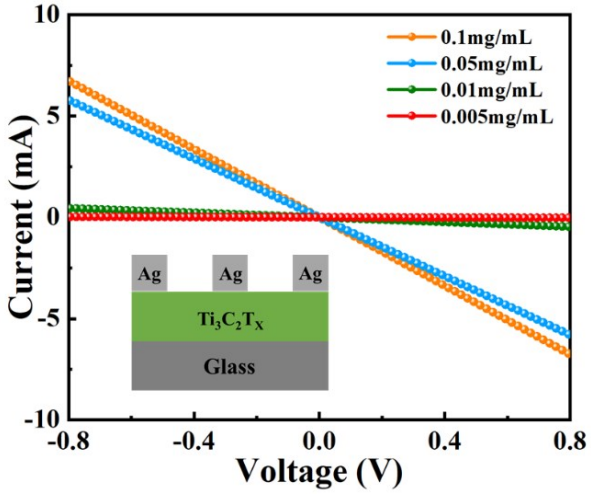
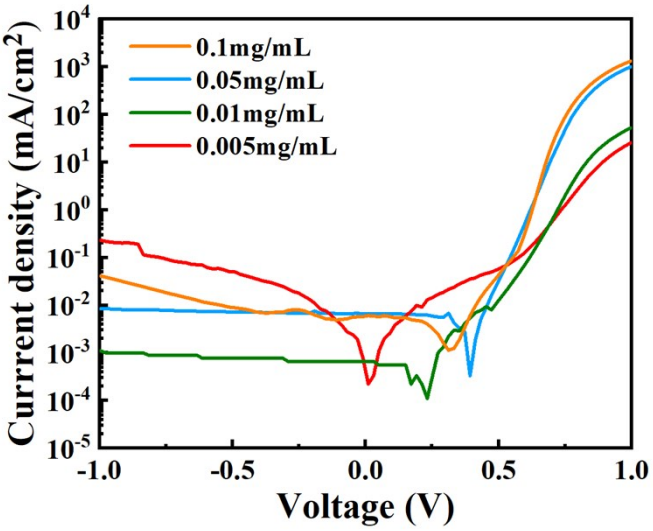


Figure S3. *I-V* characteristics of $Ti_3C_2T_X$ films prepared with various concentrations of $Ti_3C_2T_X$ solution.



FigureS4. *J-V* curves of devices fabricated by $Ti_3C_2T_X$ colloidal solution with various concentrations under dark condition.

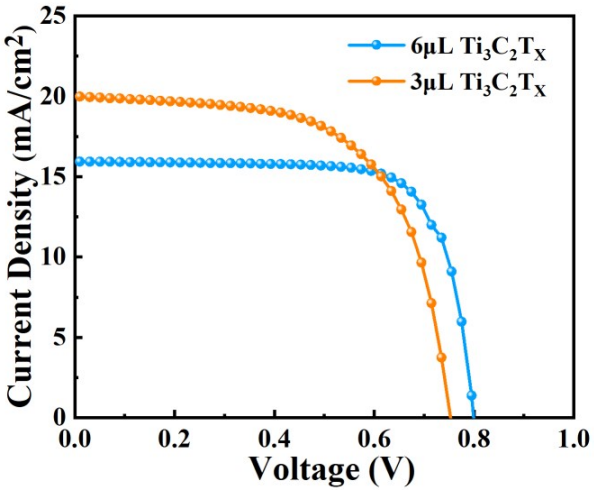
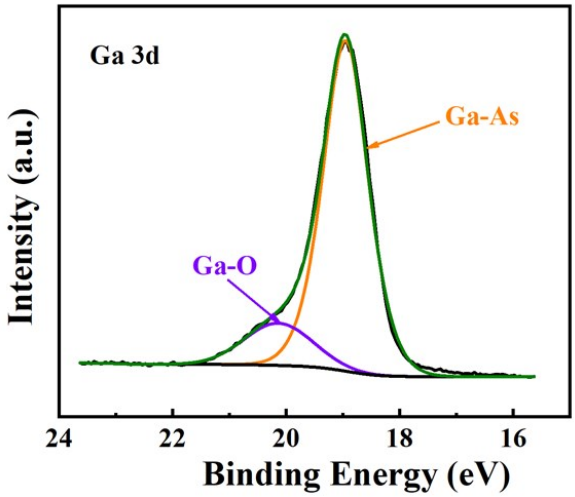


Figure S5. J-V curves of devices fabricated with 6 and 3μL $Ti_3C_2T_X$ colloidal solution under AM 1.5 illumination.



FigureS6. Ga 3d XPS spectra of MXene coated on GaAs substrate. Ga–As bond and Ga-O band is located at 18.96 eV and 20.15eV, respectively. The original proportion of Ga-O that represents the oxidation of GaAs surface is 15.25%

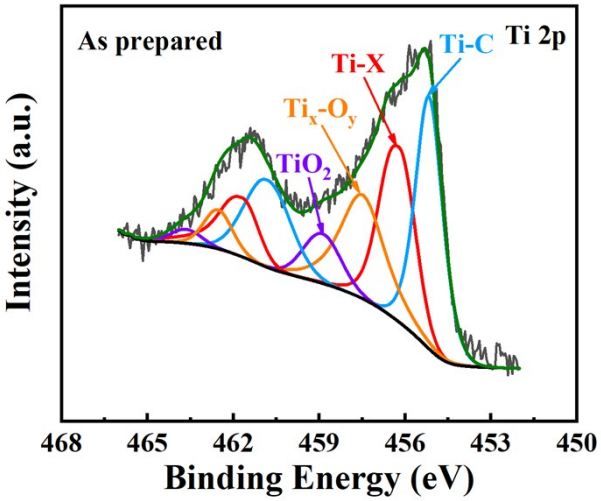


Figure S7. Ti 2p XPS spectra of as-prepared $Ti_3C_2T_x$ films

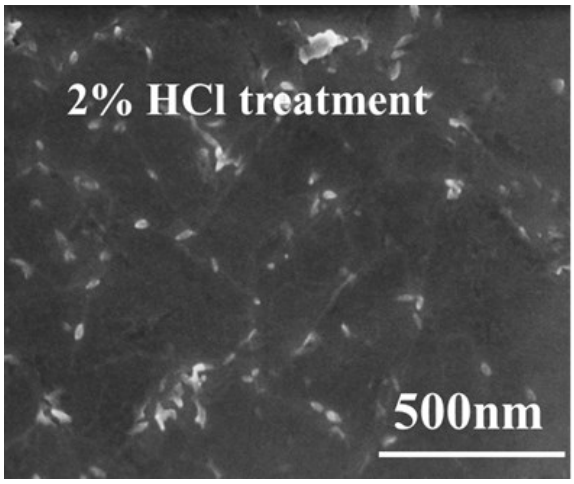


Figure S8. SEM image of 2% HCl treated $Ti_3C_2T_x$ films

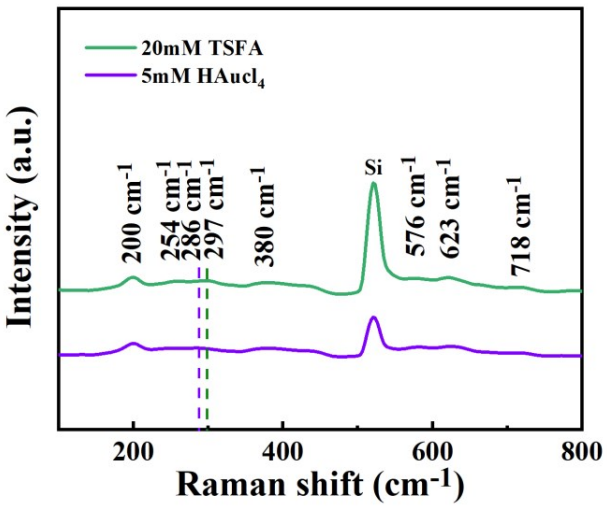


Figure S9. Raman spectra of TSFA and $HAuCl_4$ treated $Ti_3C_2T_X$ films coated on Si substrate. The Raman mode at 520 cm^{-1} correspond to the Si substrate.

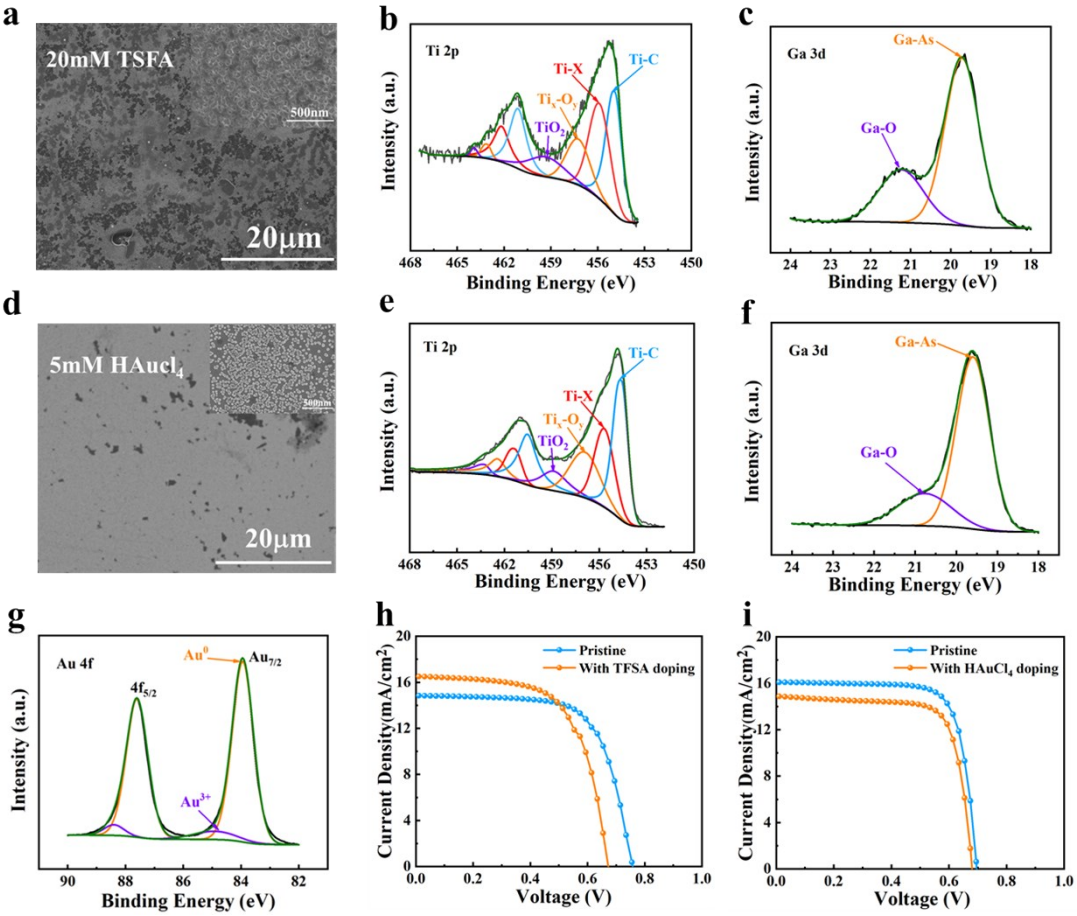


Figure S10. SEM images (a and d), Ti 2p XPS spectra (b and e) and Ga 3d XPS spectra (c and f) of 20mM TFSA and 5mM $HAuCl_4$ treated $Ti_3C_2T_X$ films. The proportion of TiO_2 and Ga-O is increased to 10.13% and 29.08% after 20mM TSFA treated. For the $HAuCl_4$ treated devices, the proportion of TiO_2 and Ga-O is increased to 9.68% and 23.08%. g) Au 4f XPS spectra of 5mM $HAuCl_4$ treated $Ti_3C_2T_X$ films. *J-V* curves of devices with and without h) 20mM TFSA and i)5mM $HAuCl_4$ treated.

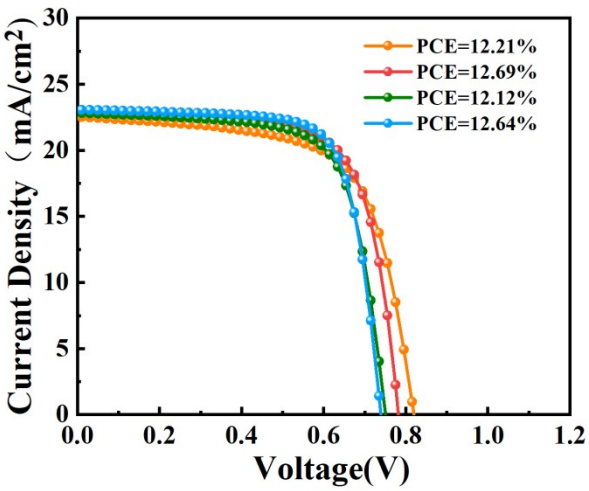


Figure S11. *J-V* curves of $Ti_3C_2T_X$/GaAs solar cells with ZnS/MgF_2 composite coating.

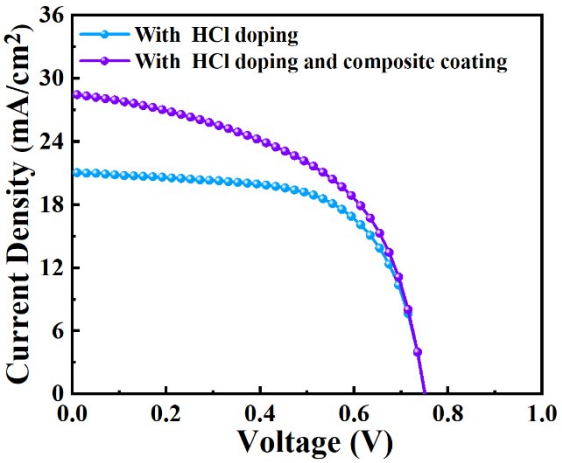


Figure S12. *J-V* curves of $Ti_3C_2T_X$/GaAs solar cells with HCl doping and ZnS/MgF_2 composite coating.