

Supplementary Information

Oxygen vacancy modulation of nanolayer TiO_x to improve hole-selective passivating contacts for crystalline silicon solar cells

Yanhao Wang,^{a,c,f} Zhaoyang Guo,^{a,f} Yongchang Li,^b Lachlan E. Black,^{c*} Daniel H. Macdonald,^c Shaojuan Bao,^d Jilei Wang,^d Yongzhe Zhang,^e Shan-Ting Zhang^{b*} and Dongdong Li^{a,b*}

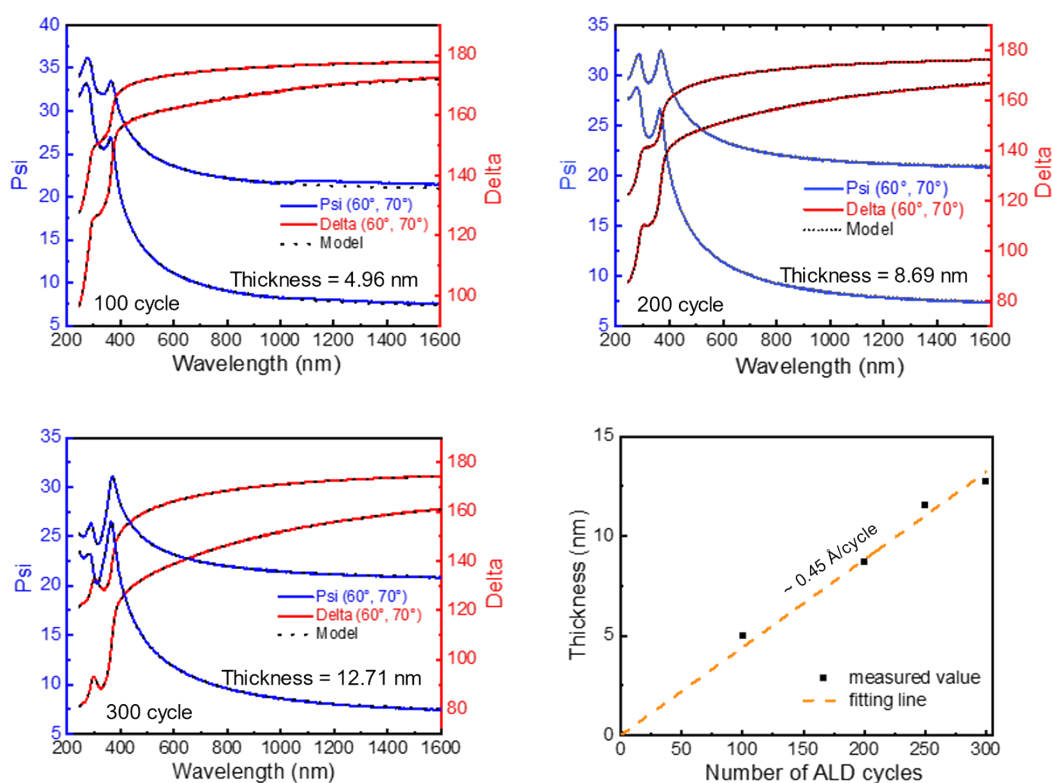


Fig. S1. The spectroscopic ellipsometry of TiO_x film with different ALD cycles and the extracted TiO_x thickness as a function of the number of ALD cycles.

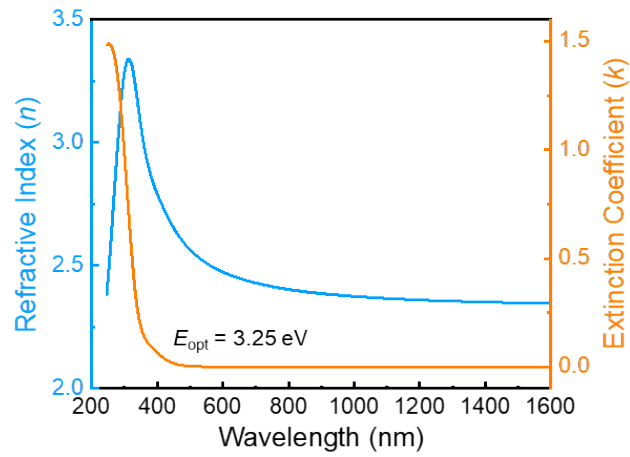


Fig. S2. Refractive index (n) and extinction coefficient (k) of the TiO_x film.

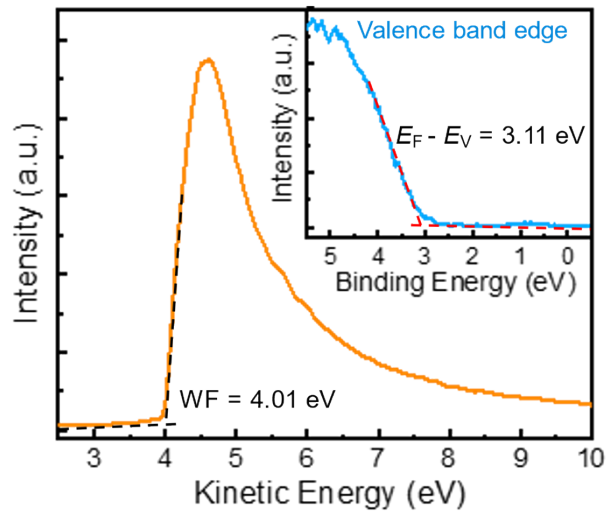


Fig. S3. Secondary electron cut-off and valence band spectra of as-deposited 15-nm TiO_x film.

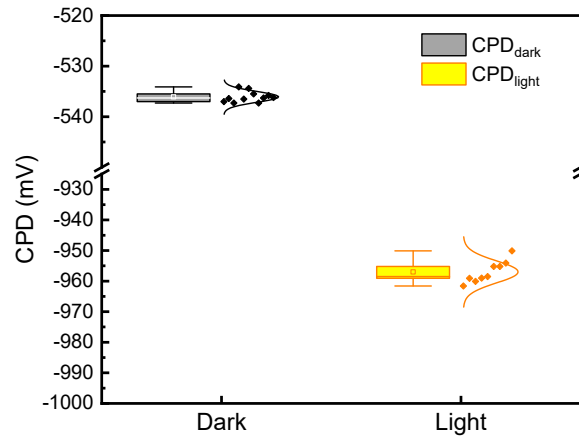


Fig. S4. Contact potential difference (CPD) measured in the dark and under illumination of Al_2O_3 film.

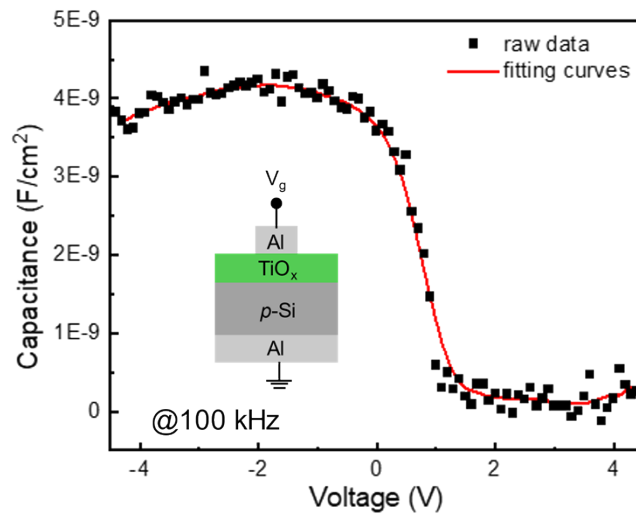


Fig. S5. The C - V measurement of the TiO_x film.

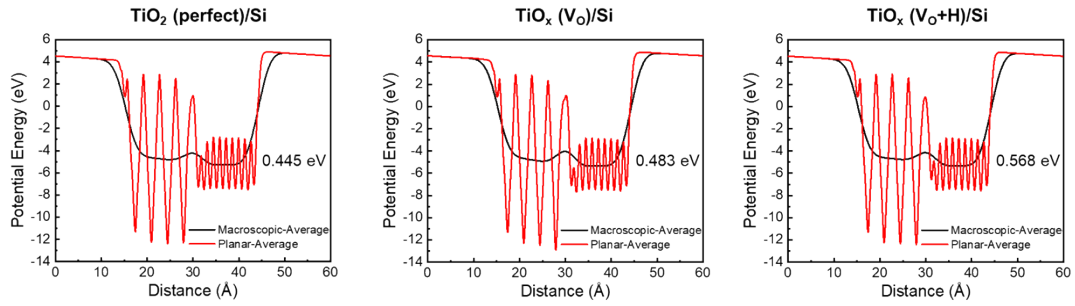


Fig. S6. The simulated macroscopic average and planar average of potential energy for the Si/TiO₂ (perfect), Si/TiO_x (V_O), and Si/TiO_x (V_O+H) structures, respectively.

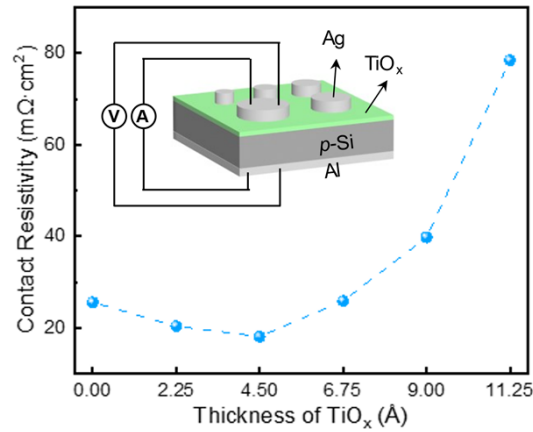


Fig. S7. Contact resistivity of *p*-Si samples with different TiO_x thicknesses.

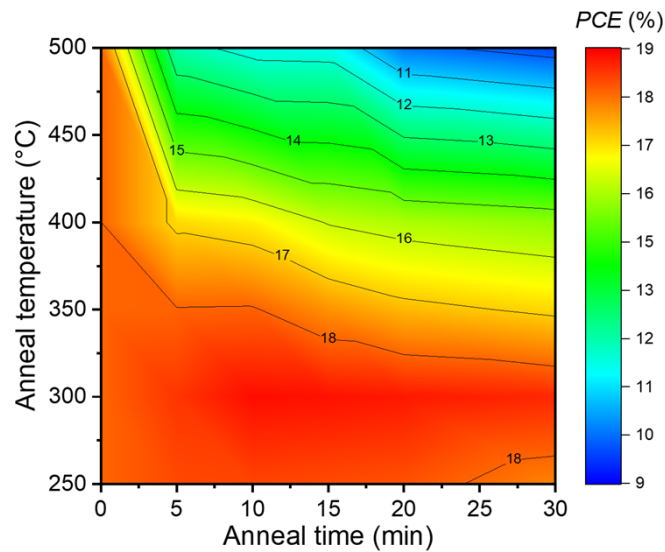


Fig. S8. *PCE* of solar cells as a function of forming gas annealing time and temperature.

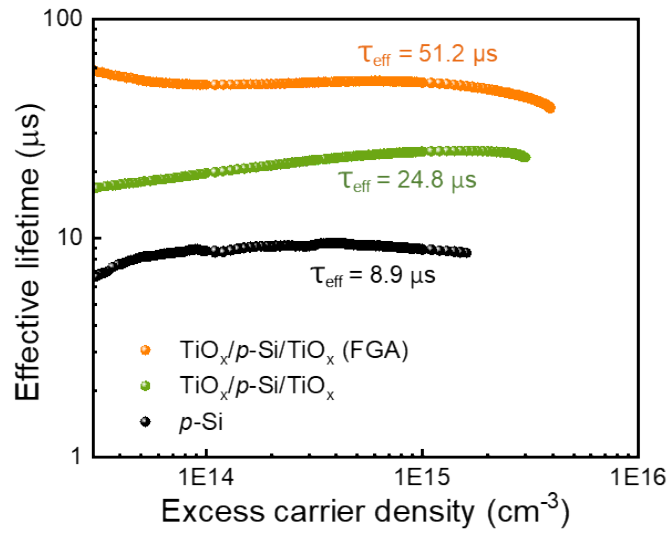


Fig. S9. Effective lifetime of the p -Si, $\text{TiO}_x/p\text{-Si}/\text{TiO}_x$, and $\text{TiO}_x/p\text{-Si}/\text{TiO}_x$ with FGA, where the τ_{eff} is indicated for excess carrier density of $1 \times 10^{15} \text{ cm}^{-3}$.

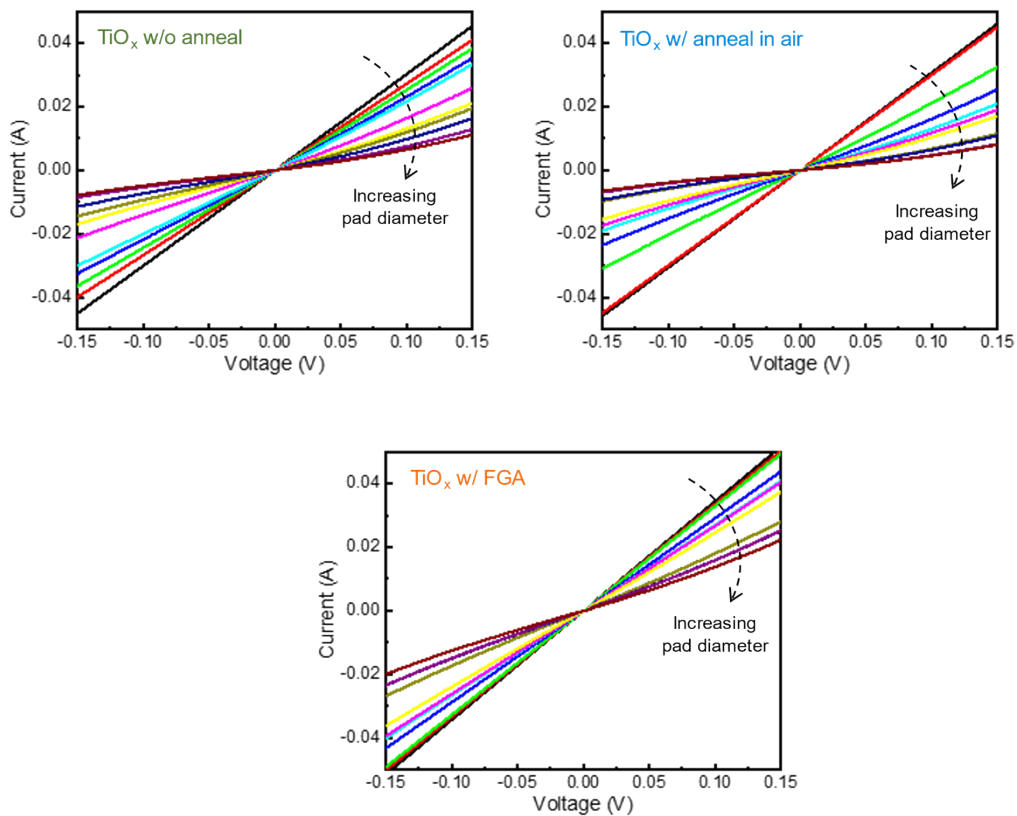


Fig. S10. The photograph of devices with different electrode pads and dark I - V curves of different contacts.

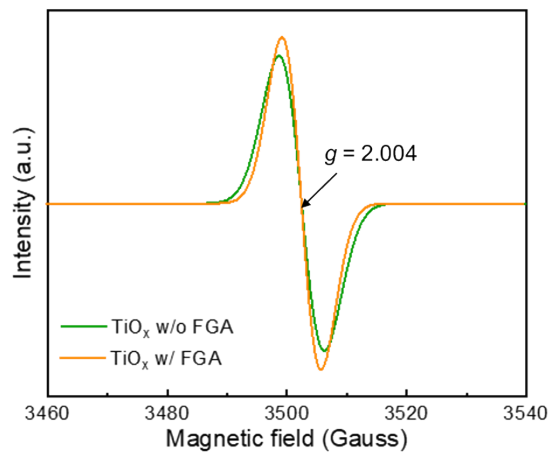


Fig. S11. Electron paramagnetic resonance (EPR) of the ultrathin TiO_x film with and without FGA treatment.

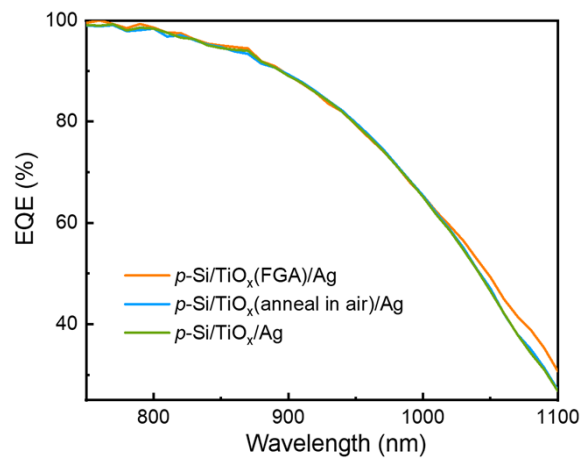


Fig. S12. EQE curves of solar cells with different TiO_x -based rear contacts.

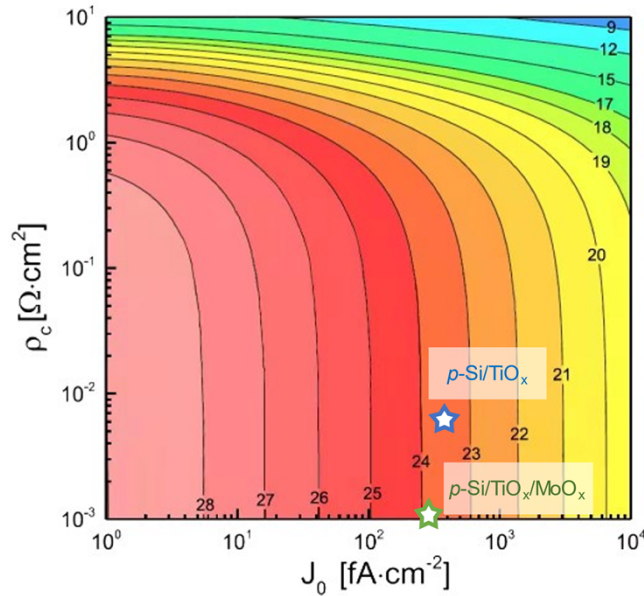


Fig. S13. Contour plot of *c*-Si solar cells featuring a full-area contact with the highest obtainable *PCE* in dependence of J_0 and ρ_c calculated from Quokka simulations. This figure has been adapted from reference [1]. The blue and green stars represent the J_0 and ρ_c values reported for *p*-Si/TiO_x and *p*-Si/TiO_x/MoO_x contacts in this work.

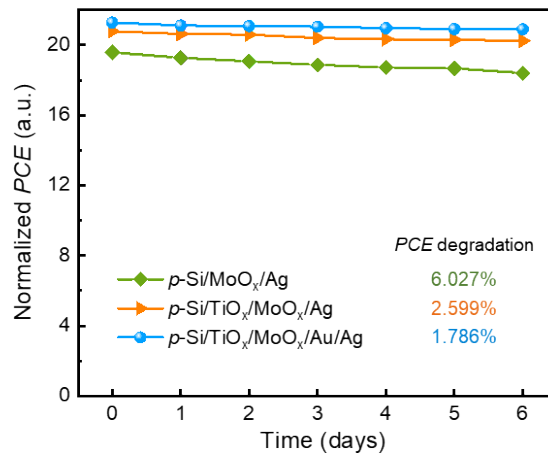


Fig. S14. Absolute *PCEs* of solar cells with different MoO_x-based HSCs as a function of storage time.

Reference

[1] Macco B, Black LE, Melskens J, et al. Atomic-layer deposited Nb2O5 as transparent passivating electron contact for *c*-Si solar cells. *Sol. Energy Mater. Sol. Cells.* 2018, 184, 98-104. doi: 10.1016/j.solmat.2018.04.037