Supporting Information

Heterojunction doping of polytriarylamine with cesium-doped vanadium oxide via interfacial electron transfer towards high-performance perovskite solar cells

Xiang Yao,[a,*] Huaxiu Geng,[a] Yunzhi Gu,[b] Hongbo Cui,[a] Guijian Guan,[a] and Mingyong Han[a,c,*]

[a] *Institute of molecular plus, Tianjin University, Tianjin 300072, P. R. China.*

[b] *Ultrafast Laser Laboratory, Key Laboratory of Opto-electronic Information Science and Technology of Ministry of Education, College of Precision Instruments and Opto-electronics Engineering, Tianjin University, 300072 Tianjin, China*

[c] *Institute of Materials Research and Engineering, 2 Fusionopolis Way, Singapore 138634*

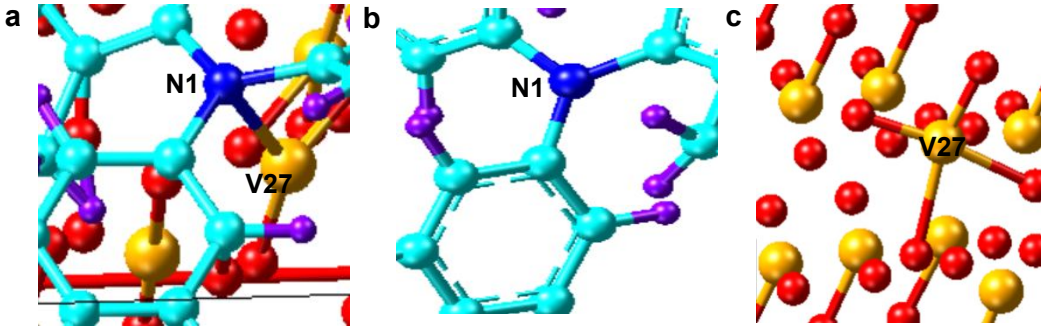
1. Density-functional theory (DFT) simulation results

2. SEM images of perovskite and histograms of statistical in-plane grain sizes

3. Hysteresis behaviors of the PSCs incorporated with different HELs

4. Steady-state measurements of V_{OC}, J_{SC}, FF and PCE for the devices

5. Stability of the PSCs with different HELs



d. Bader transfer charge states of N and V atoms at Cs-VOx/PTAA		
Conditions	N1	V27
Before doping	-1.4277	2.0873
After doping	0.4492	0.4848

Figure S1. DFT simulation for the bader transfer charge states of (a) N1 and V27 atoms of Cs-VOx/PTAA, (b) N1 atom of PTAA and (c) V27 atom of vanadium oxide. (d) Summarized bader transfer charge states of N and V atoms in the HIOS.

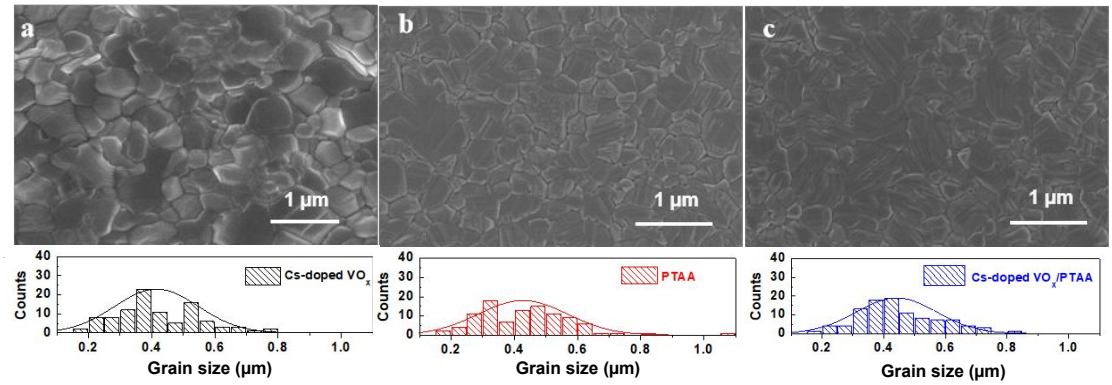


Figure S2. SEM images of $CH_3NH_3PbI_3$, and histograms of statistical in-plane grain sizes from SEM images of $CH_3NH_3PbI_3$ on the top of (a) Cs-doped VO_X, (b) PTAA, (c) Cs-doped VO_X/PTAA.

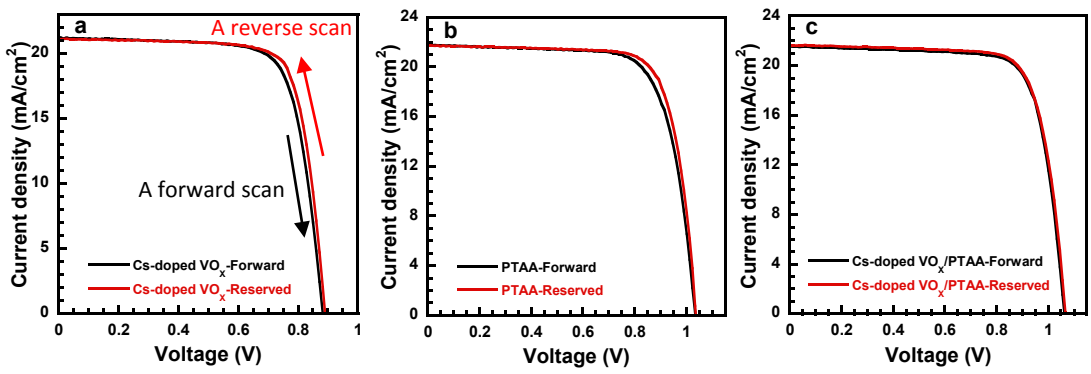


Figure S3. Hysteresis behaviors of the PSCs incorporated with different HELs. (a-c) J-V characteristics of the PSCs with (a) Cs-doped VO_X, (b) PTAA and (c) Cs-doped VO_X/PTAA HELs measured at a forward scan and a reserved scan between 0 and 1.0 V, respectively.

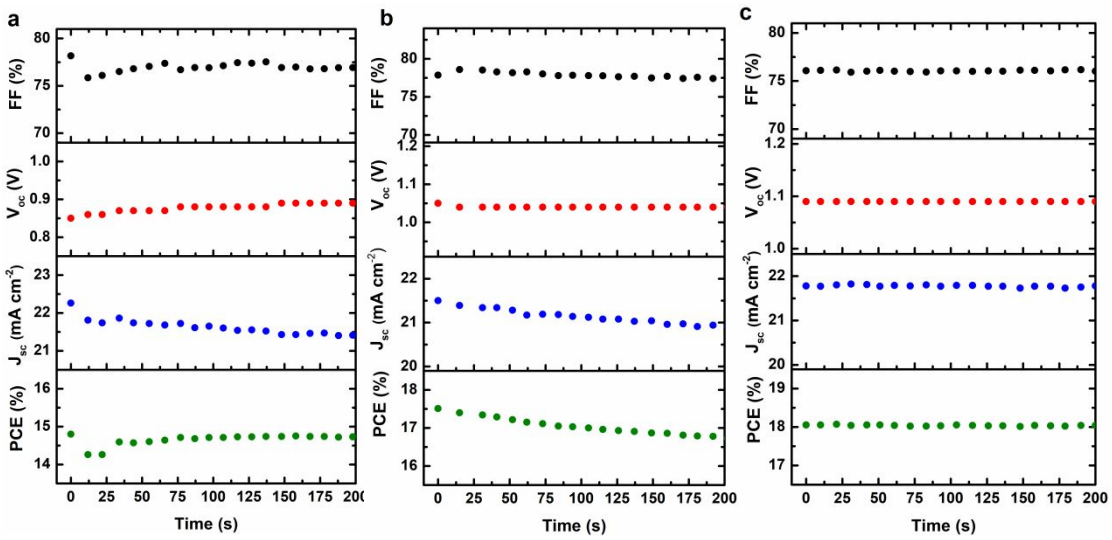


Figure S4. Steady-state measurements of V_{OC}, J_{SC}, FF and PCE for the devices with with (a) Cs-doped VO_X, (b) PTAA and (c) Cs-doped VO_X/PTAA HELs.

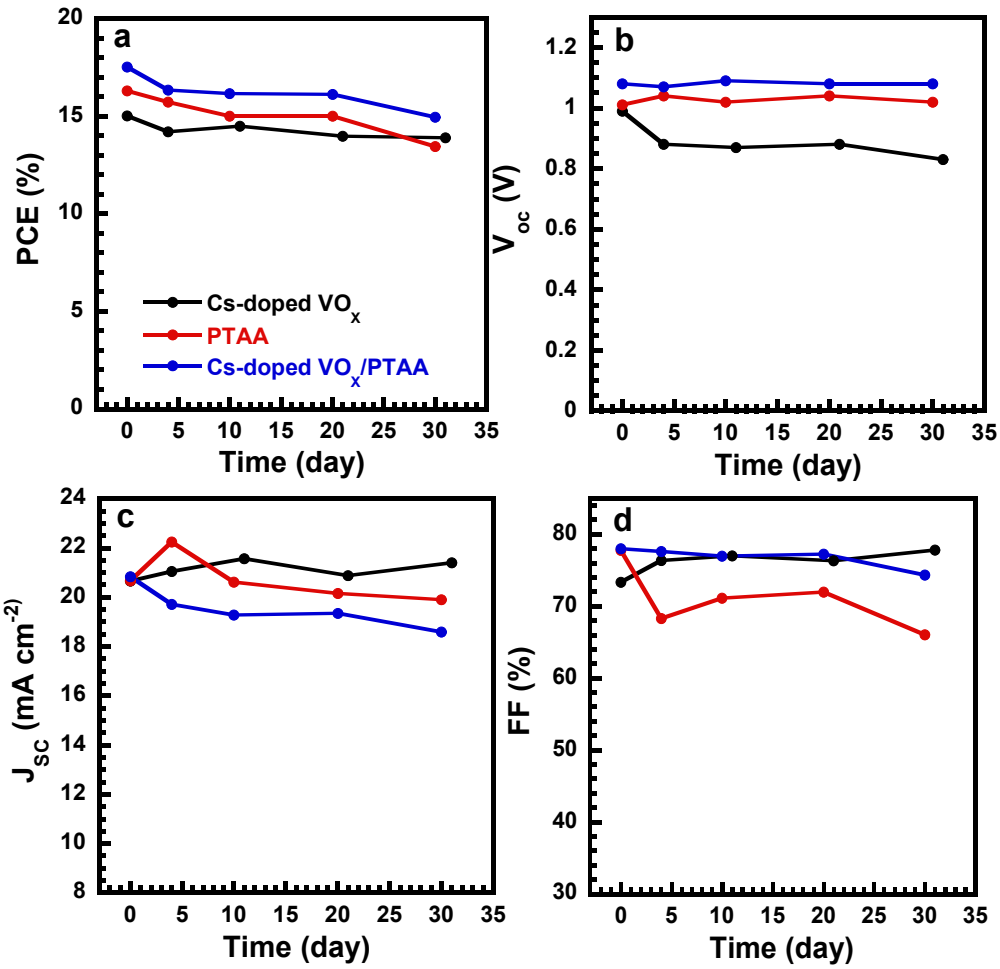


Figure S5. Evolution of J_{SC} (a), V_{OC} (b), FF (c) and PCE (d) for the device with different HELs over 30 days of storage in air.