ARTICLES

Journal of Semiconductors
(2021) 42, 112201
doi: 10.1088/1674-4926/42/11/112201

Tailoring molecular termination for thermally stable perovskite solar cells

Xiao Zhang[1, 2], Sai Ma[1, 2], Jingbi You[3, 4], Yang Bai[1, 2], and Qi Chen[1, 2, †]

[1]Beijing Key Laboratory of Nanophotonics and Ultrafine Optoelectronic Systems, School of Materials Science & Engineering, Beijing Institute of Technology, Beijing 100081, China

[2]Experimental Center of Advanced Materials, School of Materials Science & Engineering, Beijing Institute of Technology, Beijing 100081, China

[3]Key Laboratory of Semiconductor Materials Science, Institute of Semiconductors, Chinese Academy of Sciences, Beijing 100081, China

[4]Center of Materials Science and Optoelectronics Engineering, University of Chinese Academy of Sciences, Beijing 100081, China

Abstract: Interfacial engineering has made an outstanding contribution to the development of high-efficiency perovskite solar cells (PSCs). Here, we introduce an effective interface passivation strategy via methoxysilane molecules with different terminal groups. The power conversion efficiency (PCE) has increased from 20.97% to 21.87% after introducing a 3-isocyanatopropyltrimethoxy silane (IPTMS) molecule with carbonyl group, while a trimethoxy[3-(phenylamino)propyl] silane) (PAPMS) molecule containing aniline group deteriorates the photovoltaic performance as a consequence of decreased open circuit voltage. The improved performance after IPTMS treatment is ascribed to the suppression of non-radiative recombination and enhancement of carrier transportation. In addition, the devices with carbonyl group modification exhibit outstanding thermal stability, which maintain 90% of its initial PCE after 1500 h exposure. This work provides a guideline for the design of passivation molecules aiming to deliver the efficiency and thermal stability simultaneously.

Key words: perovskite solar cells; terminal groups; interfacial engineering; thermal stability

Citation: X Zhang, S Ma, J B You, Y Bai, and Q Chen, Tailoring molecular termination for thermally stable perovskite solar cells[J]. *J. Semicond.*, 2021, 42(11), 112201. http://doi.org/10.1088/1674-4926/42/11/112201

Supplement Materials

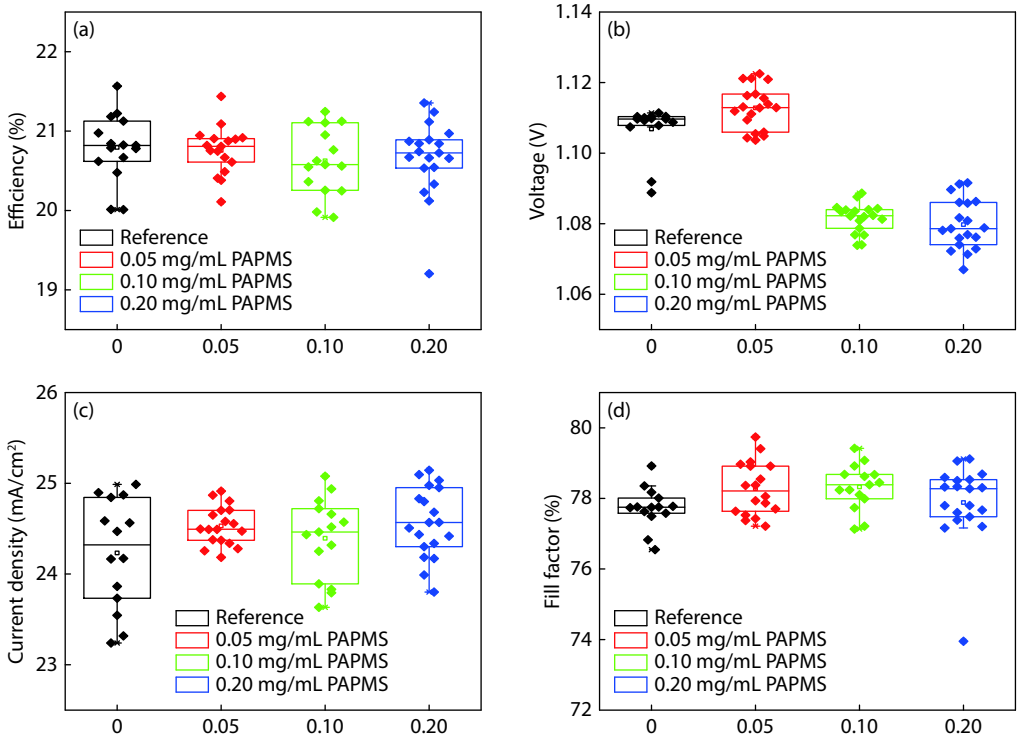

Fig. S1. Statistics of the device performance parameters for solar cells fabricated with different concentrations of PAPMS. (a) PCE. (b) V_{oc}. (c) J_{sc}. (d) FF.

Correspondence to: Q Chen, Qi Chen, qic@bit.edu.cn
Received 25 APRIL 2021; Revised 18 MAY 2021.

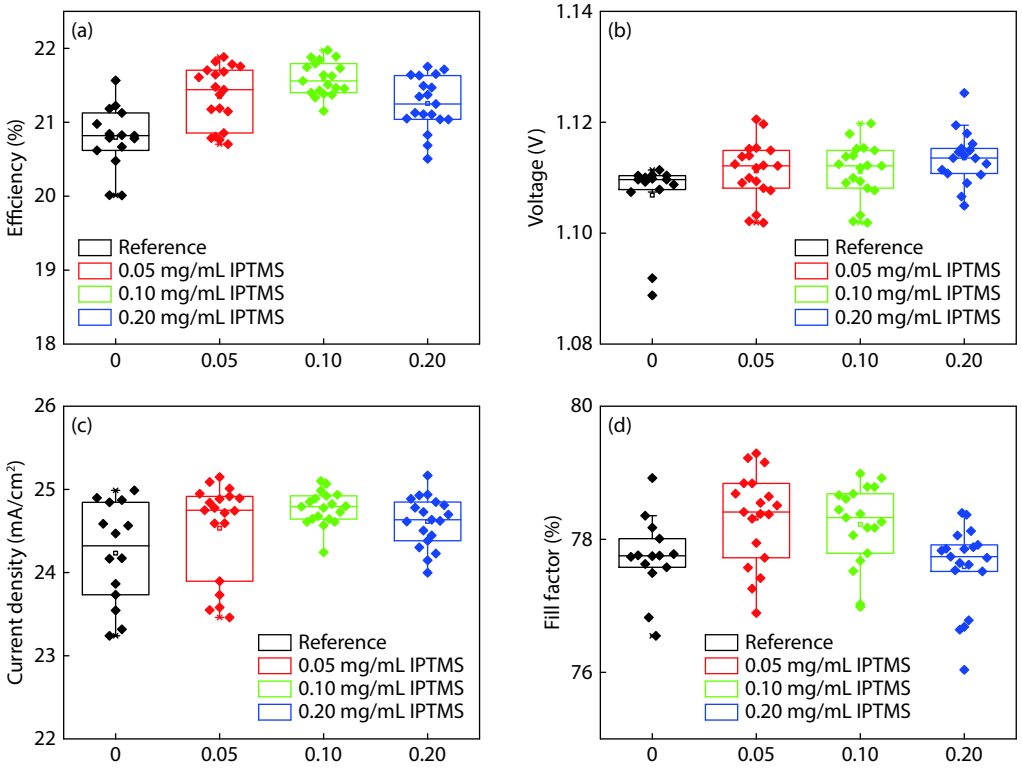

Fig. S2. Statistics of the device performance parameters for solar cells fabricated with different concentrations of IPTMS. (a) PCE. (b) V_{oc}. (c) J_{sc}. (d) FF.

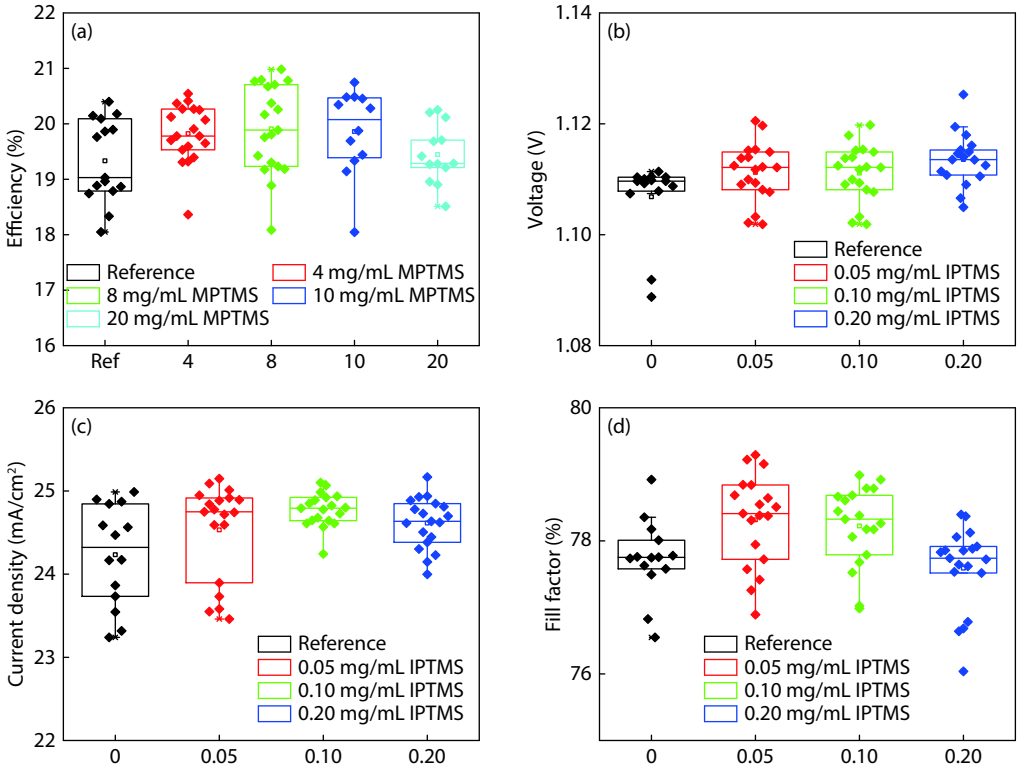

Fig. S3. Statistics of the device performance parameters for solar cells fabricated with different concentrations of MPTMS. (a) PCE. (b) V_{oc}. (c) J_{sc}. (d) FF.

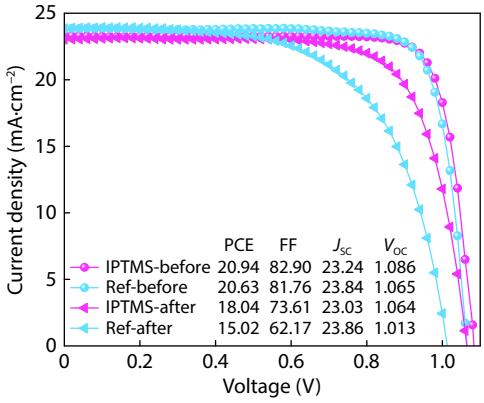

Fig. S4. *J*–*V* curve of IPTMS-treated and untreated device at 60%RH condition for 0 and 24 h.

Table 1. EIS parameters of the devices based on the pristine and IPTMS modification.

Parameter	R_{tr} (Ω)	R_{rec} (Ω)	C_1 (F)	C_2 (F)
Control	1.021×10^6	2.092×10^6	3.881×10^{-9}	6.202×10^{-8}
Target	6.413×10^5	8.233×10^6	7.227×10^{-9}	1.529×10^{-7}