Supporting materials

Critical Roles of Potassium on Charge-carrier Balance and Diffusion Induced Defects Passivation for Efficient Inverted Perovskite Solar Cells

Xuewen Yin¹, Jianhua Han¹, Yu Zhou¹, Youchen Gu¹, Meiqian Tai¹, Hui Nan¹, Yangying Zhou¹, Jianbao Li^{1,2}, Hong Lin^{1*}

¹State Key Laboratory of New Ceramics & Fine Processing, School of Materials Science and Engineering, Tsinghua University, Beijing 100084, P. R. China.

*E-mail: <u>hong-lin@mail.tsinghua.edu.cn</u>

²Key Laboratory of Ministry of Education for Advanced Materials in Tropical Island Resources, Materials and Chemical Engineering Institute, Hainan University, Haikou 570228, P. R. China.



Figure S1. Steady-state PCE (converted from steady-state photocurrent) measurement of devices based on pure NiO and NiO:5K.



Figure S2. (a) Diffuse reflectance spectra and (b) Kubelka-Munk spectra transformed

from diffuse reflectance spectra of different HTLs.



Figure S3. Ultraviolet photoelectron emission spectra of perovskite, NiO, NiO:3K, NiO:5K, NiO:7K and NiO:10K films. Black lines represent a regression analysis of measured data.



Figure S4. Schematic energy level diagrams of HTLs.



Figure S5. Deconvolution of Ni 2p, O 1s XPS spectra of NiO:3K, NiO:7K, and

NiO:10K films on FTO.



Figure S6. XRD patterns of NiO or K-doped NiO films prepared by spin-coating precursors 5 times on glasses



Figure S7. Schematic diagrams of K dopants substitute Ni atoms (a) or go into interstitial sites (b-c). (purple: K; red: O; gray: Ni.)



Figure S8. SEM images of (a) NiO:3K, (c) NiO:7K, (e) NiO:10K, and perovskites on

(b) NiO:3K, (d) NiO:7K and (f) NiO:10K.



Figure S9. Schematic diagrams of (a) perovskite, and (b) K dopant substitute Pb atom in perovskite. (amaranth: I; dark gray: Pb; purplish red: C; pink: H; blue: N; purple: K.)



Figure S10. TRPL spectra of different samples including glass/perovskite, glass/perovskite/PCBM, and glass/perovskite/spiro-OMeTAD.



Figure S11. Stability of devices based on NiO and NiO:5K without encapsulation stored in an ambient environment with 15% \pm 5% humidity.

ID	τ/ns
Perovskite/glass	245.55
NiO	53.05
NiO:3K	49.25
NiO:5K	40.88
NiO:7K	49.07
NiO:10K	50.00

Table S1. Decay time parameters of perovskites on different substrates

Table S2. EIS parameters of devices with different HTLs by fitting EIS Nyquist plots

ID	$R_{ m SR}/\Omega$	$R_{ m CT}/\Omega$	CPE1-T	CPE1-P
NiO	9.11	3974	1.58E-08	0.93
NiO:5K	6.92	898	1.33E-09	0.95