Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A. This journal is © The Royal Society of Chemistry 2019

## **Supporting Information**



Supplementary Fig. S1 The *J*–*V* curve of the recording device from KIER.



**Supplementary Fig. S2** SEM images of the Mo back contact layer surfaces for various diffusion barriers. (a) Mo/SS foil structure, (b) Mo/ZnO/SS foil structure, and (c) Mo/SiO<sub>2</sub>/SS foil structure after annealing at 800 °C for 1 hr.



**Supplementary Fig. S3** TOF-SIMS elemental depth profiles from Mo/ without barrier (a) and ZnO (b), SiO<sub>2</sub> (c) barrier/SS foil. Ion depth profiles of the samples were determined with ToF-SIMS using Cs ion guns for sputtering. It can be seen that the Cr and Fe diffusion barrier properties are excellent in SiO<sub>2</sub>. The samples without a diffusion barrier and with ZnO was especially vulnerable to Cr diffusion. Although Fe showed less diffusion compared with Cr in the samples without a barrier and with ZnO, it was not completely blocked. In the sample with the SiO<sub>2</sub> diffusion barrier, Fe and Cr were not detected in the SiO<sub>2</sub> barrier region, and thus, the SiO<sub>2</sub> diffusion barrier was sufficiently used as a diffusion barrier. In the sample of SiO<sub>2</sub>, the intensity of Si decreased sharply at the interface between the SiO<sub>2</sub> and Mo layers, and there was no difference in the intensity of Si in the Mo layer region compared with the sample without a barrier and with ZnO. That is, the diffusion of Si rarely occurs from SiO<sub>2</sub>.



**Supplementary Fig. S4** (a) The XRD patterns of CZTSSe/Mo/SS foil (black), CZTSSe/Mo/ZnO/SS foil (blue), and CZTSSe/Mo/SiO<sub>2</sub>/SS foil (red). (b) This is an XRD graph which enlarges  $26 \sim 29^{\circ}$  which is the (112), (103) peak region of CZTSSe. In the sample without a barrier, peaks were observed around  $30 \sim 31^{\circ}$  that were not found in other samples (see the red arrow in (a)). This peak is estimated to be the (111) peak of SnSe, but it is not clear whether it is due to impurity diffusion. It is estimated to be the (111) peak of SnSe (JCPDS 48–1224), but it is not clear whether it is due to impurity diffusion. As the CZTSSe (112) peak (JCPDS 04-010-6295) region was magnified, peaks at almost the same position were observed. The effect of Fe diffusion on the CZTSSe absorber will be addressed in subsequent studies.



**Supplementary Fig. S5** The statistics of (a)  $V_{OC}$ , (b)  $J_{SC}$ , (c) FF, and (d) EFF from the *J*–*V* curve of 8 CZTSSe solar cells on SS foil. The best cell was certified by KIER (supplementary Fig. S1).