Supplementary Information (SI) for Journal of Materials Chemistry C.

Supplementary Information

Delocalization and bandgap engineering in defective MoS_2 by metal-ion doping for enhanced electrical performance and efficient near-infrared detection

Minho Yoon,[a†*] Heung-Sik Kim,[b†*] Jiyoul Lee,[cd] Yong Uk Lee[d*]

[a]Department of Physics and Institute of Quantum Convergence Technology, Kangwon National University, Chuncheon, 24341, Republic of Korea

[b]Department of Energy Engineering, Korea Institute of Energy Technology, Naju-si 58217, Republic of Korea

[c]Department of Smart Green Technology Engineering, Pukyong National University, Yongso-ro 45, Nam-gu, Busan, 48513, Republic of Korea.

[d]Department of Semiconductor Engineering, Division of Nanotechnology and Semiconductor Engineering, Pukyong National University, Yongso-ro 45, Nam-gu, Busan, 48513, Republic of Korea E-mail

† Minho Yoon and Heung-Sik Kim contributed equally to this work.
*Corresponding Author: E-mail: minhoyoon78@kangwon.ac.kr, jiyoul_lee@pknu.ac.kr, yongyong@pknu.ac.kr.

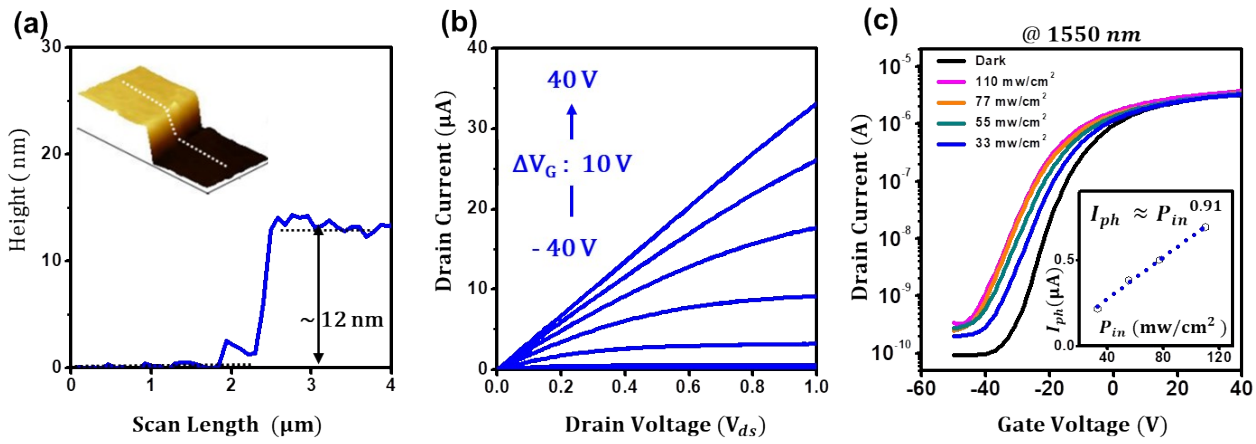

Fig. S1. (a) Thickness profiles (~12 nm) of the IGZO-coated MoS_2 FET. (b) The output characteristics (I_{ds} vs. V_{ds}) of the IGZO-coated MoS_2 FET. (c) Photo-response of the IGZO-coated MoS_2 FET as a function of power of the incident light. Inset: fitting curve with a power law.

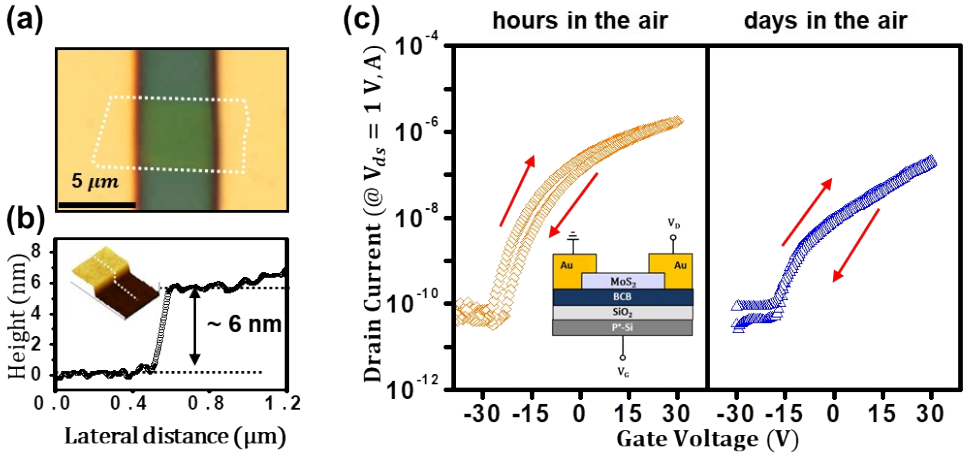

Fig. S2. (a, b) Optical microscopy (OM) image, AFM image along with channel thickness profiles (~6 nm). The channel width and length of the MoS_2 FET are 5.1 and 5.8 μm, respectively. (c) Transfer characteristics of n-type MoS_2 FET with 300 nm-thick BCB/SiO_2 dielectric with cross section scheme (inset).

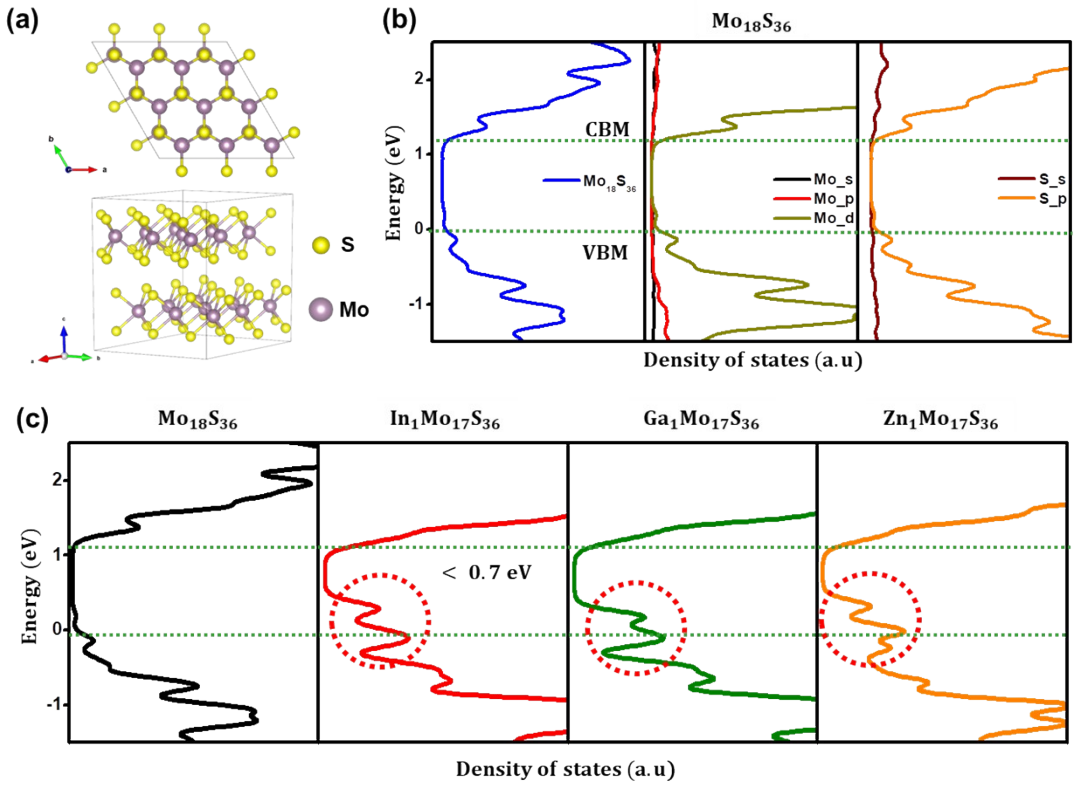

Fig. S3. (a) Constructed MoS_2 supercell. (b) Electronic density of states of MoS_2. (c) Electronic density of states of doped MoS_2 flakes, which contain metal ions such as indium (In), gallium (Ga), and zinc (Zn), respectively.

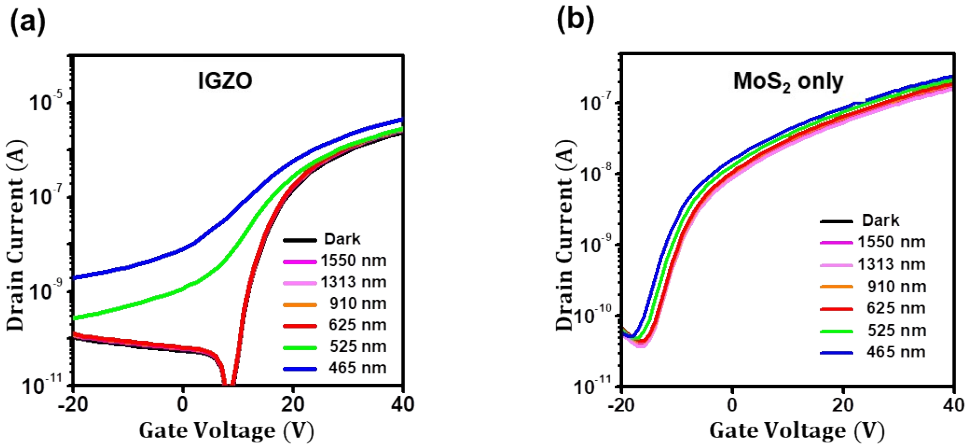

Fig. S4. (a, b) Photo-detecting properties of the IGZO and MoS_2 FET, respectively.

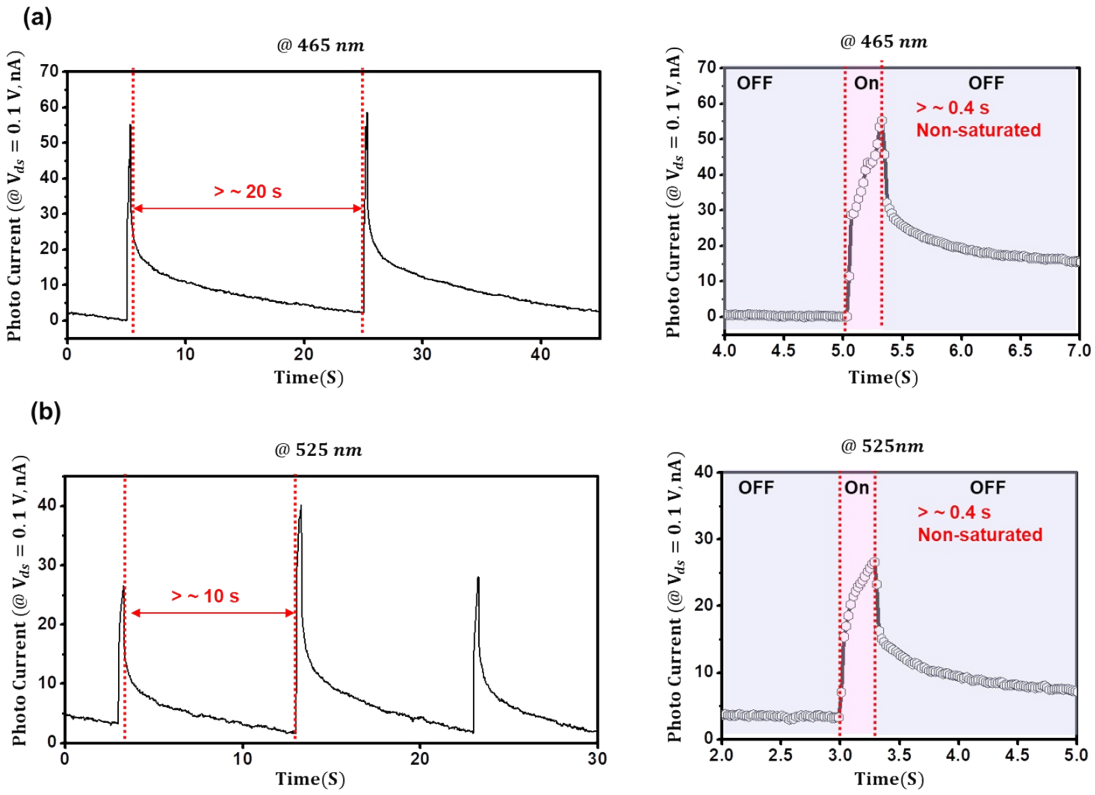

Fig. S5. (a, b) Dynamic photoresponse of the IGZO-coated MoS_2 phototransistor to visible lights (465 , 525 nm), respectively.

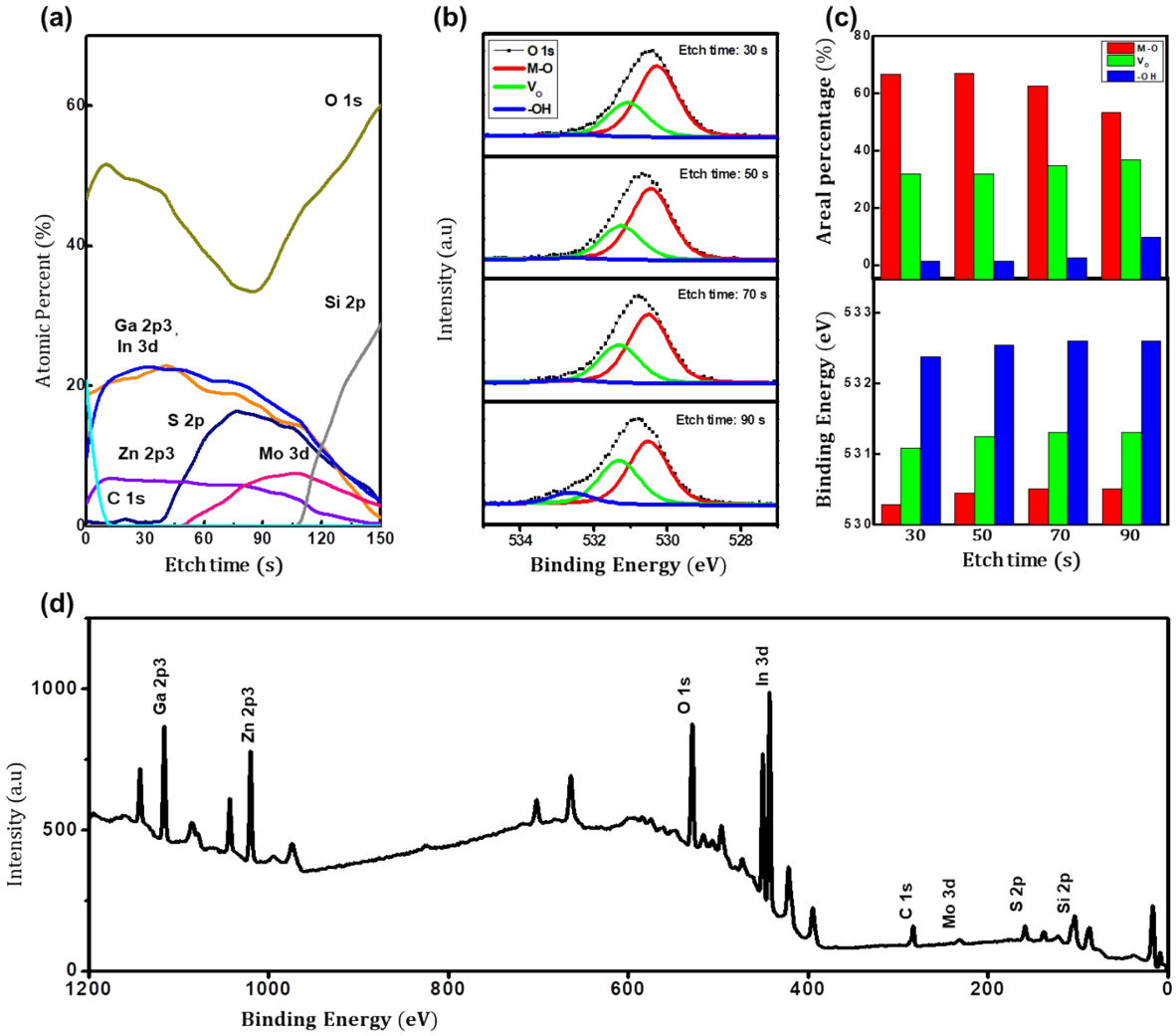

Fig. S6. XPS analyses of the IGZO-coated MoS_2. (a) XPS depth profile (b) O1s spectrum changes as a function of etch time. (c) Areal percentage and binding energy shift of O1s spectra. (d) Survey scan of the surface of the IGZO-coated MoS_2.

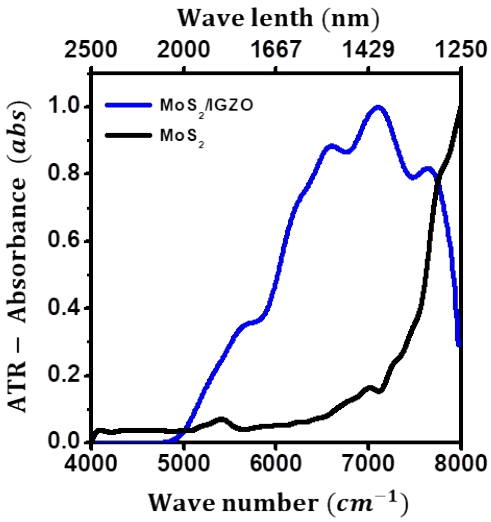

Fig. S7. Near-infrared absorption spectra of the MoS_2-only and MoS_2/IGZO flakes, respectively.

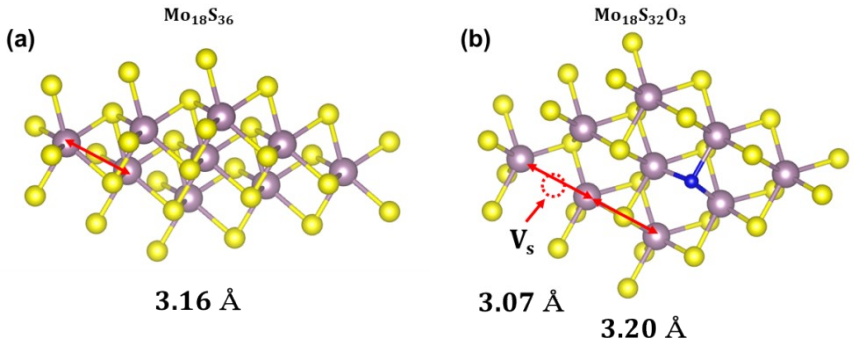

Fig. S8. (a, b) Fully relaxed crystal structure of MoS_2 and defective MoS_2, respectively.

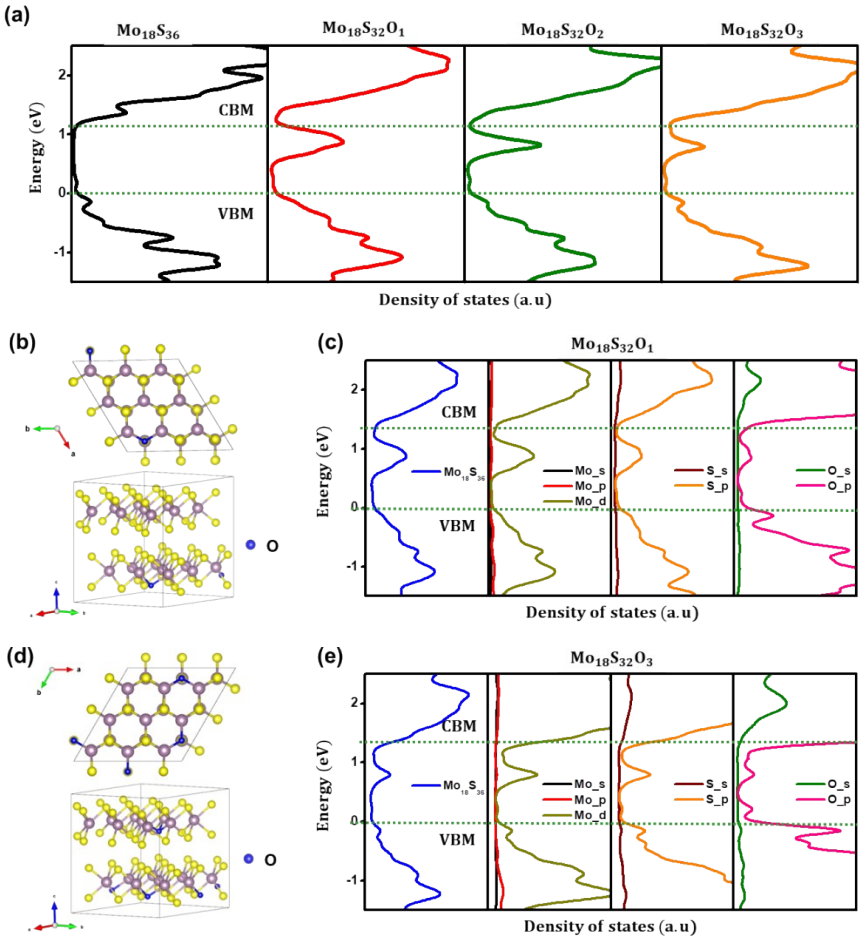

Fig. S9. (a) Electronic density of states of the defective MoS_2 according to the stoichiometry. (b, c) Constructed supercell and electronic density of states of defective MoS_2 ($Mo_{18}S_{32}O_1$). (d, e) Constructed supercell and electronic density of states of defective MoS_2 ($Mo_{18}S_{32}O_3$).

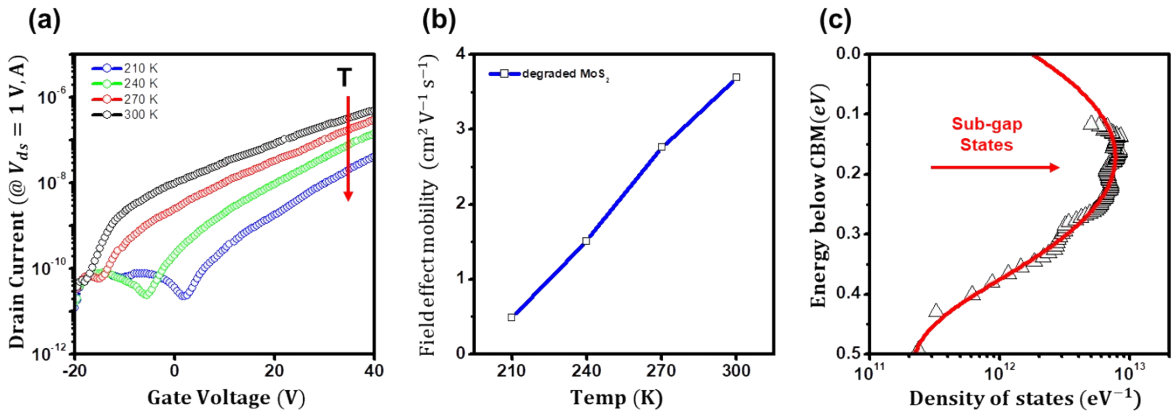

Fig. S10. (a, b) Temperature dependence of the transfer curves and field-effect mobility of the degraded MoS_2 FETs c Extracted charge trap density of states (DOS) of the degraded MoS_2 FET.