Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C. This journal is © The Royal Society of Chemistry 2024

### Supplementary information

# Modulating Fermi energy in few layer MoS<sub>2</sub> via metal passivation with enhanced detectivity for Near IR Photodetector

R. Abinaya<sup>1</sup>, E. Vinoth<sup>1</sup>, S. Harish<sup>1, 2</sup>, S. Ponnusamy<sup>1</sup>, J. Archana<sup>1\*</sup>, M. Shimomura<sup>2</sup>, M. Navaneethan<sup>2, 3\*</sup>

<sup>1</sup>Functional Materials and Energy Devices Laboratory, Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur-603 203, India

<sup>2</sup>Graduate School of Science and Technology, Shizuoka University, 3-5-1 Johoku, Naka-Ku,

Hamamatsu, Shizuoka 432-8011, Japan

<sup>3</sup>Nanotechnology Research Centre (NRC), Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur-603 203, India

## \*Corresponding author (s):

#### Dr. M. Navaneethan

e-mail- navaneem@srmist.edu.in

#### Dr. J. Archana

e-mail- archanaj@srmist.edu.in



Scheme S1. Fabricated actual device



**Fig S1.** FESEM images (a), Mo (a1), S (a2), Zn (a3) distribution of Zn-MoS<sub>2</sub>, FESEM images (b), Mo (b1), S (b2), Zn (b3) distribution of Fe-MoS<sub>2</sub>, EDS spectra of Zn-MoS<sub>2</sub> (c) and Fe-MoS<sub>2</sub> (d).



Fig S2. XPS results of Mo (a), S (b) for MoS<sub>2</sub>, Zn-MoS<sub>2</sub> and Fe-MoS<sub>2</sub>.

Further, cyclic current-voltage (I-V) measurements have been performed in the dark environment as well as under illumination to study the transport of charge carriers through the device from -5V to +5V. In the I-V hysteresis the trace path denoted as 0V to -5V and retrace path as -5V to 0V. Here we observed that the photoconduction were enhanced under illumination in forward bias and area of hysteresis enhanced in reverse bias for the passivated devices. This can be explained by the obtained hysteresis I-V the basis charge curve on of transport(trapping/detrapping) properties of the photodiode. Here the role of Fe and Zn passivation layer acts as nano structuring, leads the surface defects/traps present in it. Under the light illumination, we observed the no photovoltaic effect as the device has no open circuit voltage. Thus, the fraction of photogenerated charge carriers are expected to be trapped in the surface defect states. On the reverse current, the trapping rate could be depended on the flow of current through the device and the number of empty traps. But in the forward current, it depends on the density of filled states. Thus, the passivated photodetectors capture the photo generated electron-hole pairs and recombines at the interface gets easier leads the enhanced photoconduction of the devices.



Fig S3. Cyclic current-voltage (I-V) characteristics of MoS<sub>2</sub>, Zn-MoS<sub>2</sub> and Fe-MoS<sub>2</sub>.



Fig S4. Wavelength dependent photocurrent and rectification ratio.



Fig S5. Temporal response at bias voltage of 1.5 and 4.5 V of MoS<sub>2</sub>, Zn-MoS<sub>2</sub> and Fe-MoS<sub>2</sub>.

For  $MoS_2$ , the current lies in the range of  $10^{-6}$  A, however under illumination, the slight increment in magnitude is observed for all temperatures than under dark. For Fe-MoS<sub>2</sub>, no significant enhancement between dark and light illumination with respect to applied temperature has been observed. But in case of Zn-MoS<sub>2</sub>, under illumination, the values are increased tremendously to mA range at all temperature and the maximum achieved value is  $0.171 \times 10^{-3}$  A at 323 K. This huge increment in the photocurrent is not only been raised from the light illumination, but also the effect of applied temperature. This indicates that the device could perform as photothermoelectric based detectors.



Fig S6. Temperature dependent (I-V) characteristics of MoS<sub>2</sub>, Zn-MoS<sub>2</sub> and Fe-MoS<sub>2</sub>.