Electronic Supplementary Material (ESI) for Nanoscale Horizons.
This journal is © The Royal Society of Chemistry 2024

Supporting Information

Synergistic Heterojunction of SnS_2/SnSSe Nanosheets on GaN for Advanced Self-powered Photodetectors

Sukhendu Maity and Praveen Kumar*

School of Materials Science, Indian Association for the Cultivation of Science, Kolkata, 700032, India

Contents

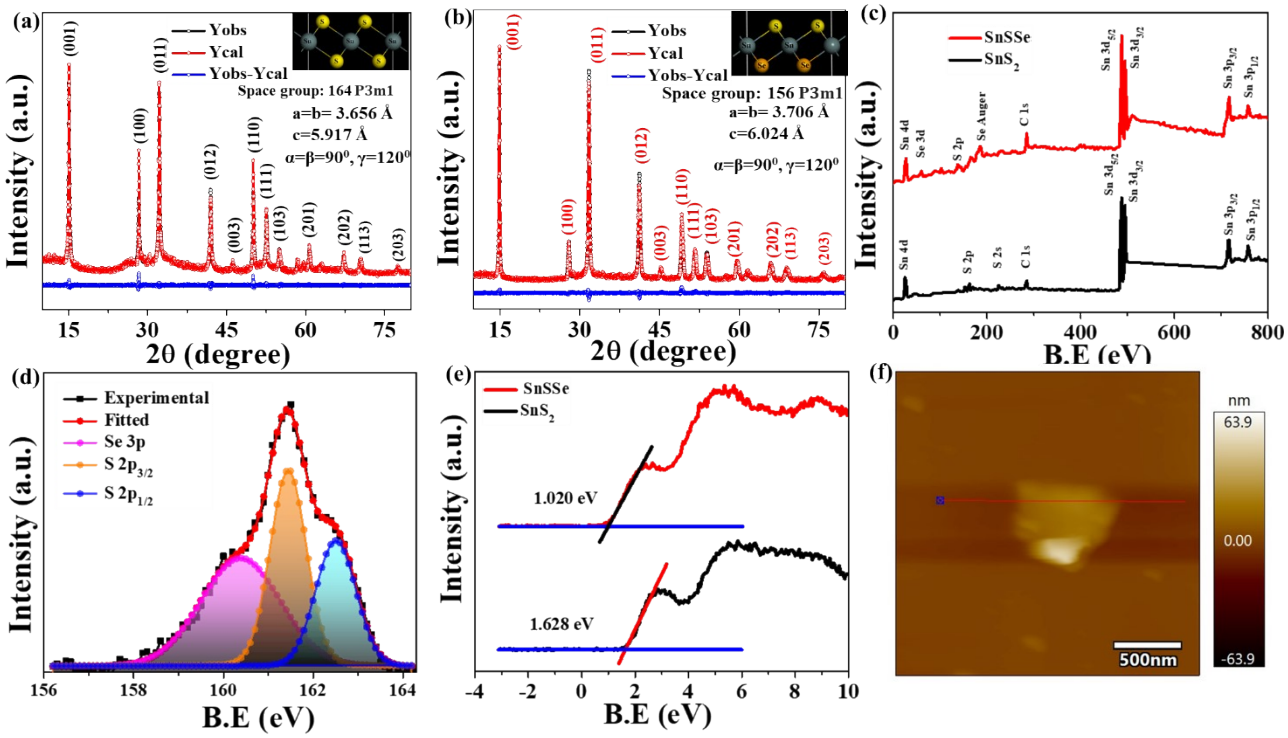

Figure. S1. (a), (b) Rietveld refinement of SnS_2 and SnSSe bulk powder respectively, (c) XPS survey spectrum of SnS_2 and SnSSe, (d) High resolution XPS of deconvoluted S 2p for SnSSe, (e) High resolution XPS of deconvoluted S 2p for SnS_2, (e) valence band spectrum with respect to the Fermi level of SnS_2 and SnSSe, (f) AFM images of SnSSe 2d sheet.

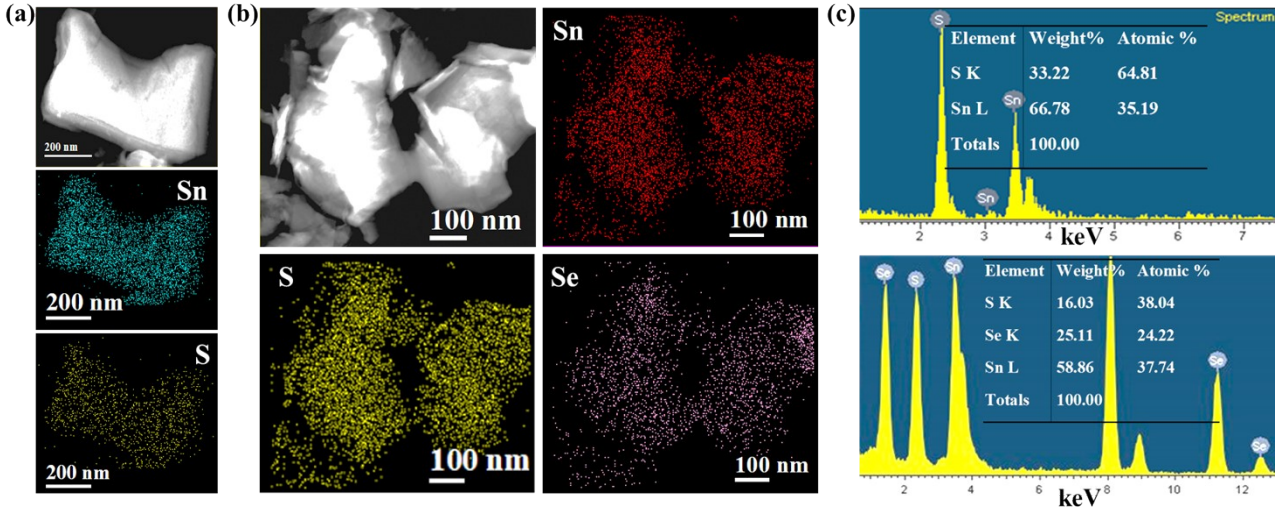

Figure. S2. (a) HAADF mapping of SnS_2 nanosheet (b), HAADF mapping of SnSSe nanosheet (c) EDX spectra of SnS_2 and SnSSe nanosheets.

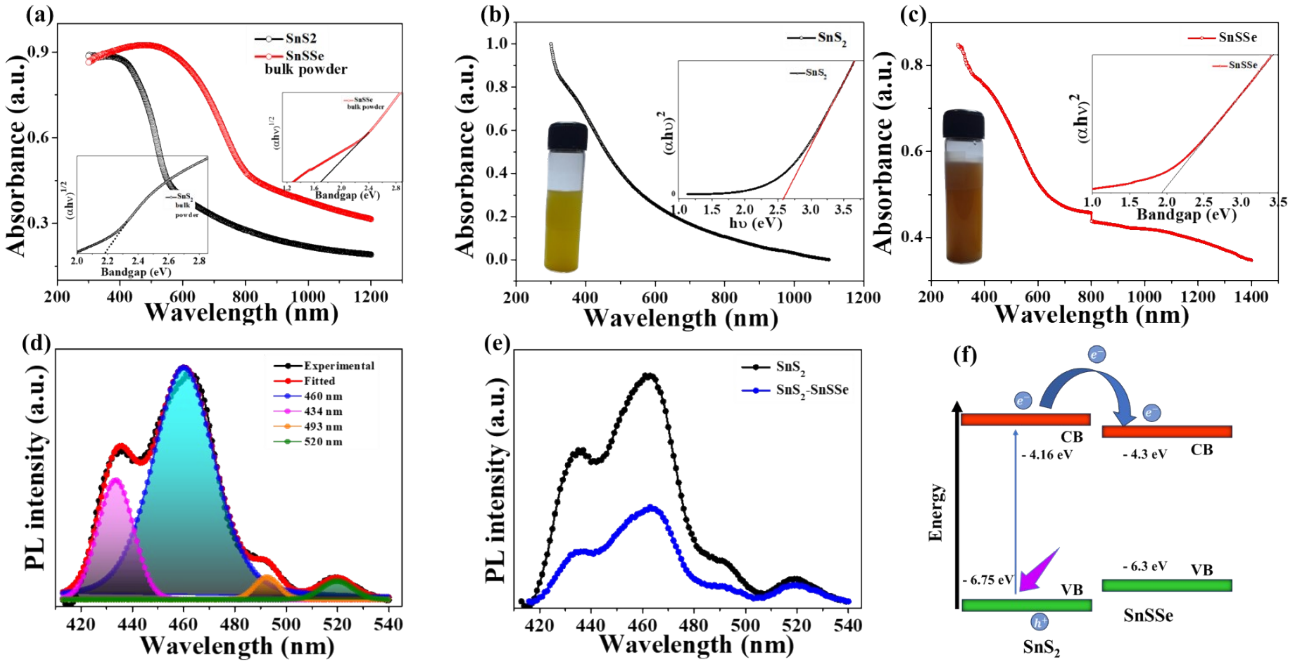

Figure. S3. (a) Absorbance spectra for bulk SnS_2 and SnSSe powder sample, (b), (c) Absorbance spectra for exfoliated SnS_2 and SnSSe in isopropanol solvent, (d) Deconvoluted PL spectrum of exfoliated SnS_2, (e) PL quenching of SnS_2 in presence of SnSSe, (f) schematic representation of the electron transfer process from SnS_2 to SnSSe.

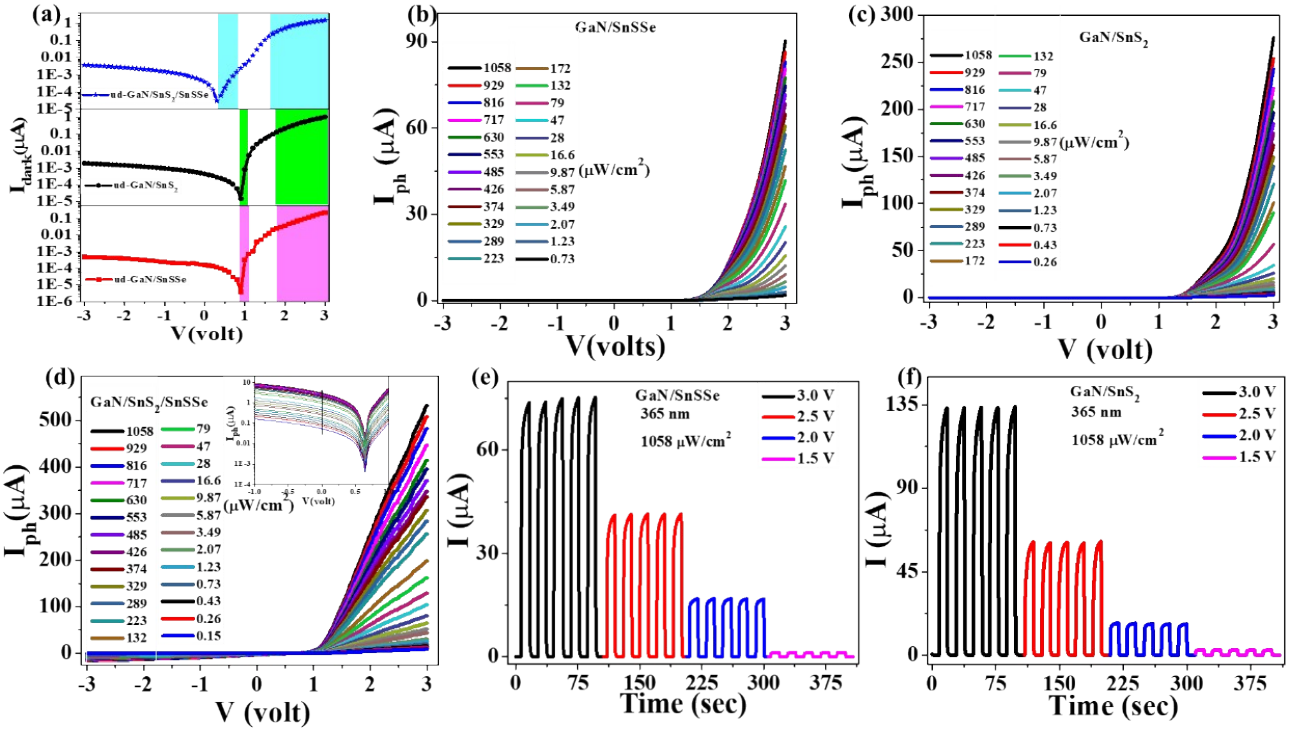

Figure. S4. (a) semi-logarithmic I-V curves of the fabricated devices, (b)- (c) Photoresponse recorded with varying intensity under 365 nm illumination, (e)-(f) Bias

dependent photo switching of the device D_1 and D_2 at fixed intensity of 1058 μW/cm^2.

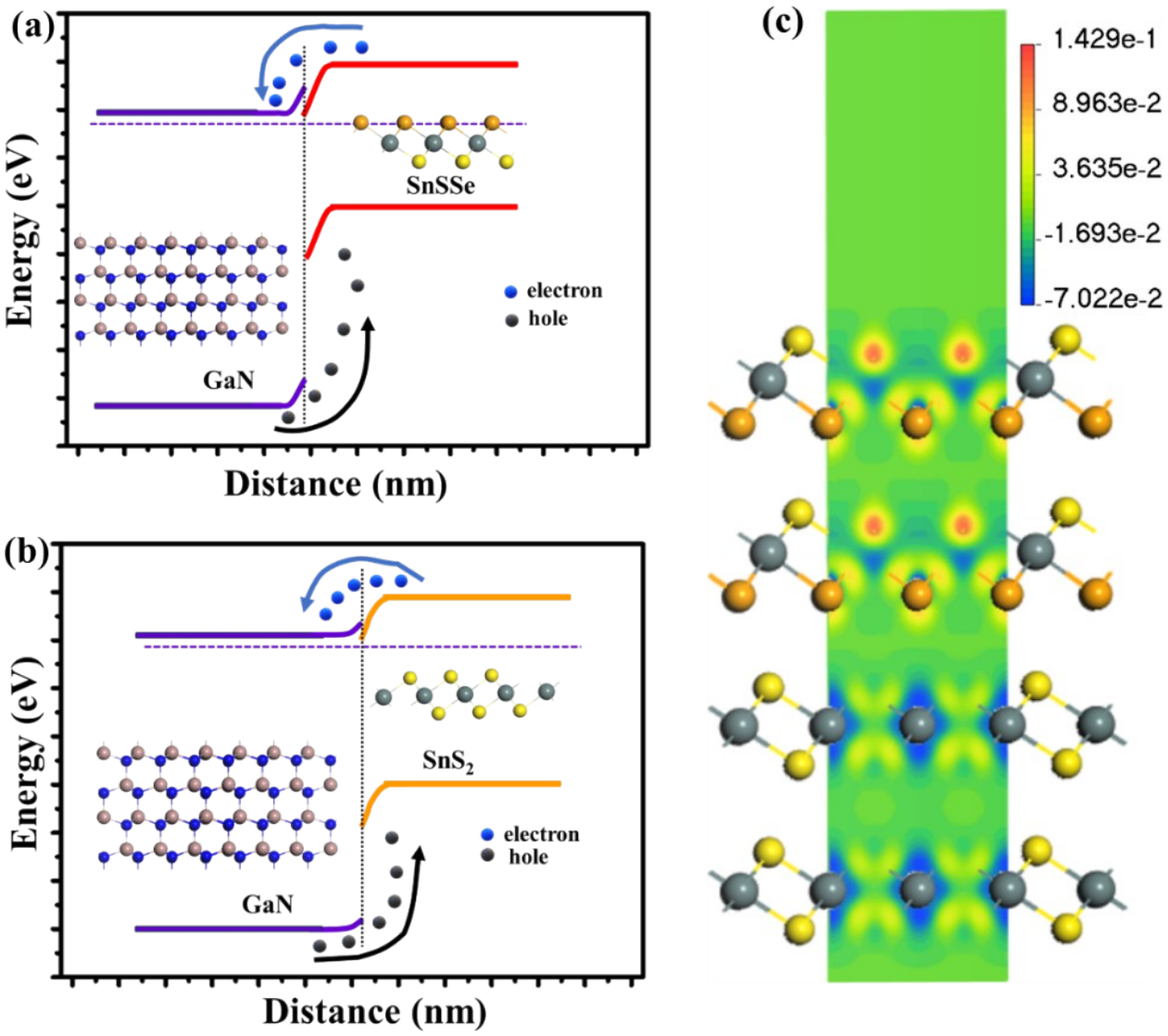

Figure. S5. (a), (b) Schematics of energy band diagram for $D_1$and D_2 device configuration, (c) Simulated electron density distribution of SnS_2/SnSSe heterostructure.

Table ST1. Parameters to calculate the average photoluminescence lifetime of carriers

$T= A+B_1*exp(-i/T_1) + B_2*exp(i/T_2)$

Sample	Excitation (nm)	Emission (nm)	Average life time (ns)	T_1 (ns)	T_2 (ns)	B_1	B_2
SnS_2			2.629	0.914461	6.04562	66.57	33.43
	375	**460**					
SnS_2 - SnSSe			**1.483**	**0.900447**	**5.2463**	**86.59**	**13.41**

Table ST2. Parameters to calculate the average photoluminescence lifetime of carriers.

$T= A+B_1*exp(-i/T_1) + B_2*exp(i/T_2)$

Device configuration	Excitation (nm)	Emission (nm)	Average life time (ns)	T_1 (ns)	T_2 (ns)	B_1	B_2
GaN/SnS_2			6.692	0.52091	7.36049	9.76	90.23
GaN/SnSSe	**375**	**460**	6.603	0.29676	7.25718	9.39	90.60
GaN/SnS_2 /SnSSe			**4.931**	**0.71218**	**7.37601**	**36.69**	**63.31**

Table ST3. Performance comparison of our fabricated device with other reported work.

Device configuration	Wavelength (nm)	Bias (volt)	R (A/W)	EQE (%)	D* (Jones)	Refer.
CTS QDs/SnS_2	320	5	53.88	20,878	3.2×10^{13}	1
SnS_2/ITO	405	3	58×10^{-3}	17.9	1.53×10^{10}	2
Cr: Au/SnS_2/Cr: Au	365	1	112	3.7×10^{4}	1.18×10^{11}	3
Ag/SnS_2/Ag	365	5	5.5	1868	1.72×10^{13}	4
Si/SnS_2	405	-2	0.12		9.35×10^{10}	5
SnS_2/Si NW	340	2	100	3.64×10^{4}	1.14×10^{14}	6
Au/In-SnS_2/Au	405	5	153.8	4.72×10^{4}	5.81×10^{12}	7
SnS_2/PEDOT: PSS	300	-1	182.89	7.55×10^{4}	1.44×10^{12}	8
Al/SnS_2/CuO/ PEDOT: PSS/ITO	300	-1	1.87	775.41	1.10×10^{11}	9
SnS_2/Ag_2S	405	2	4.52		3.53×10^{11}	10
SnS_2/GaN	265	0	3.52		1.76×10^{14}	11
p-Si/SnS_2	365	0	0.0125		2.85×10^{7}	12
InSe/SnS2/GeSe	355	0	1.87	656	8.39×10^{12}	13
SnO_2/In_2O_3/SnS_2	555	0	2.9×10^{-3}		5.9×107	14
ITO/SnS_2/$ZnO_{1-x}S_x$/Au	365	0	8.28×10^{-3}		5.09×10^{10}	15
Ud-GaN/SnS_2/SnSSe	365	3	314.96	10.7×10^{4}	2.00×10^{14}	This work
		0	1.52	519	6.06×10^{13}	

Table ST4. Population analysis (Mulliken and Hirshfeld) for geometry optimized SnS_2.

Atomic Populations (Mulliken)								Hirshfeld Analysis		
Species	Ion	s	p	d	f	Total	Charge (e)	Species	Ion	Hirshfeld Charge (e)
S	1	1.89	4.57	0.00	0.00	6.46	-0.46	S	1	-0.14
S	2	1.89	4.57	0.00	0.00	6.46	-0.46	S	2	-0.14
Sn	1	1.16	1.92	0.00	0.00	3.08	0.92	Sn	1	0.28

Table ST5. Population analysis (Mulliken and Hirshfeld) for geometry optimized SnSSe.

Atomic Populations (Mulliken)								Hirshfeld Analysis		
Species	Ion	s	p	d	f	Total	Charge (e)	Species	Ion	Hirshfeld Charge (e)
S	1	1.90	4.56	0.00	0.00	6.46	-0.46	S	1	-0.15
Se	1	1.79	4.45	0.00	0.00	6.24	-0.24	Se	1	-0.11
Sn	1	1.31	1.99	0.00	0.00	3.30	0.70	Sn	1	0.26

Table ST6. Population analysis for SnS_2/ SnSSe heterostructures.

Atomic Populations (Mulliken)								Hirshfeld Analysis		
Species	**Ion**	**s**	**p**	**d**	**f**	**Total**	**Charge (e)**	**Species**	**Ion**	**Hirshfeld Charge (e)**
S	1	1.89	4.56	0.00	0.00	6.46	-0.46	S	1	-0.14
S	2	1.90	4.56	0.00	0.00	6.46	-0.46	S	2	-0.14
S	3	1.90	4.55	0.00	0.00	6.45	-0.45	S	3	-0.15
S	4	1.90	4.56	0.00	0.00	6.45	-0.45	S	4	-0.14
S	5	1.89	4.57	0.00	0.00	6.47	-0.47	S	5	-0.15
S	6	1.89	4.57	0.00	0.00	6.47	-0.47	S	6	-0.15
Se	1	1.75	4.45	0.00	0.00	6.21	-0.21	Se	1	-0.11
Se	2	1.81	4.45	0.00	0.00	6.26	-0.26	Se	2	-0.11
Sn	1	1.18	1.91	0.00	0.00	3.09	0.91	Sn	1	0.29
Sn	2	1.18	1.90	0.00	0.00	3.08	0.92	Sn	2	0.29
Sn	3	1.31	2.01	0.00	0.00	3.32	0.68	Sn	3	0.25
Sn	4	1.27	2.01	0.00	0.00	3.27	0.73	Sn	4	0.25

Reference:

1 S. M. Yadav and A. Pandey, *IEEE Trans. Electron Devices*, 2020, **67**, 2008–2015.

2 H. Tian, C. Fan, G. Liu, Y. Zhang, M. Wang and E. Li, *J. Mater. Sci.*, 2019, **54**, 2059–2065.

3 H. Ying, X. Li, Y. Wu, Y. Yao, J. Xi, W. Su, C. Jin, M. Xu, Z. He and Q. Zhang, *Nanoscale Adv.*, 2019, **1**, 3973–3979.

4 S. M. Yadav and A. Pandey, *IEEE Trans. Nanotechnol.*, 2020, **19**, 301–307.

5 J. Xu, H. Zhang, Z. Song, Y. Xu, Q. Peng, X. Xiu, Z. Li, C. Li, M. Liu and B. Man, *Appl. Surf. Sci.*, 2020, **506**, 144671.

6 S. Das, K. J. Sarkar, B. Pal, H. Mondal, S. Pal, R. Basori and P. Banerji, *J. Appl. Phys.*, 2021, **129**, 053105.

7 C. Fan, Z. Liu, S. Yuan, X. Meng, X. An, Y. Jing, C. Sun, Y. Zhang, Z. Zhang, M. Wang, H. Zheng and E. Li, *ACS Appl. Mater. Interfaces*, 2021, **13**, 35889–35896.

8 A. K. Dwivedi, R. Tripathi, S. Tripathi, S. Jit and S. Tripathi, *IEEE Electron Device Lett.*, 2022, **43**, 1913–1916.

9 A. K. Dwivedi and S. Tripathi, *IEEE Trans. Electron Devices*, 2023, **70**, 2378–2383.

10 H. Zhang, H. Li, H. Yu, F. Wang, X. Song, Z. Xu, D. Wei, J. Zhang, Z. Dai, Y. Ren, Y. Ye, X. Ren and J. Yao, *Mater. Lett.*, 2023, **330**, 133037.

11 T. Chen, Q. Feng, W. Feng and X. Yang, *J. Alloys Compd.*, 2024, **971**, 172657.

12 M. Kumar, B. R. Huang, A. Saravanan, H. Sun and S. C. Chen, *Adv. Electron. Mater.*, 2024, **10**, 2400164.

13 Y. Yan, J. Li, H. Li, S. Li, Z. Li, W. Gao, Y. Jiang, X. Song, C. Xia and J. Li, *Appl. Phys. Lett.*, 2023, **122**, 043505.

14 S. Abbas, D. K. Ban and J. Kim, *Sensors Actuators, A Phys.*, 2019, **293**, 215–221.

15 J. Jiang, J. Huang, Z. Ye, S. Ruan and Y. J. Zeng, *Adv. Mater. Interfaces*, 2020, **7**, 2000882.