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

A high-performance organic-inorganic self-powered broadband photodetector based on PANI/Bi_2O_2S nanocomposites

Bingwei Li [a,1], Kai Wang [b,1], Nanyin Zhao [a], Zhentao Fu [a], Mingtao Wang [a], Zhuoqiao Xie [a], Jun Li [a*]

a. Hunan Provincial Key Laboratory of Micro-Nano Energy Materials and Devices and School of Physics and Optoelectronics, Xiangtan University, Hunan 411105, P R China

b. Key Laboratory of MEMS of the Ministry of Education Southeast University Nanjing 210096, China

[1] These authors contributed equally to this work.

[*] Corresponding author. E-mail addresses: lijun@xtu.edu.cn

Theoretical calculation

In this paper, the Density Functional Theory (DFT) calculations were performed by the Vienna Ab-initio Simulation Package (VASP).[1, 2] Also, The Bi_2O_2S was optimized with a less than 0.01 eV atom-1 residual force on per atom. For the exchange-correlation potentials, we adopted Perdew-Burke-Ernzerhof (PBE) within the Generalized Gradient Approximation (GGA).[3] The energy cutoff was 500 eV, and the Brillouin zone integration was performed using a k-point grid of (16×16×16). After optimization, the lattice constants of Bi_2O_2S are 3.85 Å along the x and y directions and 12.06 Å along the z direction. The Bi-O and Bi-Bi bond lengths are 2.319 Å and 3.444 Å, respectively.

Table S1 Responsivity in different wavelength

Wavelength Concentration	Power Density	Photocurrent Density	Responsivity
350nm	100 μW/cm^2	2.95 μA/cm^2	29.5 mA/W
365nm	150 μW/cm^2	1.72 μA/cm^2	11.5mA/W
546nm	100 μW/cm^2	1.15 μA /cm^2	11.5mA/W
630nm	150 μW/cm^2	1.00 μA/cm^2	6.0mA/W
660nm	170 μW/cm^2	0.78 μA/cm^2	4.6mA/W
700nm	110 μW/cm^2	0.58 μA/cm^2	5.3mA/W
760nm	90 μW/cm^2	0.15μA /cm^2	1.7mA/W

Calculated by formula:

$$R=Ip / PS$$

(Where R is the photoresponsivity, Ip is the photocurrent, P and S is the Power density and Irradiation area, respectively)

Table S2 Performance comparison

Material	Electrolyte Concentration	Responsivity	Photoresponse Time (s)	Potential (V)	Ref.
This work	0.5M, KOH	29.5 mA/W	0.1	0	
Bi QDs	0.1M KOH	8.64 μA/W	0.2	0.6	[4]
$SnSe_2/WSe_2$	0.5M KOH	1.03 mA/W	0.05	0.6	[5]
InSe NSs	0.3M KOH	10.14 mA/W	0.002	0	[6]
Ga_2O_3	0.5M Na_2SO_4	3.81 mA/W	0.5	0	[7]
GeH NSs	0.5M Na_2SO_4	24 μA/W	0.24	0	[8]
Sb NSs	0.5M KOH	1.5μA/W	1	0.6	[9]
GeSe NSs	0.5M H_2SO_4	0.16μA/W	0.855	-0.3	[10]

The charge transfer mechanism can be explained by the following equation:

$$h^+ + OH^- \rightarrow OH\cdot \qquad (1)$$

$$e^- + OH\cdot \rightarrow OH^- \qquad (2)$$

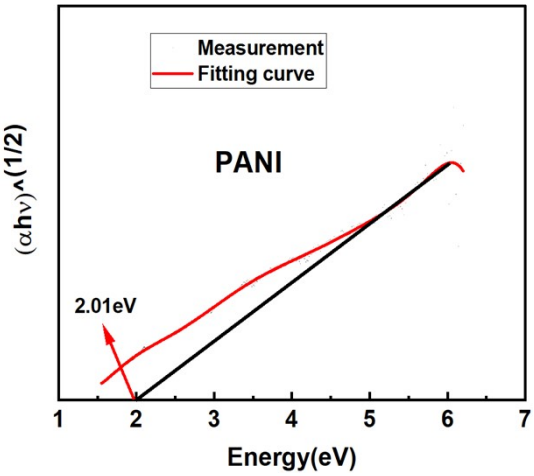

Figure S1 Theoretical prediction of the band structure of Bi_2O_2S.

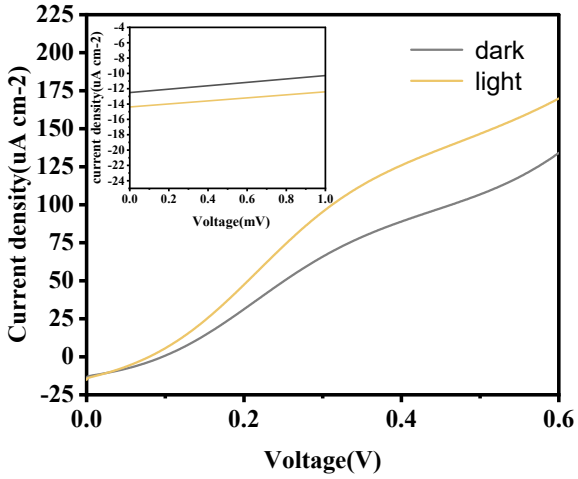

Figure S2 Linear Sweep Voltammetry (LSV) characteristic curves of PANI/Bi_2O_2S under dark and light conditions.

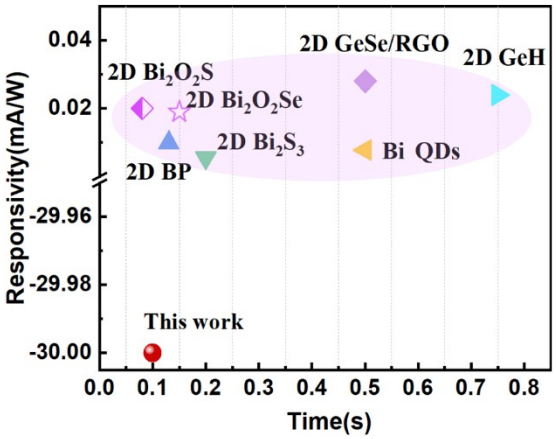

Figure S3 Performance comparison between different semiconductor materials.

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