Electronic supplementary information

A graphene-Mo₂C heterostructure for a highly responsive broadband

photodetector

Xiaozhi Bao,^a Tian Sun,^b Yan Liu,^b Chuan Xu,^c Weiliang Ma,^b Junpo Guo,^a Yun Zheng,^a Shivananju Bannur Nanjunda,^d Huating Liu,^e Zongyu Huang,^e Shaojuan Li,^{b,f} Shenghuang Lin,^g Guichuan Xing,^a Wencai Ren,^{c,*} Qiaoliang Bao,^{b,*} Huaiyu Shao^{a,*}

^a Guangdong-Hong Kong-Macau Joint Laboratory for Photonic-Thermal- Electrical Energy Materials and Devices, Institute of Applied Physics and Materials Engineering, University of Macau, Avenida da Universidade, Taipa, Macao SAR 999078, China.

^b Institute of Functional Nano and Soft Materials (FUNSOM), Soochow University, Suzhou 215123, P. R. China

^c Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, Shenyang 110016, P. R. China

^d Department of Electrical Engineering, Centre of Excellence in Biochemical Sensing and Imaging Technologies (Cen-Bio-SIM), Indian Institute of Technology Madras, Chennai 600036, India

^e Hunan Key Laboratory for Micro-Nano Energy Materials and Devices, School of Physics and Optoelectronic, Xiangtan University, Hunan 411105, China

^f State Key Laboratory of Applied Optics, Changchun Institute of Optics, Fine Mechanics and Physics, Chinese Academy of Sciences, Changchun, Jilin, 130033, China

^g Songshan Lake Materials Laboratory, Dongguan 523808, China

Corresponding authors: Huaiyu Shao (E-mail: hshao@um.edu.mo) or Wencai Ren (wcren@imr.ac.cn) or Qiaoliang Bao (E-mail: qiaoliang.bao@gmail.com)

Heterostructure	Condition	Responsivity	Response	wavelength	Ref.
		AW^{-1}	time		
Graphene-Cu _{3-x} P	$V_{sd} = 1 V$		540 ms	405-1550 nm	1
	405 nm	$1.59 \times 10^5 \text{AW}^{-1}$			
Graphene-Au NRs	$V_{sd} = 1 V$				2
	1300nm	$4 \times 10^4 \text{ AW}^{-1}$	8200 ms	400-1310 nm	
Graphene-MoTe ₂	$V_{sd} = 1 V$	972 AW ⁻¹	78 ms	532-1064 nm	3
	1064 nm				
Perovskite-organic	$V_{sd} = -0.1 V$	0.43 AW ⁻¹	56 ns	300-1000 nm	4
	720 nm				
Graphene-Mo ₂ C	V _{sd} =1 V				This
	405 nm	9381.4 AW ⁻¹	5.4 ms	405-1550	work

Table S1. Comparison between graphene- Mo_2C device and other similar devicesbased on graphene or other composite materials.

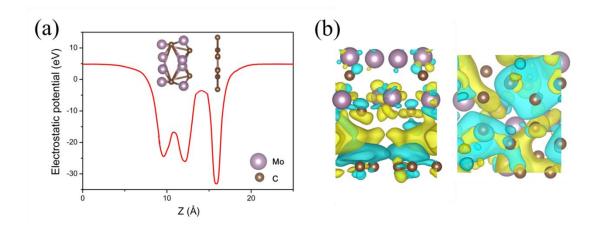


Figure S1. a) Effective electrostatic potential profile of graphene- Mo_2C heterostructure. The corresponding structure diagram is shown in the illustration. b) Side view and top view of charge density difference for graphene- Mo_2C heterostructure. The blue areas indicate the depletion of electrons and yellow areas indicate the accumulation of electrons.

Computing method:

The first-principles calculation method based on density functional theory is adopted, and the whole calculation process is performed in Vienna ab initio simulation package (VASP). The van der Waals correction of opt-PBE is taken into account in the calculation. The plane-wave basis cutoff energy is uniformly set at 400 eV. The atomic positions were optimized until the forces on atoms were less than 10^{-2} eV Å⁻¹, and the criterion of 10^{-6} eV per unit cell was sufficiently strict to obtain during the during structural relaxation. To eliminate the spurious interaction between the periodically repeated images of the slabs, the vacuum layer was set to more than 20 Å. The 6×6×1 Monkhorst-Pack K mesh was for the geometric optimization and state calculation.

Notes and references

- T. Sun, Y. Wang, W. Yu, Y. Wang, Z. Dai, Z. Liu, B. N. Shivananju, Y. Zhang, K. Fu and B. Shabbir, *Small*, 2017, **13**, 1701881.
- 2. Z. Xia, P. Li, Y. Wang, T. Song, Q. Zhang and B. Sun, *ACS applied materials & interfaces*, 2015, **7**, 24136-24141.
- W. Yu, S. Li, Y. Zhang, W. Ma, T. Sun, J. Yuan, K. Fu and Q. Bao, *Small*, 2017, 13, 1700268.
- 4. C. Li, H. Wang, F. Wang, T. Li, M. Xu, H. Wang, Z. Wang, X. Zhan, W. Hu and L. Shen, *Light: Science & Applications*, 2020, **9**, 1-8.