Supporting Information for

Multilayered PtSe₂/pyramid-Si heterostructures array with light confinement effect for high-

performance photodetection, image sensing and light trajectory tracking applications

Mengru Ma,¹ Huahan Chen,¹ Kunnan Zhou,¹ Chao Xie,^{1*} Yi Liang,¹ Li Wang,¹ Chunyan Wu,¹ Wenhua Yang,¹ Jiawen Guo³ and Linbao Luo^{1*}

¹ School of Electronic Science and Applied Physics and Anhui Provincial Key Laboratory of Advanced Functional Materials and Devices, Hefei University of Technology, Hefei, Anhui 230009, P. R. China

² School of Physics and Engineering and Key Laboratory of Material Physics of Ministry of Education, Zhengzhou University, Zhengzhou, Henan 450052, P. R. China

* Email: chao.xie@hfut.edu.cn, luolb@hfut.edu.cn



Figure S1. Optical images of (a) the pyramid-Si microstructures array, (b) the pyramid-Si microstructures array covered with PtSe₂ films, and (c) the heterostructrure-based photodetectors array.



Figure S2. (a) High-resolution XPS spectra of (a) Pt 4f and (b) Se 3d of the PtSe₂ sample. (c) XRD pattern of the PtSe₂ sample. (d) TEM and (e) HRTEM images of the PtSe₂ sample.



Figure S3. (a) The dimeter and (b) height distribution of the pyramid-Si microstructures.



Figure S4. (a) *I-V* curves in dark, (b) dark current at zero bias, (c) *I-V* curves under 810 NIR illumination, and (d) time-dependent photoresponse under 810 NIR illumination of PtSe₂/planar-Si heterostructure, PtSe₂/pyramid-Si heterostructures with and without AlO_x passivation layer.



Figure S5. (a) The plot of $\ln I - V$ curve for estimating the diode ideality factor (*n*). (b) The plot of $\ln J - V$ curve for calculating the barrier height of the heterostructure.

Calculation of the barrier height (ϕ_{BH}) of the heterostructure: The diode properties of the heterostructure is described by thermionic emission theory of majority charge carriers over a potential zero bias barrier Φ_{BH} , from the pyramid-Si to the PtSe₂:^{S1}

$$J(T,V) = J_S(T) \left[\exp\left(\frac{eV}{nk_BT}\right) - 1 \right]$$
(1)

Where J(T, V) is the current density across the PtSe₂/pyramid-Si interface, V is the applied voltage, e is the elementary charge, $k_{\rm B}$ is the Boltzmann constant, T is the temperature, and n is the ideality factor. The saturation current density $J_{\rm S}(T)$ is defined by

$$J_{S}(T) = A^{*}T^{2}exp^{[i0]}(-\frac{e\Phi_{BH}}{k_{B}T})$$
(2)

Where A^* is the effective Richardson constant, which is 252 A/(cm²K²) for n-type Si.^{S2} $J_{\rm S}(T)$ = 3.88 10⁻⁵ mAcm⁻² is deduced from the ln*J*-*V* curve in Fig. S5(b). Therefore, based on eqn (2), the barrier height $\Phi_{\rm BH}$ is estimated to be 880.5 meV,



Figure S6. (a) Time-dependent photoresponse of the heterostructure under NIR illumination with different intensities. (b) $I_{\text{light}}/I_{\text{dark}}$ ratio of the heterostructure as a function of incident light intensity. (c) Dark current at zero bias as a function of time. (d) Analysis of the noise spectral density of the heterostructure.



Figure S7. (a) Time-dependent photoresponse of the heterostructure under light illuminations with wavelength of (a) 200 nm, (b) 1300 nm and (c) 1550 nm. (d) Absorbance spectra of PtSe₂ layer, pyramid-Si and PtSe₂/pyramid-Si heterostructure.



Figure S8. (a) *I-V* curves of all 64 device units in darkness. (b) 3D diagram of the rectification ratio for each device unit.

Supporting Information References:

- S1. C. Xie, B. Nie, L. Zeng, F.-X. Liang, M.-Z. Wang, L. Luo, M. Feng, Y. Yu, C.-Y. Wu, Y. Wu and S.-H. Yu, ACS Nano, 2014, 8, 4015–4022.
- S2. S. M. Sze and K. K. Ng, *Physics of Semiconductor Devices*, John Wiley & Sons: Hoboken, NJ, 2007..