Supporting Information

Self-powered high performance UV-Vis-NIR broadband photodetector based on β-Bi_2O_3 nanoparticles through defect engineering

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S 1. Theoretical calculation of tetragonal Bi_2O_3 crystal structure

Tetragonal Bi_2O_3 crystal structure was calculated using the projector-enhanced wave (PAW) method and based on the generalized Kohn-Sham theory,[1,2] as implemented in the Vienna ab-initio simulation package (VASP).[3-5] The atomic structure was derived from the Materials Project database.[6] 5d, 6s, and 6p electrons were selected as the valence electrons of Bi, and the 2s and 2p electrons were selected as the valence electrons of O. The PBE function and the Monkhorst-Pack k-points setting of the 9 × 9 × 15 mesh were used for geometric optimization.[7] The positions of the atom were relaxed until all the forces on the atoms were below 0.01 eV/Å, and the cut-off energy of the basis function was 400 eV. The calculated atomic structure was observed through the post-processing program VESTA.[8]

Reference

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S 2. The EDS spectrum, TEM and HRTEM images of the raw material Bi_2O_3

As shown in Fig. S1(a) EDS spectrum of the raw material Bi_2O_3, the atomic ratio of Bi to O is 25.93:74.07 (less than the stoichiometric ratio of 2:3), which can be attributed to the elemental O in the test environment. Additionally, signals for elements C, Al, Si, and Pt are also detected, which can also be attributed to the test environment. Furthermore, the morphology and structure of the raw material Bi_2O_3 were also characterized using TEM. As shown in Fig. S1(b), the raw material Bi_2O_3 is formed by agglomerates of blocks with a length of about 1.2 μm and a width of about 1.0 μm, which is consistent with the SEM analysis results. The HRTEM image (Fig. S1(c)) shows that the crystallographic planes d-spacing of the raw material Bi_2O_3 is 0.24 nm, which corresponds to the (130) plane of the monoclinic α-Bi_2O_3, which is consistent with the XRD analysis results.

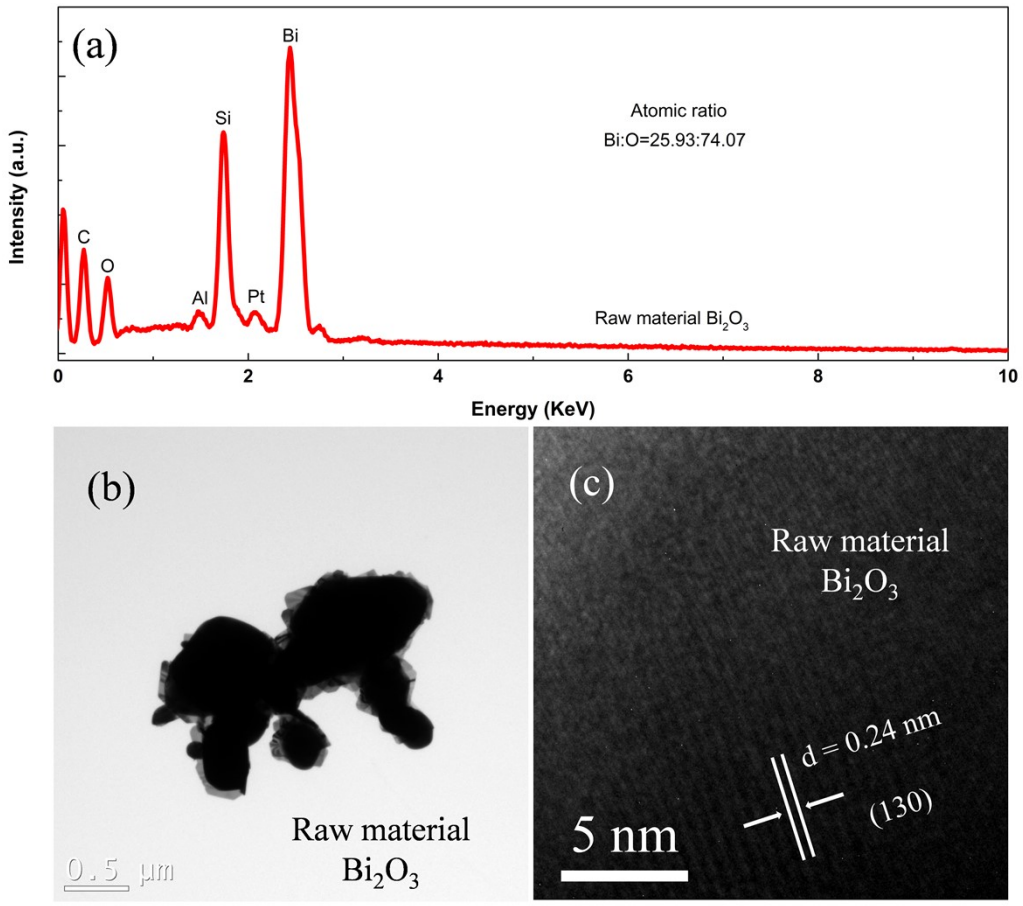

Fig. S1 EDS spectrum (a), TEM (b), and HRTEM images (c) of the raw material Bi_2O_3.

S 3. XPS spectra of raw material Bi_2O_3

From the XPS survey in Fig. S2(a), only the characteristic peaks of Bi, O, and C are observed. The characteristic peak of C can be attributed to CO_2 in the atmosphere. In the high-resolution XPS spectrum of Bi 4f (Fig. S2(b)), the raw material Bi_2O_3 also exhibits two characteristic peaks at 163.6 and 158.3 eV, which can be attributed to Bi^{3+} in Bi_2O_3. In the high-resolution XPS spectrum of O 1s (Fig. S2(c)), the raw material Bi_2O_3 also exhibits an asymmetric broad band in the range of 533 to 528 eV, which can be fitted to two peaks at 530.2 and 529.0 eV by Gaussian fitting. They can also be assigned to V_o and Bi-O, respectively, and the intensity ratio of the two peaks is 1.0.

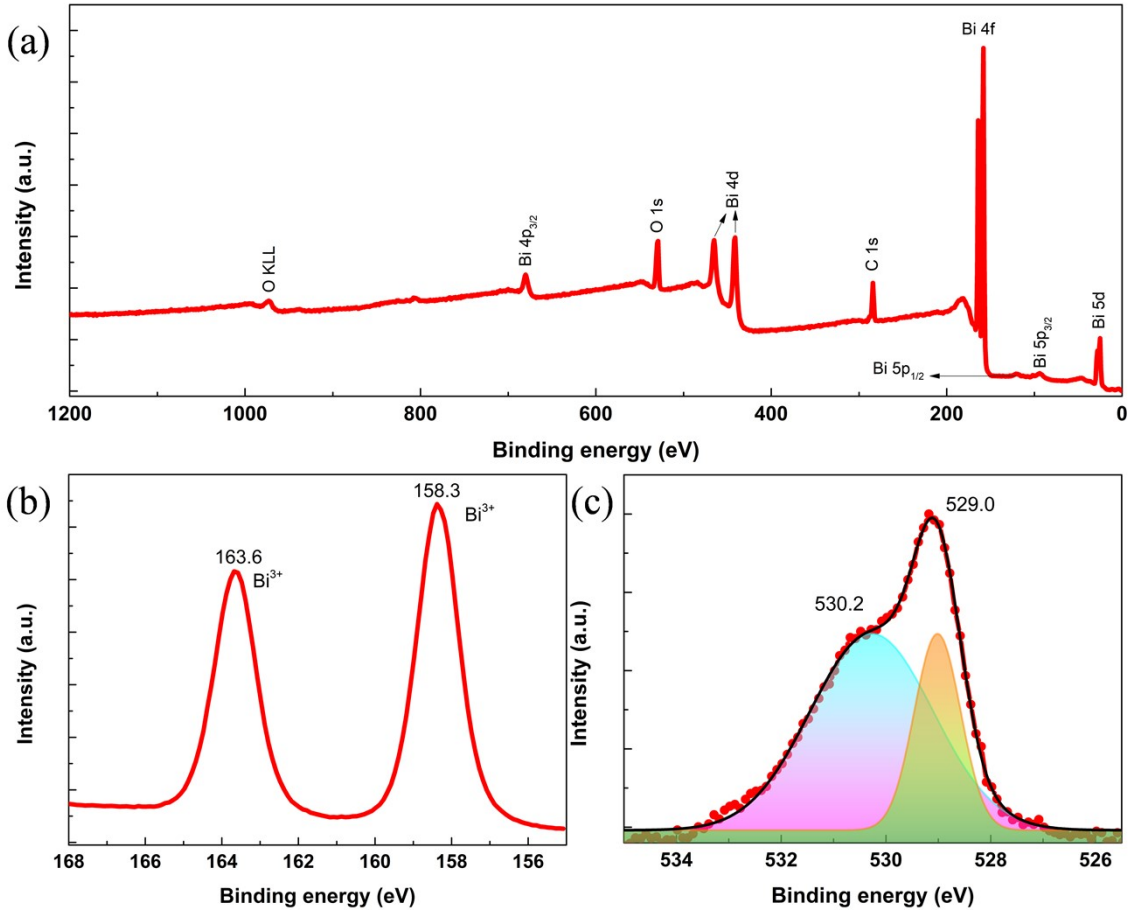

Fig. S2 XPS spectra of raw materia Bi_2O_3: (a) survey spectrum; (b) Bi 4f spectrum; (c) O 1s spectrum.

S 4. Photoresponse spectrum of bare FTO without Bi_2O_3 nanoparticles

As shown in Fig. S3, the device based on bare FTO mainly has a weak photoresponse under monochromatic light illumination with wavelength of 365 nm.

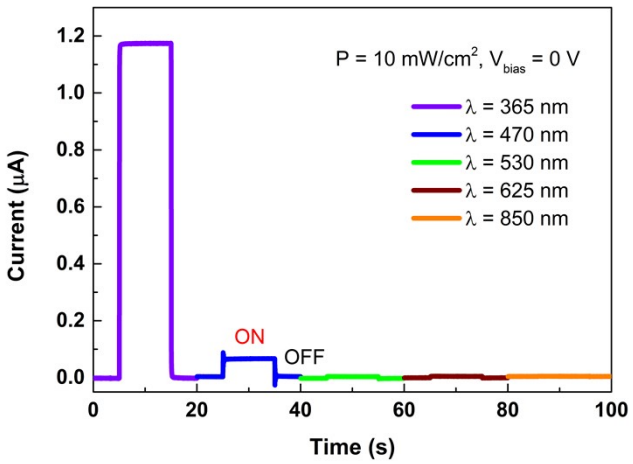

Fig. S3 Photoresponse spectra of bare FTO without Bi_2O_3 nanoparticles illuminated by various wavelengths (365, 470, 530, 625 and 850 nm) with power of 10 mW/cm^2.