

Supplementary Information for:

Low-temperature abnormal behavior of continuous photocurrent in Bi₂S₃ nanowires

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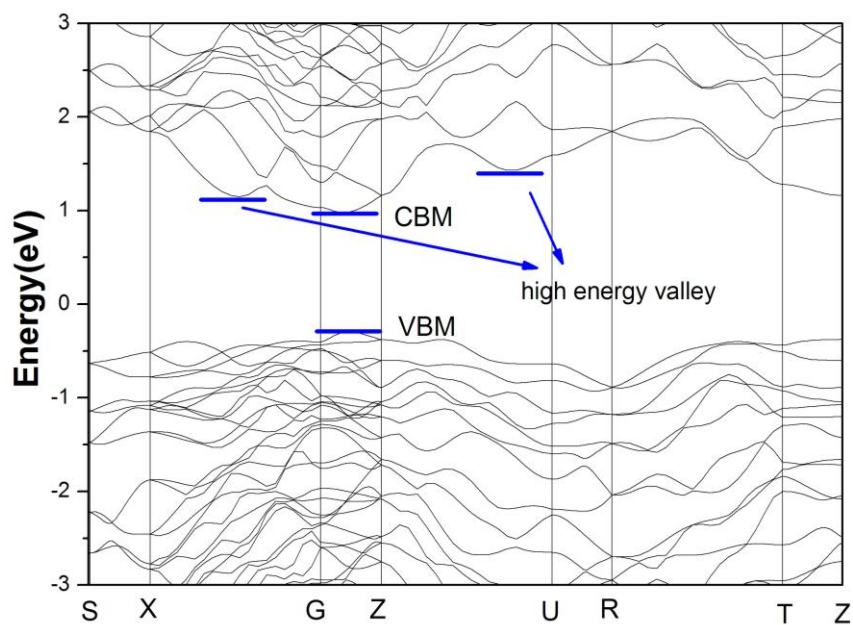


Figure S1. Band structure of calculated Bi₂S₃ NWs. The blue lines indicate the high energy valleys located in conduction band (including the bottom of conduction band).

Electronic structure calculations were performed using the Vienna ab initio simulation package (VASP).¹ The generalized gradient approximation (GGA) of Perdew, Burke, and Ernzerhof was used for the exchange and correlation potentials.² The experimental lattice constants were used for the calculation ($a = 11.305 \text{ \AA}$, $b = 11.147 \text{ \AA}$, $c = 3.981 \text{ \AA}$).³ The cutoff energy of the plane-wave basis was 500 eV, and $6 \times 6 \times 6$ k-point meshes were used for the Brillouin zone integration. The atomic relaxation was carried out until forces were less than 0.02 eV \AA^{-1} . The calculation result showed that the Bi_2S_3 had the fundamental gap and the direct band. The difference between direct and indirect gaps was about 0.05 eV. This suggested Bi_2S_3 can be seen as a nearly direct band gap of 1.24 eV.

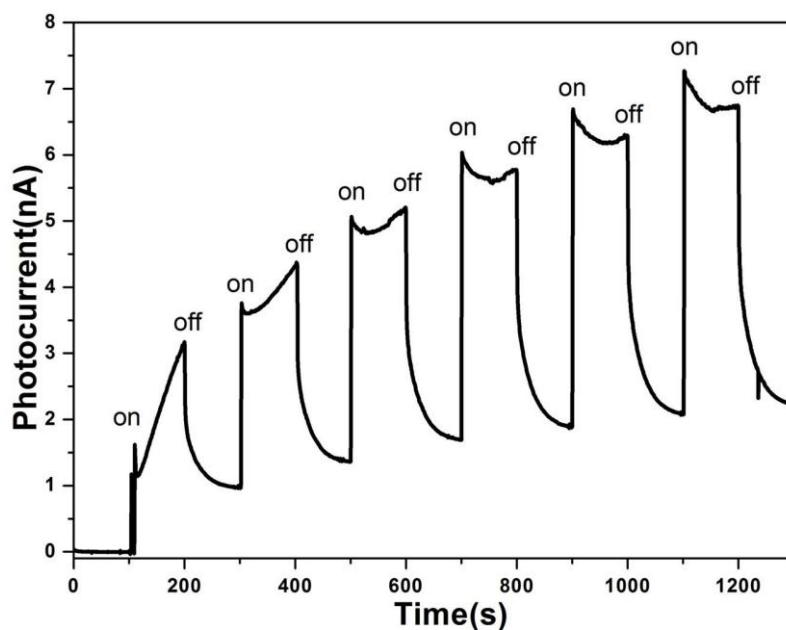


Figure S2. The first six periods of photocurrent at 50 K with an intensity of 195 mW cm^{-2} (bias voltage: 5 V). The photocurrent gradually increases to get the steady, and the abnormal behavior shows more obviously, too.

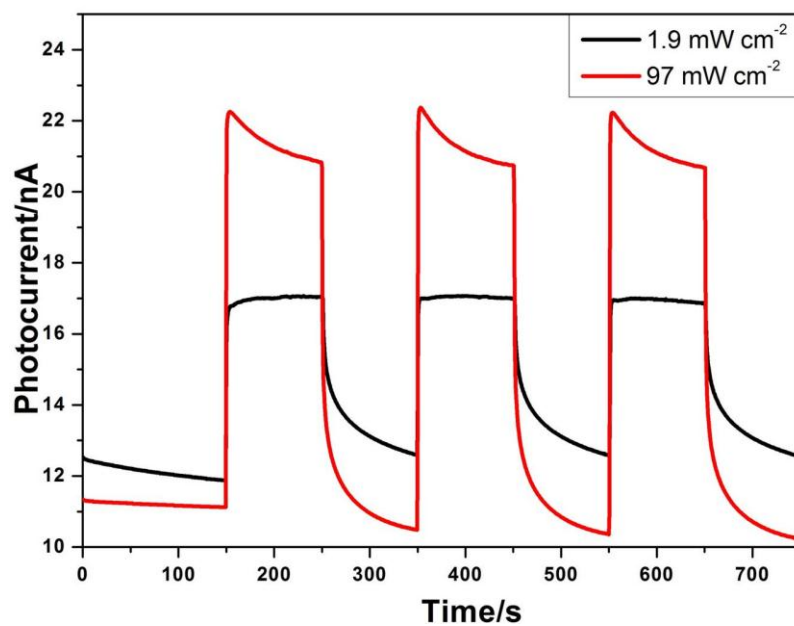


Figure S3. Photoresponsive curves measured under different laser irradiating intensity (bias voltage, 5 V; temperature, 50 K).

References:

- 1 G. Kresse and Furthmüller, *J. Phys. Rev. B*, 1996, 54, 11169.
- 2 J. P. Perdew, K. Burke and M. Ernzerhof, *Phys. Rev. Lett.*, 1996, 77, 3865.
- 3 R. Caracas and X. Gonze, *Phys. Chem. Minerals*, 2005, 32, 295.