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Supplementary Information

Optical, Electrical and Photoelectric Properties of Layered-perovskite Ferroelectric Bi_2WO_6 Crystals

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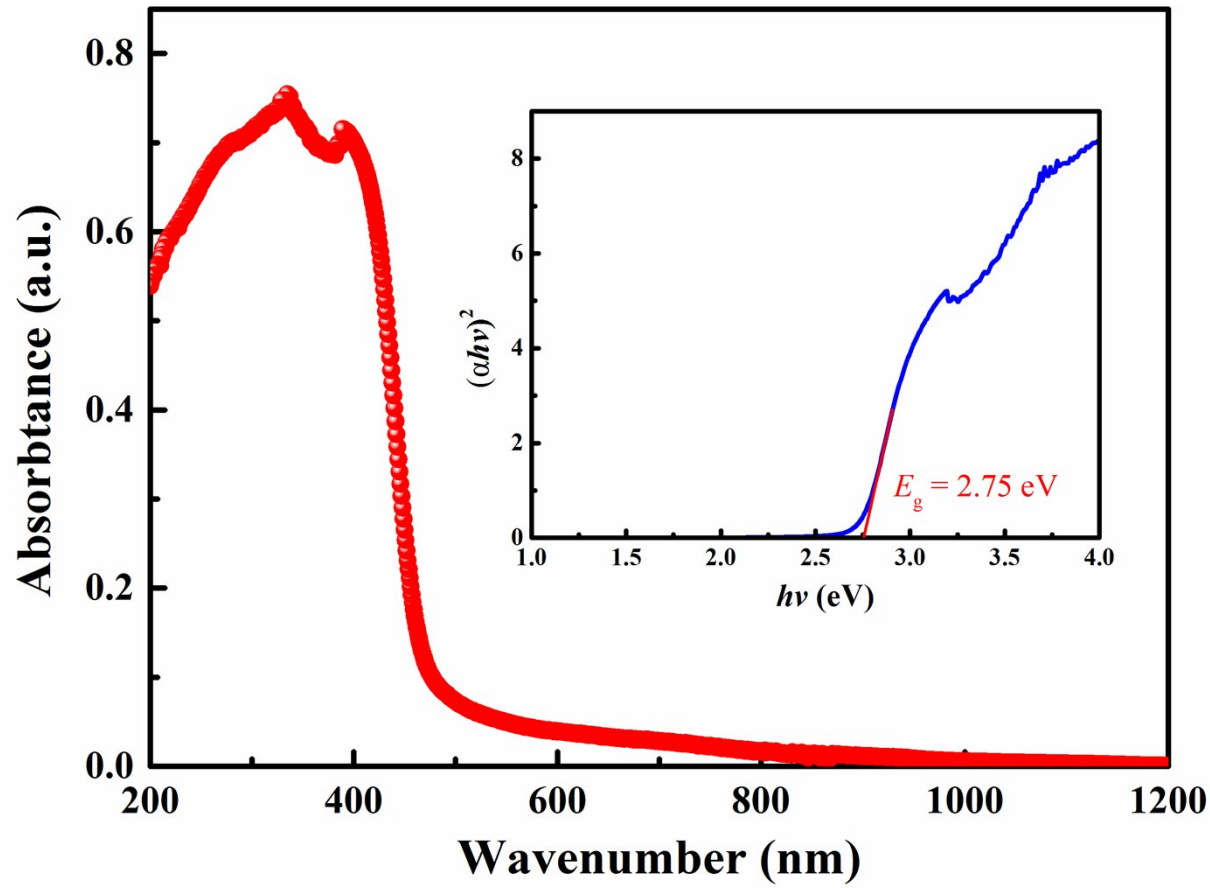

Fig. S1 The determination of the band gap for Bi_2WO_6.

Near the cut-off of the optical transmission, the band gap, the absorption and the wave frequency obey the equation:

$$\alpha hv = A(hv - Eg)^{n/2},$$

where α, v, A, and E_g are absorption coefficient, light frequency, proportionality constant, and band gap, respectively. In the equation, n decides the characteristics of the transition in a semiconductor (n=1, direct absorption; n=4, indirect absorption). The values of n and Eg were determined by the following steps: first, plot ln(αhv) vs ln(hv - Eg) using the approximate Eg value, and then determine the value of n with the slope of the straight line near the band edge; second, plot $(\alpha hv)^{1/n}$ vs hv and then obtain the band gap Eg by extrapolating the straight line to the hv axis intercept.

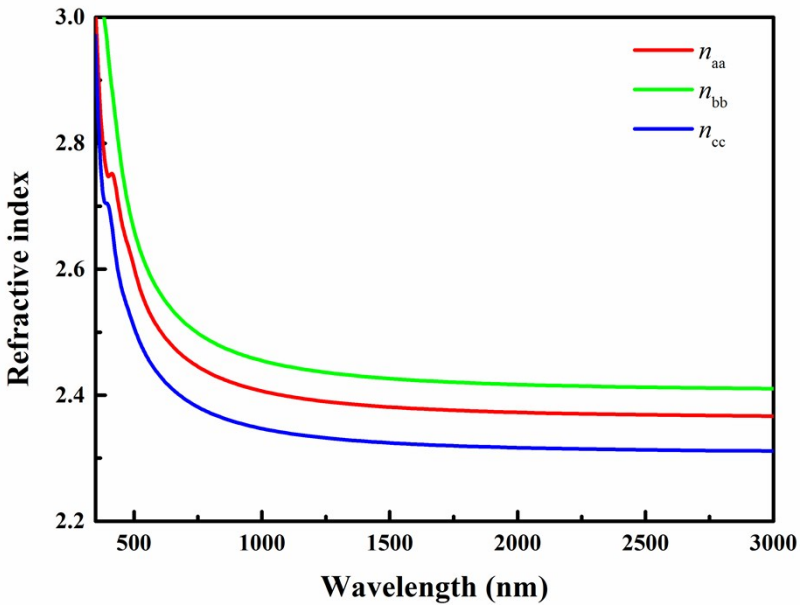

Fig. S2 Calculated refractive index of Bi_2WO_6.

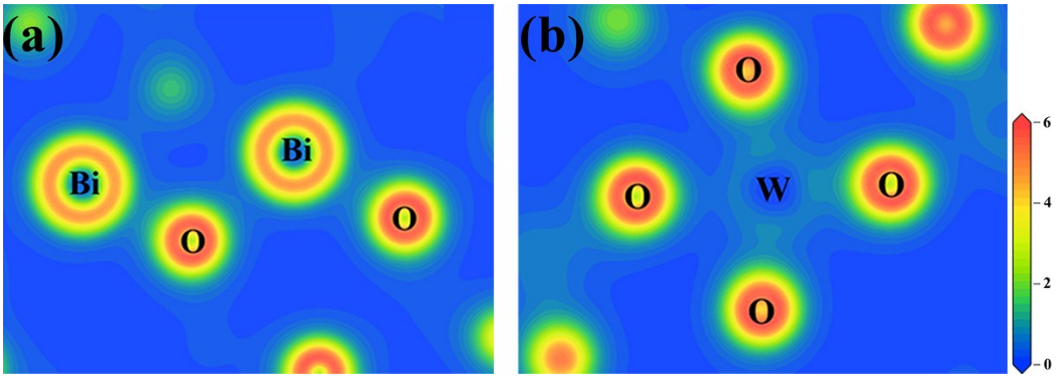

Fig. S3 Electric charge density distribution of Bi_2WO_6: (a) Bi-O and (b) W-O.

The birefringence of nonlinear optical material is a very important parameter for phase-matching range. One can see that the calculated birefringence is about 1.1-1.5 for BWO (Fig. S2). Fig. S3 shows the valence charge density around the constituent ions in BWO crystals. As we can see, the electrons around the Bi-O and W-O bonds form orbitals with strong covalent characteristics, while the charge densities located on the other cations and groups are almost spherical which lead the differences response to the incident light. The energy difference between the covalent-interaction Bi-O and W-O bond states along different directions play a crucial role in the origin of the large birefringence for the BWO crystals.