

– Supporting Information –

**Antiperovskite oxides as promising candidates for
high-performance ferroelectric photovoltaics: First-
principles investigation on Ba₄As₂O and Ba₄Sb₂O**

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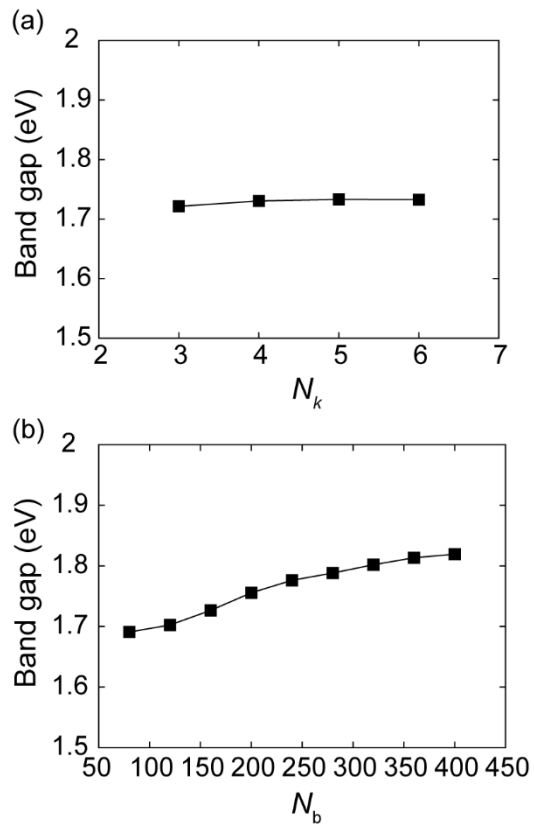


Figure S1. Convergence test of a GW band gap with respect to (a) the k-point grid ($N_k \times N_k \times N_k$) and (b) number of bands (N_b). The tested material is Ba₄As₂O.

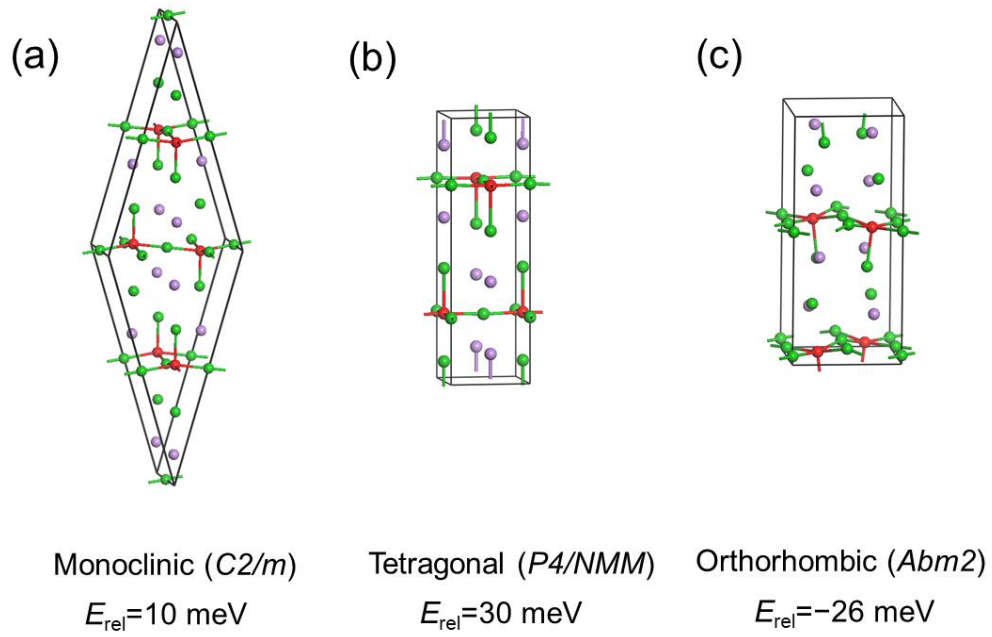
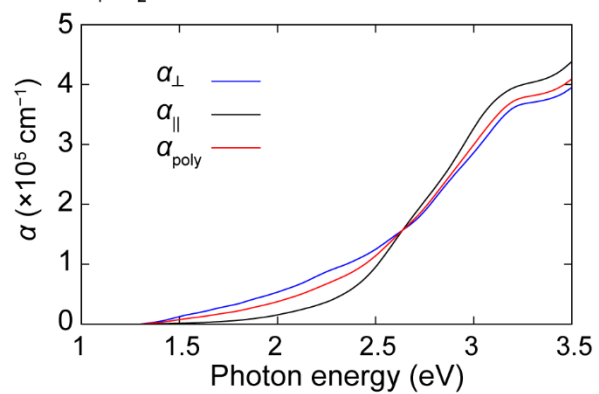


Figure S2. Possible crystal structures of $\text{Ba}_4\text{As}_2\text{O}$ characterized by (a) monoclinic, (b) tetragonal, and (c) orthorhombic lattice. E_{rel} denotes the DFT energy relative to that of the ferroelectric phase. Red, green, and purple balls indicate O, Ba, and As atoms, respectively.

(a) Ba₄As₂O



(b) Ba₄Sb₂O

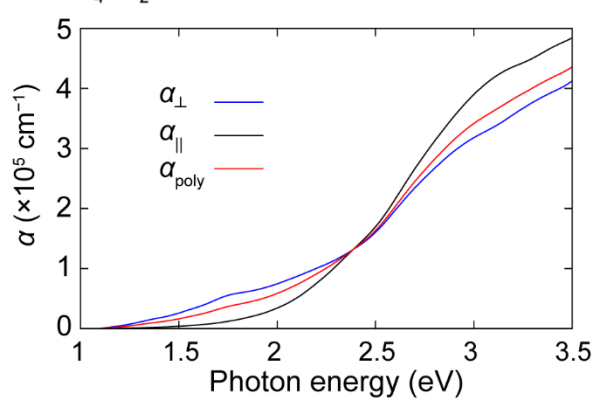


Figure S3. Anisotropy in absorption coefficients of (a) Ba₄As₂O and (b) Ba₄Sb₂O.

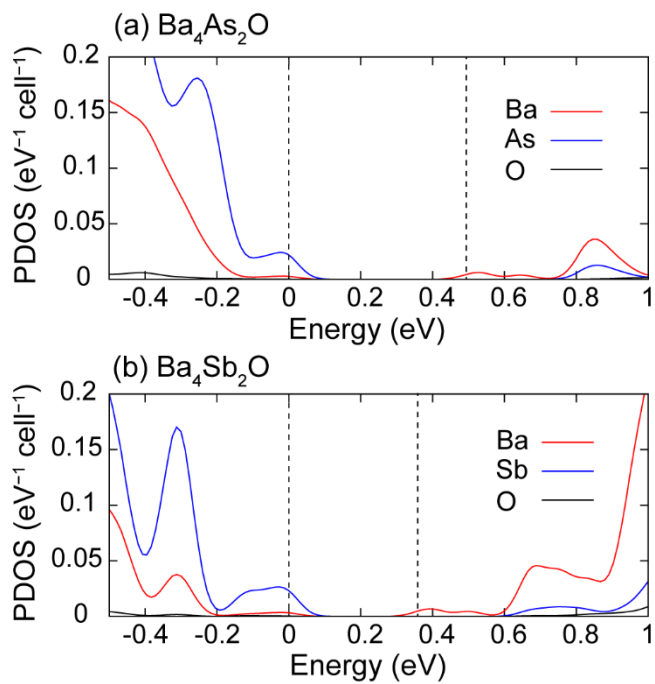


Figure S4. Atom-resolved partial density of states (PDOSs) of (a) Ba₄As₂O and (b) Ba₄Sb₂O (PBE calculations). The valence band maximum is set to 0 eV. The dashed vertical lines denote the band edge positions.

Table S1. PBE+SOC calculation results (band gap and total energy) depending on the cutoff energy (E_{cut}) and a k-point grid.

	Band gap (eV)	Total energy (eV)
$E_{\text{cut}} = 500$ eV and k-point=4x4x6	0.49	-33.07
$E_{\text{cut}} = 600$ eV and k-point=4x4x6	0.49	-33.08
$E_{\text{cut}} = 500$ eV and k-point=6x6x8	0.49	-33.07