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Refractive properties of the α-$BaGeO_3$ crystal and their origins: a density function theory study

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Table S1 Convergence test for the total energy of $Ba_2MgGe_2O_7$ with respect to the *Γ*-centered *k*-point grid (The energy cutoff is fixed at 900 eV)

k-point	total energy (eV)
1 × 1 × 1	−12465.43013
1 × 1 × 2	−12465.56520
2 × 2 × 3	−12465.37235
3 × 3 × 4	−12465.37167

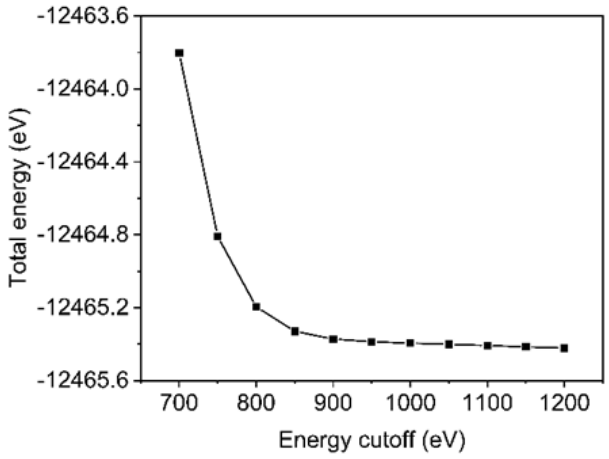

Fig. S1 Convergence test for the total energy of $Ba_2MgGe_2O_7$ with respect to the energy cutoff (The *Γ*-centered *k*-point grid is fixed at 2 × 2 × 3).

Table S1 and Fig. S1 present the results of convergence tests for the total energy of $Ba_2MgGe_2O_7$ with respect to the *Γ*-centered *k*-point grid and the energy cutoff, respectively. The results show that an energy cutoff of 900 eV and a *Γ*-centered *k*-point grid of 2 × 2 × 3 are sufficient to yield a converged total energy.

Table S2 Convergence test for the total energy of α-$BaGeO_3$ with respect to the *Γ*-centered *k*-point grid (The energy cutoff is fixed at 800 eV)

k-point	total energy (eV)
1 × 1 × 1	−12600.76069
2 × 2 × 2	−12600.97733
3 × 3 × 3	−12600.97682

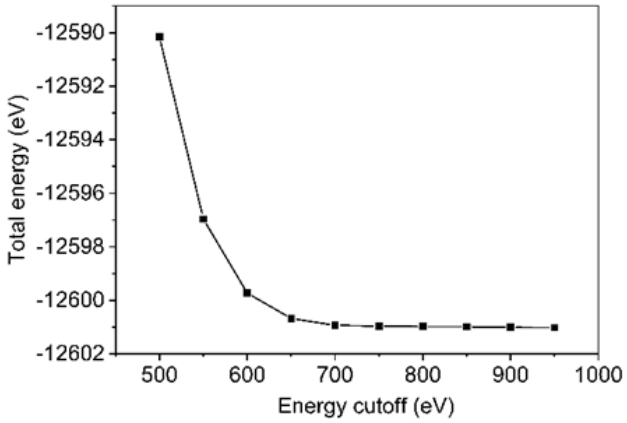

Fig. S2 Convergence test for the total energy of α-$BaGeO_3$ with respect to the energy cutoff (The *Γ*-centered *k*-point grid is fixed at 2 × 2 × 2).

Table S2 and Fig. S2 present the results of convergence tests for the total energy of α-$BaGeO_3$ with respect to the *Γ*-centered *k*-point grid and the energy cutoff, respectively. The results show that an energy cutoff of 800 eV and a *Γ*-centered *k*-point grid of 2 × 2 × 2 are sufficient to yield a converged total energy.

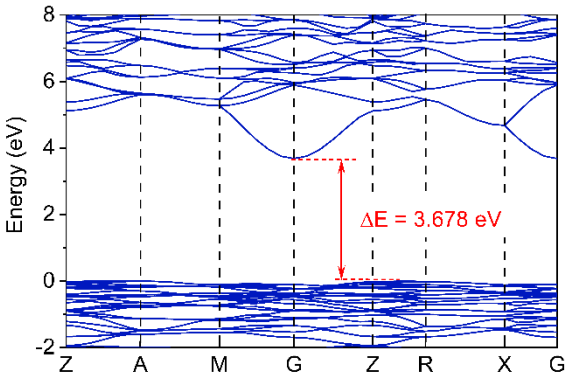

Fig. S3 Calculated band structure of $Ba_2MgGe_2O_7$.

Fig. S3 presents the calculated band structure of $Ba_2MgGe_2O_7$. The crystal is an indirect band material with a calculated band gap of 3.678 eV. As compared with the experimental band gap of 5.124 eV, a scissors operator of 1.446 eV was used to compensate the underestimation of the band gap on the $Ba_2MgGe_2O_7$ optical properties.

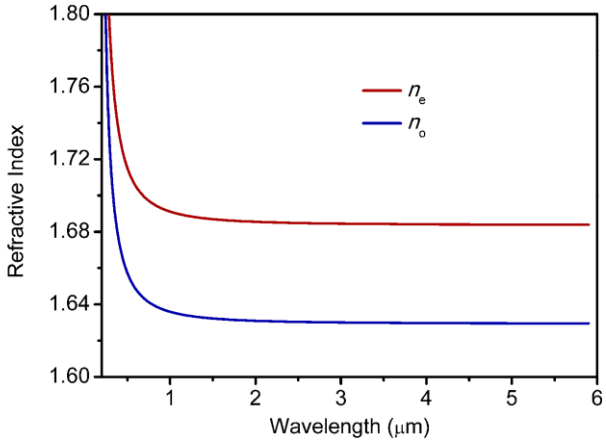

Fig. S4 Calculated refractive dispersion curves of α-$BaGeO_3$ when a light beam propagates along the crystallographic *a* axis with the polarized directions perpendicular/parallel to the *ac* crystallographic plane.

Fig. S4 presents n_o and n_e of α-$BaGeO_3$ as a function of wavelength when a light beam propagates along the crystallographic *a* axis, which reveals that calculated refractive index and birefringence are almost invariable with the wavelength in the mid-IR region.