Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Linear π-conjugated units of the $D_{\infty h}$ point group as superior ultraviolet birefringent units

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Calculations detials

The electronic structures and optical properties were obtained on the basis of ab initio calculations implemented in the CASTEP package through density functional theory (DFT).[1] The generalized gradient approximation (GGA)[2] was adopted, and Perdew-Burke-Ernzerhof (PBE)[3] functional was chosen to calculate the exchange-correlation potential, with an energy cutoff of 750 eV. The numerical integration of the Brillouin zone was performed using a 3 × 3 × 2 Monkhorst-Pack *k*-point sampling. Norm-conserving pseudopotentials were used with the following valence electron configurations: Li-$2s^1$,Na-$2s^22p^63s^1$, Si-$3s^23p^2$, C-$2s^22p^2$, N-$2s^22p^3$, B-$2s^22p^1$, O-$2s^22p^4$ and F-$2s^22p^5$. In addition, B3LYP (Becke, three-parameter, Lee-Yang-Parr) exchange-correlation functional with the Lee-Yang-Parr correlation functional at the 6-311G basis set in Gaussian was employed to calculate the groups.

Table S1 Performances of (BO_2)- and $(BO_3)^{3-}$anions

	BO_2	BO_3
Polarizability anisotropy	9.2	8.3
HOMO-LUMO gap	14.4	7
Type of hybrid orbitals of B atom in ground state	sp	sp^2
Theoretical bond angle of O–B–O (°)	180	120

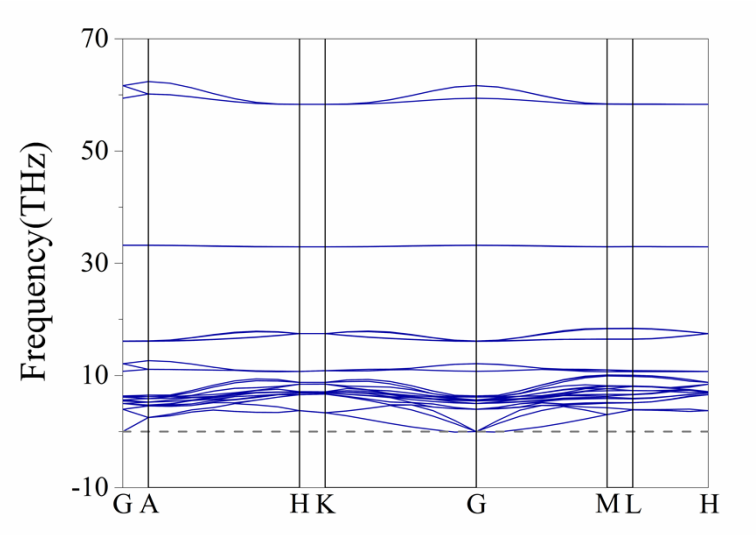

Figure S1 Calculated phonon dispersion curves of $NaBO_2$.

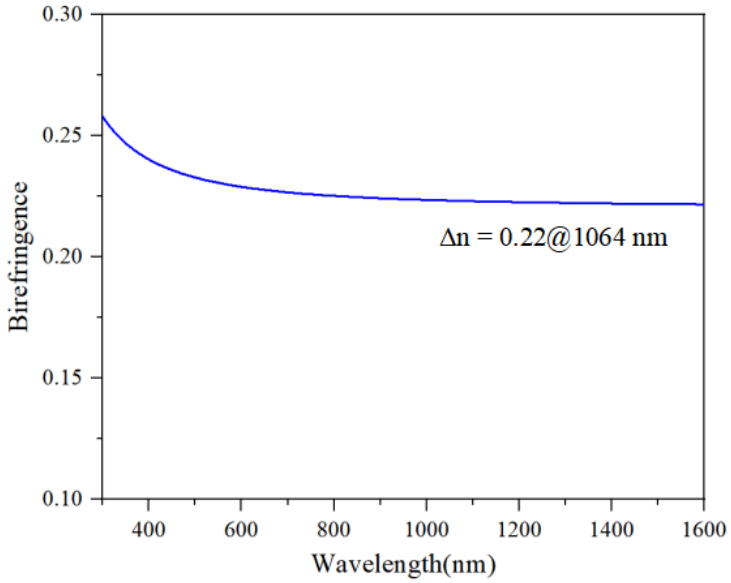

Figure S2 Calculated birefringence dispersion curves of $NaBO_2$

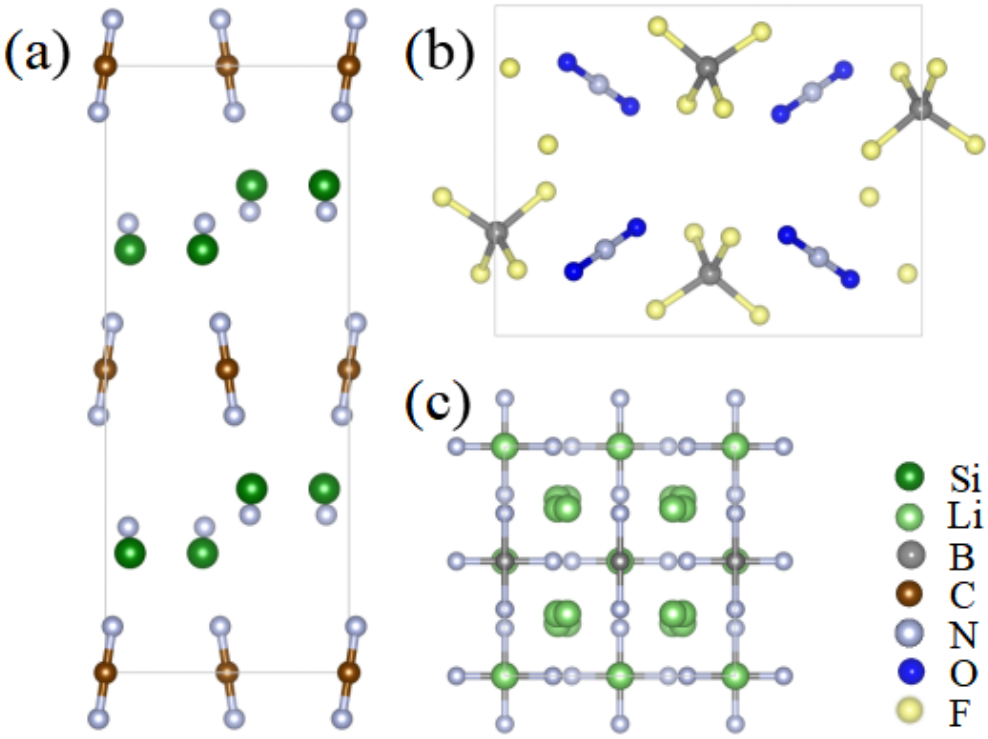

Figure S3 Crystal structure of (a) Si_2CN_4, (b) BF_4NO_2, and (c) Li_3BN_2

References

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3 Rappe, A.; Rabe, K.; Kaxiras, E.; Joannopoulos, J. D. *Phys. Rev. B* **1990**, **41**, 1227.