Electronic Supplemental Information

Straight and Twisted Open Nodal-line Phonon States in CaI_2 Family of Materials

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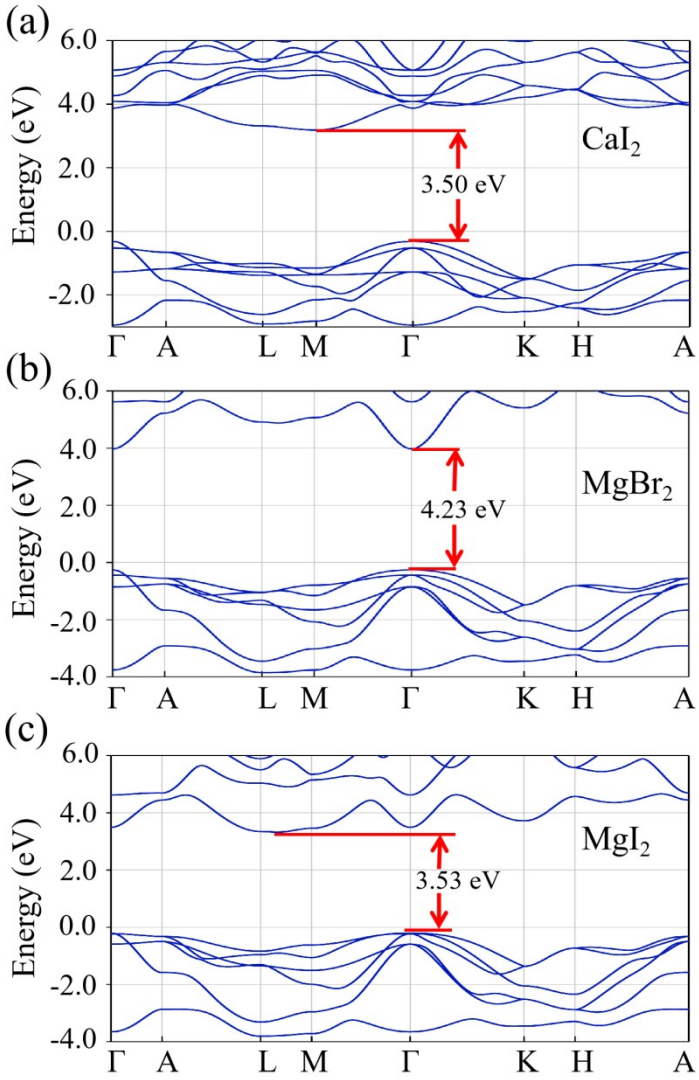

Figure S1. Band structures of CaI_2 (a), $MgBr_2$ (b) and MgI_2 (c). One can find CaI_2, $MgBr_2$ and MgI_2 are semiconductors with an indirect gap 3.50 eV, a direct gap 4.23 eV and an indirect gap 3.53 eV, respectively.

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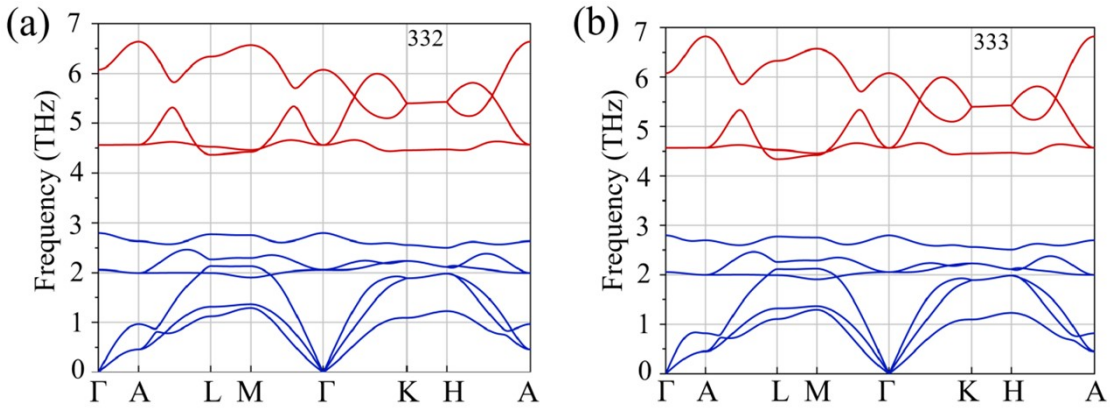

Figure S2. Phonon spectra of CaI_2 for the 3×3×2 supercell (a) and the 3×3×3 supercell (b).

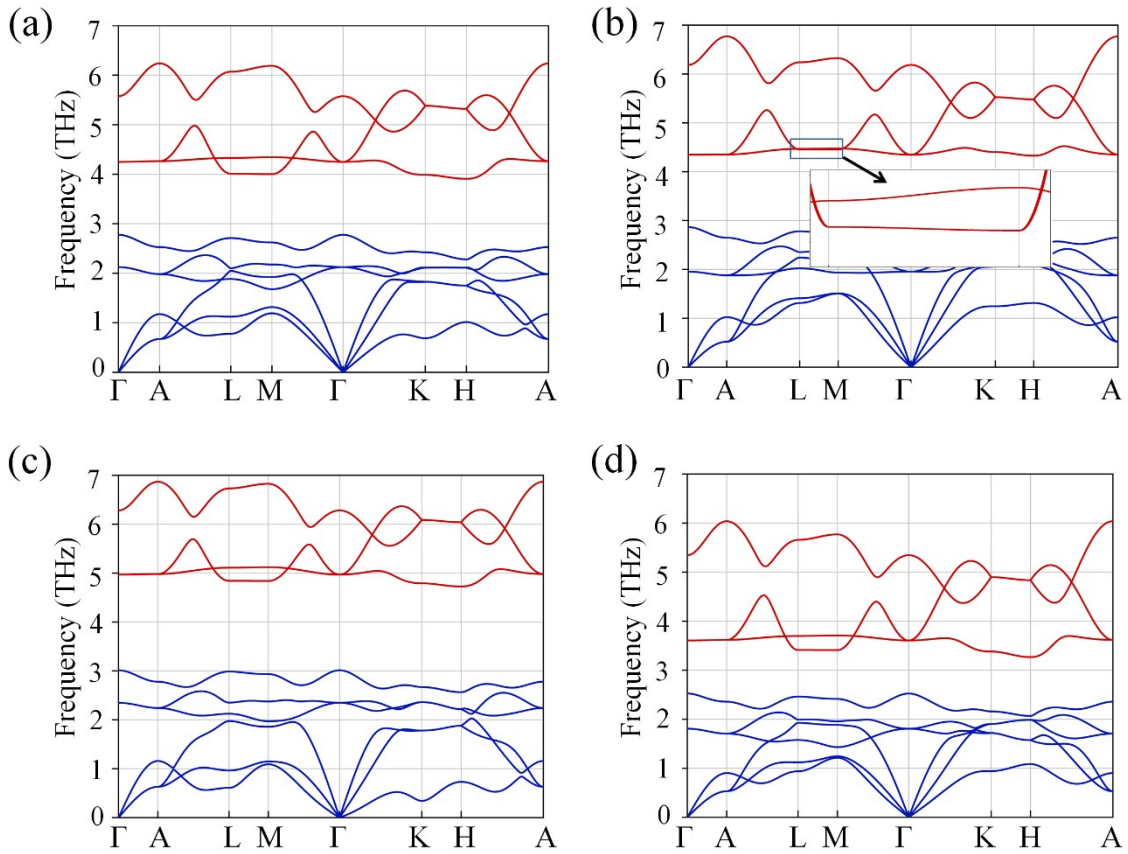

Figure S3. The computed phonon spectra of CaI_2 under -3% uniaxial strain on the *c* axis (a), +3% uniaxial strain on the *c* axis (b), -2% uniform strain (c) and + 2% uniform strain (d). The inset in (b) is an enlarge view for the rectangle.

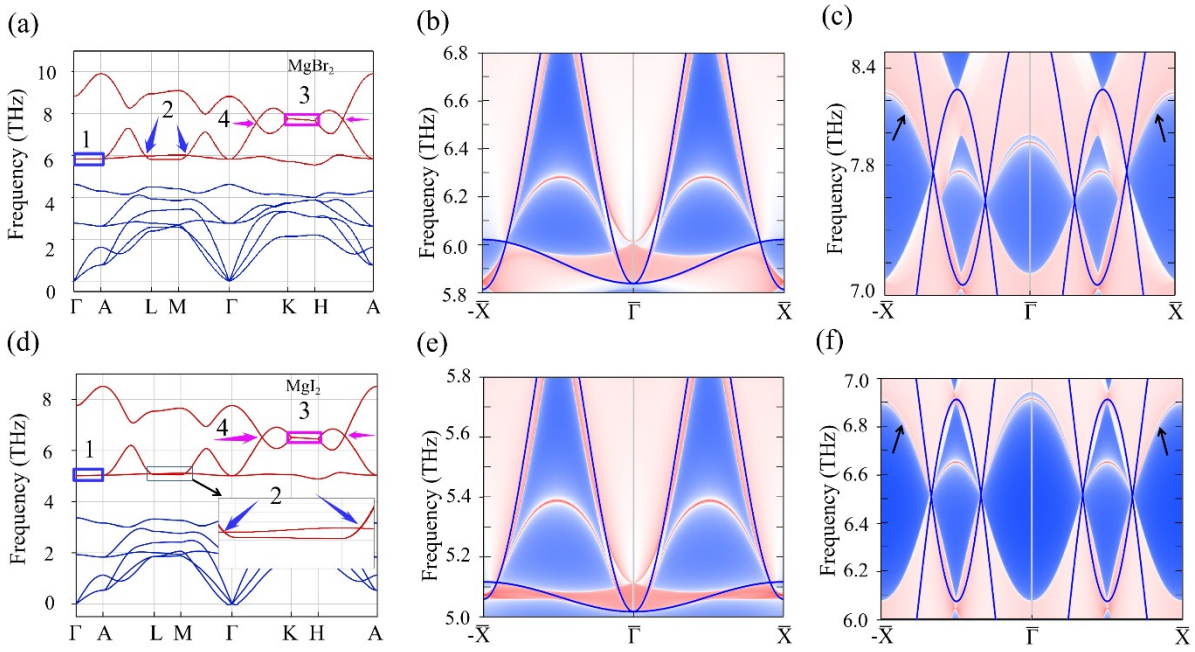

Figure S4. The calculated phonon spectra, phonon DOS and surface states for $MgBr_2$ (a-c) and MgI_2 (d-f). The numbers 1, 2, 3 and 4 indicate four sets of open PWNLs. The blue lines in (b-c) and (e-f) indicate the phonon spectra along selected high symmetry lines. The black arrows in (c) and (f) indicate the surface states connecting to the projected PWNL3.

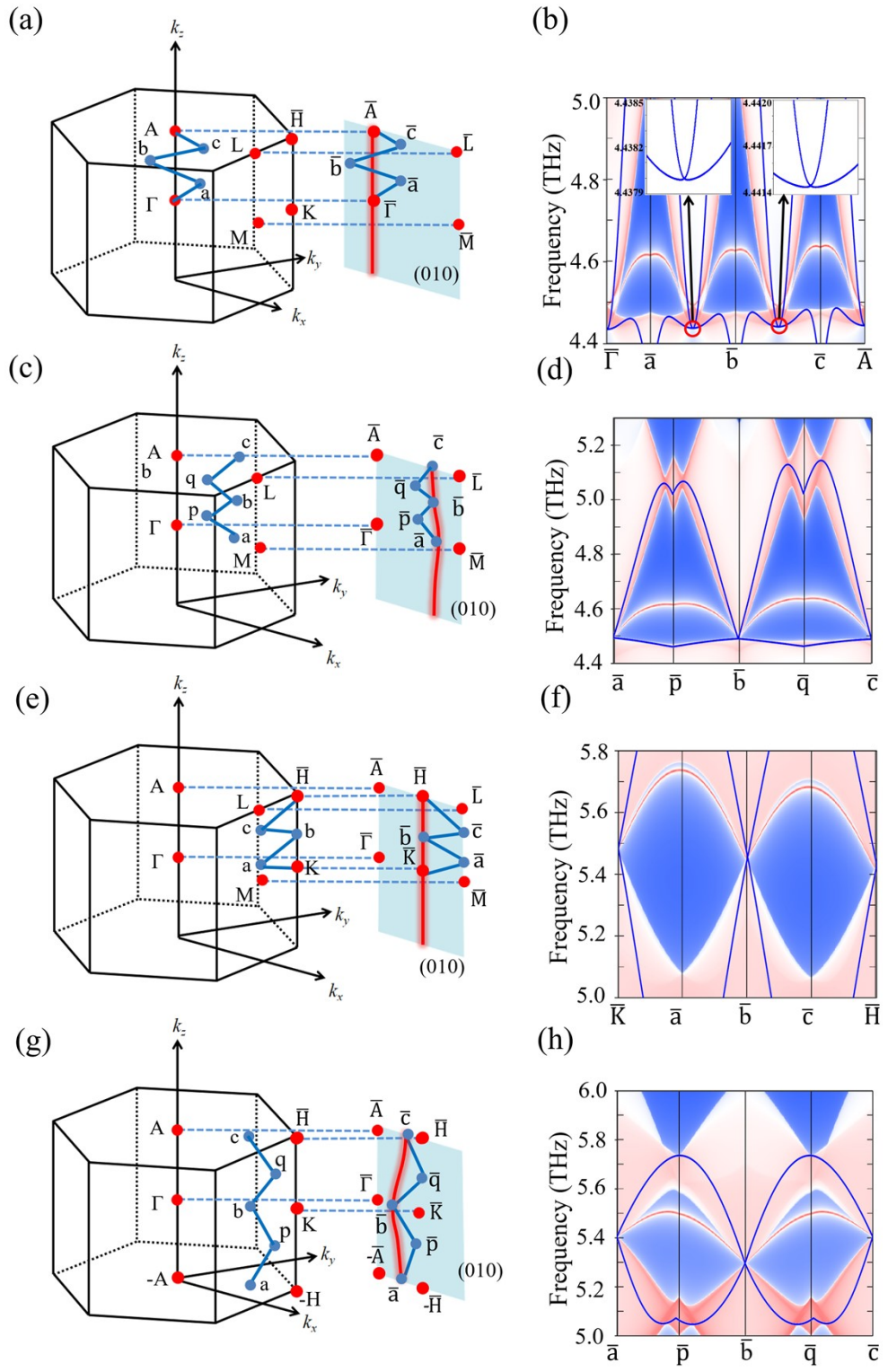

Figure S5. Bulk BZ with specific symmetry points and their projections on the (010) plane as well as the corresponding surface states along given paths for CaI_2. Figure (a-b), (c-d), (e-f) and (g-h) correspond to the open PWNL1, 2, 3 and 4 (see Figure 2(a)), respectively. The red lines in the (010)-projected plane stand for the projections of the open PWNL1, 2, 3 and 4, respectively. The solid blue lines in the surface states indicate the phonon spectra along selected routes. The insets in (b) are enlarge views of the BCPs with linear dispersions.

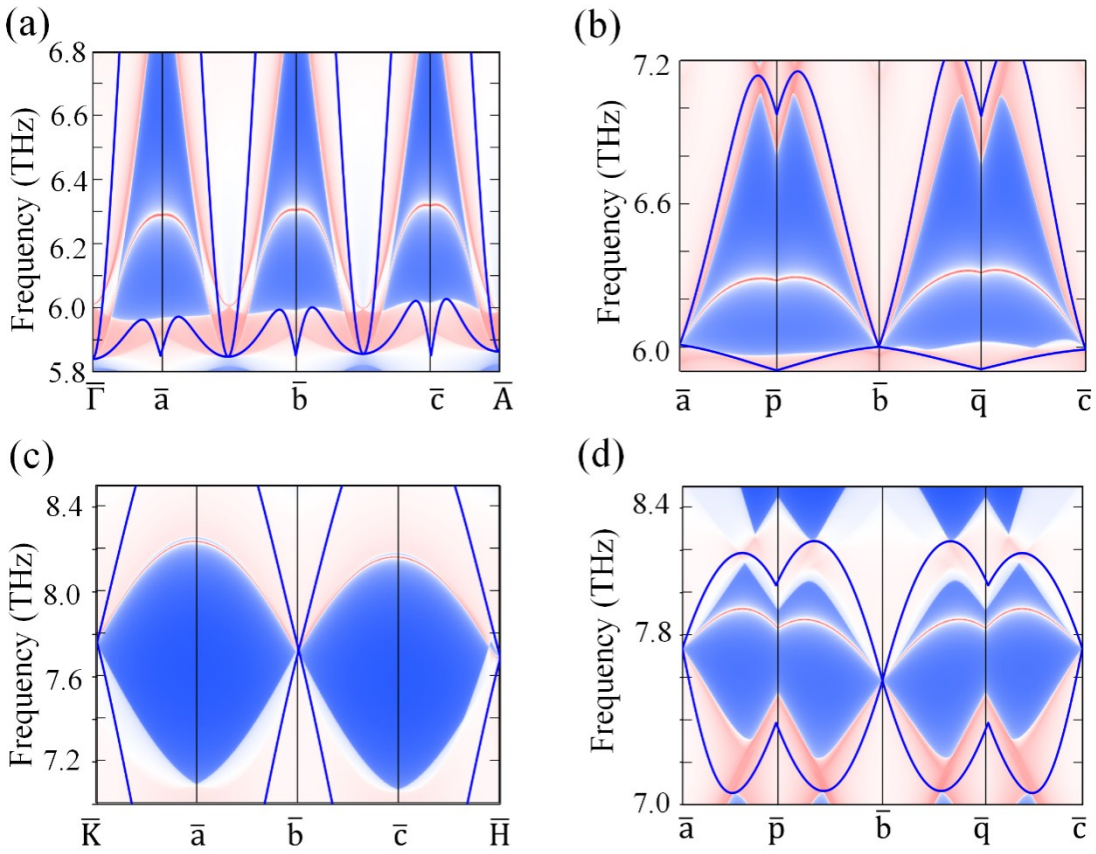

Figure S6. The calculated surface states for $MgBr_2$ along similar routes in Figure S5 for PWNL1 (a), PWNL2 (b), PWNL3 (c), and PWNL4 (d), respectively. The solid blue lines illustrate the phonon spectra along selected routes.

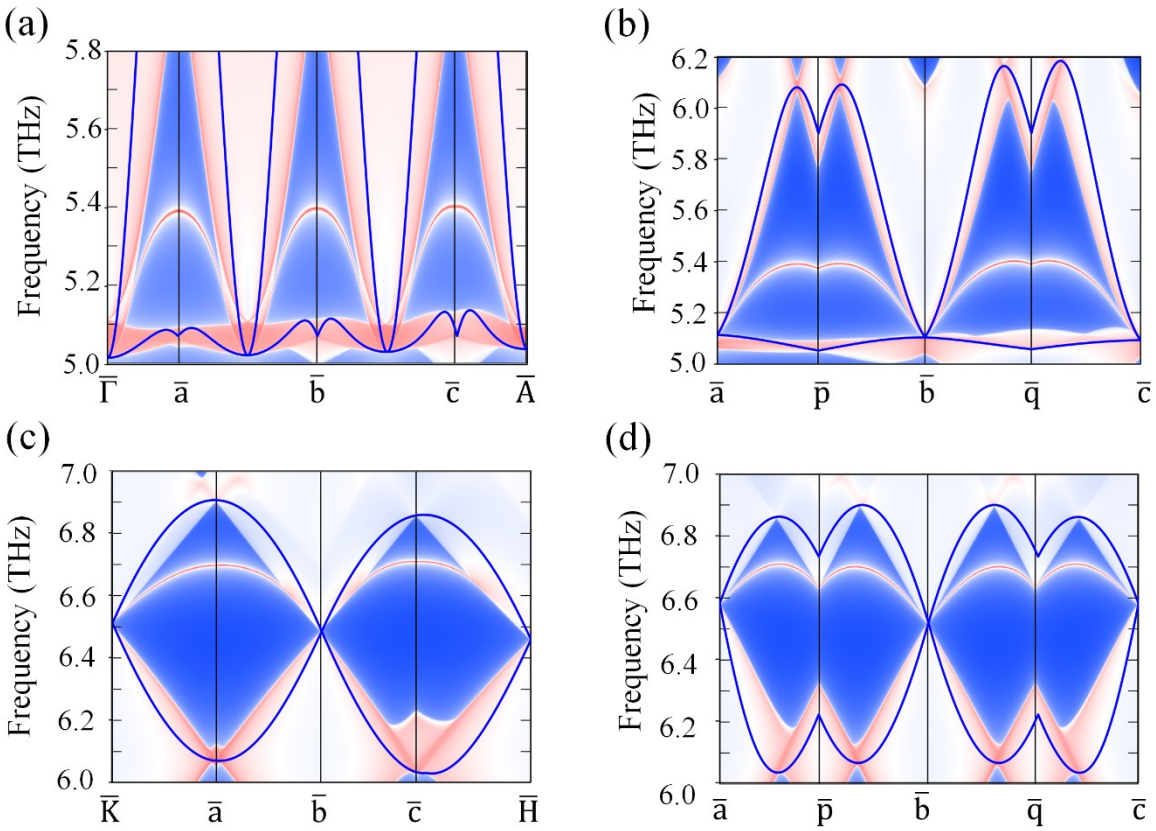

Figure S7. The calculated surface states for MgI_2 along analogous routes in Figure S5 for the open PWNL1 (a), PWNL2 (b), PWNL3 (c), and PWNL4 (d), respectively. The solid blue lines stand for the phonon spectra along selected routes.

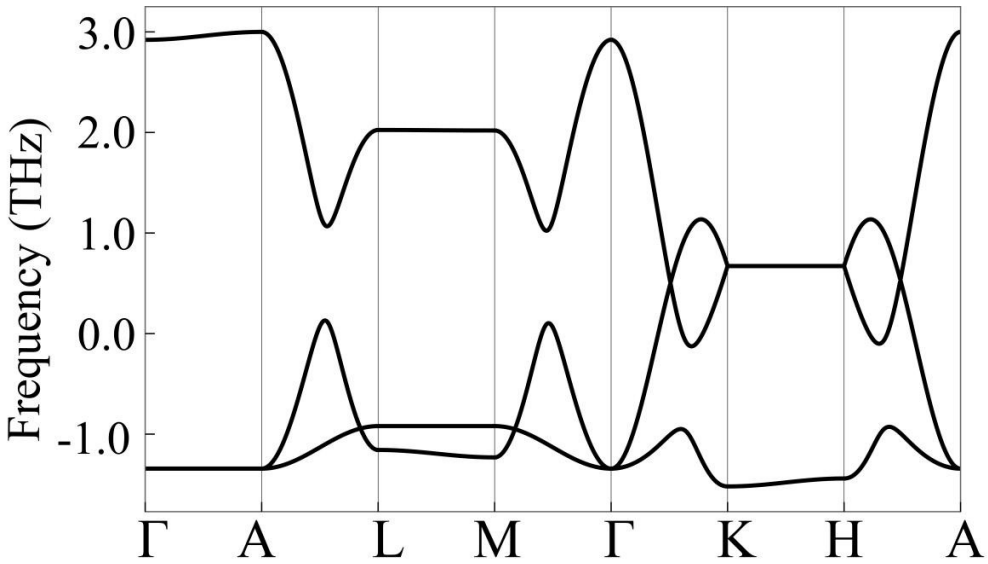

Figure S8. The calculated phonon spectra based on the phononic tight-binding model, which is consistent with the first-principles calculations results (the highlighted red lines in Figure 2 (a))

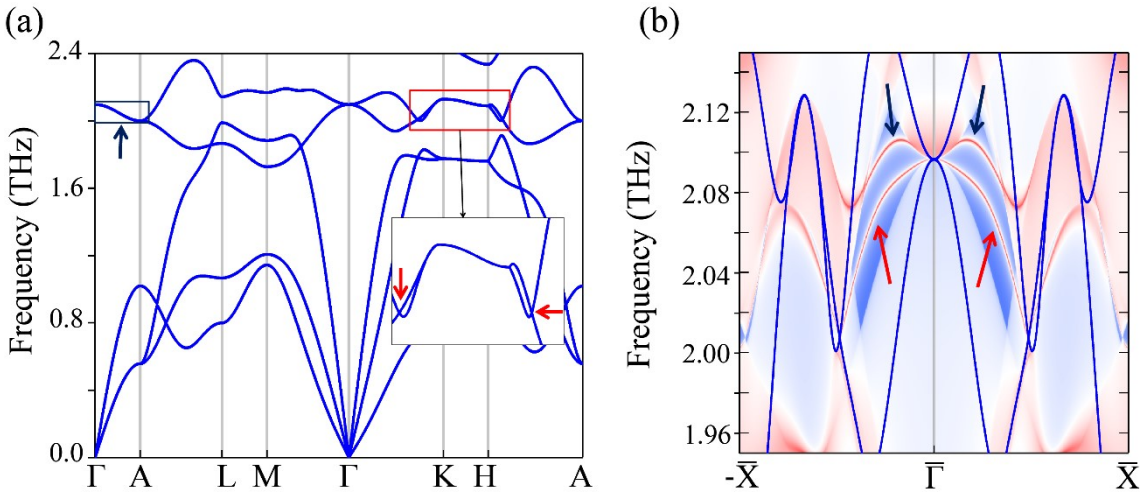

Figure S9. (a) The phonon spectra for CaI_2 in the range of 0-2.4 THz. The black rectangle and arrows indicate the PWNL along Γ-A. The inset is an enlarge view of the red rectangle where the red arrows stand for the BCPs along Γ-K and H-A. (b) The calculated surface states near 2 THz. The black arrows indicate the surface states stemming from PWNL along Γ-A. The red arrows indicate the surface states coming from the PWNL crosses Γ-K and H-A. The surface states from the PWNL along K-H are buried in the bulk states.

Table 1. The experimental and calculate lattice parameters (in units of Å) by PBE and vdW corrections.

	Experimental[1]		PBE[2]		vdW[2]	
Compound	*a*	*c*	*a*	*c*	*a*	*c*
CaI_2	4.490	6.975	4.543	7.881	4.478	7.022
$MgBr_2$	4.154	6.865	4.204	7.836	4.159	6.944
MgI_2	3.810	6.260	3.878	7.138	3.838	6.219

[1] References 1-3.

[2] Present work

Table 2. The calculated elastic constants C_{ij} (GPa), the bulk modulus B (GPa), the shear modulus G (GPa), Young's modulus E (GPa), Poisson's ratio ν and Pugh's ratio B/G for CaI_2, $MgBr_2$ and MgI_2, respectively.

Compound	C_{11}	C_{12}	C_{13}	C_{14}	C_{33}	C_{44}	B	G	E	ν	B/G
CaI_2	29.6	8.40	6.42	-1.66	15.68	3.91	12.40	6.40	16.38	0.280	1.937
$MgBr_2$	60.80	18.28	8.91	-1.56	27.30	5.90	15.78	8.70	22.04	0.267	1.814
MgI_2	45.99	13.64	5.58	-0.86	18.07	4.05	22.48	11.92	30.38	0.274	1.887

References

[1] H. Blum, Z Phys. Chem. **22**, 298-304 (1933).

[2] C. M. Widdifield, and D. L. Bryce, Phys. Chem. Chem. Phys. **11**, 7120-7122 (2009).

[3] I. W. Bassi, F. Polato, M. Calcaterra, and J. C. J. Bart, Z. Krist-Cryst. Mater. **159**, 297-302 (1982).