Supplementary Materials

Negative thermal expansion and electronic structure variation of chalcopyrite type LiGaTe$_2$

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Table S1. Fractional atomic coordinates and isotropic displacement parameters (Å$^2$) of LiGaTe$_2$

|   | x      | y      | z      | $U_{iso}$   |
|---|--------|--------|--------|-------------|
| Te | 0.26834 (18) | 3/4 | 1/8 | 0.0138 (5) |
| Ga | 0 | 0 | 1/2 | 0.0201 (11) |
| Li | 0 | 0 | 0 | 0.0126 |
Table S2. Main bond lengths (Å) of LiGaTe$_2$

| Bond        | Length (Å) | Symmetry Code |
|-------------|------------|---------------|
| Ga—Te$^i$   | 2.6086 (7) |               |
| Li—Te$^{ii}$| 2.7462 (7) |               |

Symmetry codes: (i) -y+1/2, x-1/2, -z+1/2; (ii) x, y, z.
| T, K | Space group | Cell parameters (º, Å), Cell volume (Å³) | $R_{DDM}$, $R_B$ (%) | $\chi^2$ |
|-----|-------------|------------------------------------------|---------------------|--------|
| 303 | $I-42d$     | $a = 6.33859$ (11), $c = 11.7040$ (2), $V = 470.24$ (2) | 14.64, 6.7 | 1.14   |
| 323 | $I-42d$     | $c = 11.7030$ (3), $V = 470.55$ (3) | 15.24, 7.85 | 1.21   |
| 343 | $I-42d$     | $a = 6.34095$ (16), $c = 11.7011$ (4), $V = 471.06$ (3) | 15.30, 7.90 | 1.16   |
| 363 | $I-42d$     | $c = 11.6991$ (4), $V = 471.41$ (3) | 15.60, 7.79 | 1.16   |
| 383 | $I-42d$     | $a = 6.34710$ (16), $c = 11.6979$ (4), $V = 471.74$ (3) | 15.60, 8.21 | 1.12   |
| 403 | $I-42d$     | $a = 6.35063$ (16), $c = 11.6969$ (3), $V = 471.74$ (3) | 16.17, 7.21 | 1.15   |
| 423 | $I-42d$     | $c = 11.6955$ (5), $V = 472.02$ (4) | 16.4, 8.57 | 1.10   |
| 443 | $I-42d$     | $a = 6.35603$ (16), $c = 11.6914$ (2), $V = 472.17$ (2) | 13.52, 8.17 | 1.18   |
| 463 | $I-42d$     | $c = 11.6900$ (2), $V = 472.51$ (2) | 14.25, 7.73 | 1.20   |
| 483 | $I-42d$     | $a = 6.36001$ (11), $c = 11.6875$ (2), $V = 472.51$ (2) | 13.86, 8.10 | 1.20   |
| 503 | $I-42d$     | $a = 6.3626$ (1), $c = 11.6854$ (2), $V = 473.05$ (2) | 14.00, 8.37 | 1.19   |
| 523 | $I-42d$     | $c = 11.6826$ (2), $V = 473.26$ (2) | 14.84, 7.99 | 1.22   |
| 543 | $I-42d$     | $a = 6.36473$ (12), $c = 11.6805$ (2), $V = 473.59$ (2) | 14.86, 9.01 | 1.21   |
| 563 | $I-42d$     | $a = 6.3700$ (1), $c = 11.6779$ (2), | 15.69, 8.35 | 1.23   |
\( \nu = 473.85 \) (2)
Figure S1. The diagram of vibrational mode of 75.14 cm$^{-1}$. 
Fig 2. Survey photoelectron spectrum of LiGaTe$_2$. 
Figure S3. C 1s core level.
Figure S4. O 1s band.
Figure S5. Electronic band structure of LiGaTe$_2$, calculated by PBE functional.
Figure S6. The calculated density of states of LiGaTe$_2$. (a) GGA+U, (b) GGA.
Figure S7. The calculated refractive indexes and birefringence of LiGaTe$_2$ crystal.