Electronic Supplementary Information

Investigation into the optimized growth, anisotropic properties and theoretical calculations of the polar material Cs₂TeW₃O₁₂

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1. Figure S1. Experimental and calculated powder X-ray diffraction patterns of $Cs_2TeW_3O_{12}$ polycrystalline.

2. Figure S2. (a) and (b) Photographs of the as-grown $Cs_2TeW_3O_{12}$ crystals in a narrow and large thermostatic field, respectively.

3. Figure S3. Viscosity versus temperature curves in different flux systems, where the viscosity of the TeO_2 -Cs₂CO₃ flux system is evidently lower than that of the TeO_2 flux system.

4. Figure S4. Specific heat vs. temperature for $Cs_2TeW_3O_{12}$.

5. Figure S5. The processing orientations of $Cs_2TeW_3O_{12}$ crystal for measuring the thermal diffusion and thermal conductivity coefficients.

6. Table S1. Observed Raman wavenumbers (cm⁻¹) and vibrational assignments for $Cs_2TeW_3O_{12}$ crystal.



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Figure S3. Viscosity versus temperature curves in different flux systems, where the viscosity

of the TeO₂-Cs₂CO₃ flux system is evidently lower than that of the TeO₂ flux system.



Figure 4. Specific heat vs. temperature for the Cs₂TeW₃O₁₂ crystal.



Figure S5. The processing orientations of $Cs_2TeW_3O_{12}$ crystal for measuring the thermal

diffusion and thermal conductivity coefficients.

| Raman spectra (cm ⁻¹) | Assignments |
|-----------------------------------|---|
| 146.55 (vs) | translational motions of W ⁶⁺ , Te ⁴⁺ and Cs ⁺ cations |
| 200-600 (w) | bending modes of W-O bonds, Te-O bonds, and W-O-Te bridges |
| 665.52 (s) | W-O bonds and W-O-Te bridges |
| 674.14 (s) | W-O bonds and W-O-Te bridges |
| 910.34 (vs) | stretching vibrations of the short W-O bonds |
| 937.94 (m) | stretching vibrations of the short W-O bonds |
| | |

Table S1. Observed Raman wavenumbers (cm⁻¹) and vibrational assignments for the $Cs_2TeW_3O_{12}$ crystal.¹⁻³

In the table, vs: very strong; s: strong; m: medium; w: weak;

References

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