Supplementary Information

Excellent thermoelectric properties of Tl₂S₃ monolayer for medium-temperature applications

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Figure S1. (a)-(d) Convergence of electron and hole mobilities with respect to k and q grids at room temperature. It is found that $360 \times 360 \times 1$ k grids with $180 \times 180 \times 1$ q grids ensure the convergence of electron mobility within 2%, whereas the hole mobility converges at $180 \times 180 \times 1$ k grids with $180 \times 180 \times 1$ k grids.

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Figure S2. Free energy fluctuations with respect to time in AIMD simulations at different temperatures and the structures for 2D Tl_2S_3 obtained by AIMD simulations at 300-700 K.



Figure S3. (a)-(b) The electronic band structures of novel 2D Tl_2S_3 and projected density of stat es.



Figure S4. The electronic band structures of novel 2D Tl_2S_3 are calculated by QE, the electronic band and Wannier fitted electronic band.