

Supporting Information (SI)

Physical Insights on the Ultralow Lattice Thermal Conductivity and High Thermoelectric Performance of Bulk LiMTe₂ (M=Al, Ga)

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S1. Convergence of κ_l with respect to q-grid

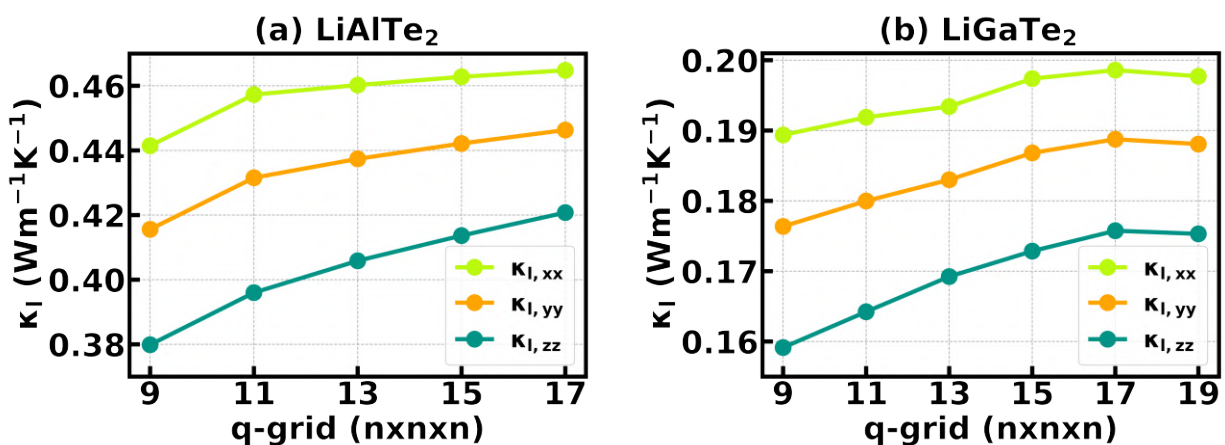


Figure S1: Convergence of κ_l at 300 K with respect to q-grid

S2. Convergence of κ_l with respect to number of nearest neighbour atoms

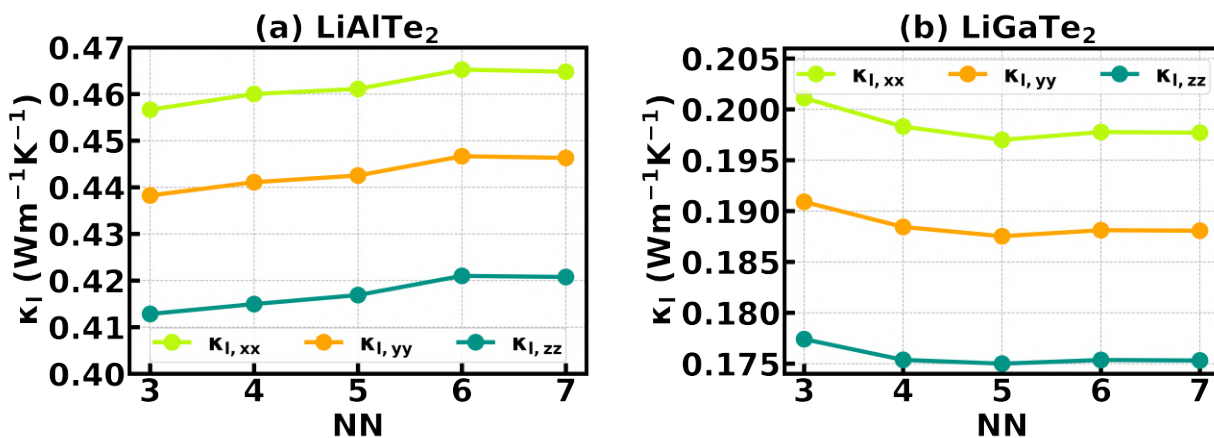


Figure S2: Convergence of κ_l at 300 K with respect to number of nearest neighbour atoms

S3. AIMD

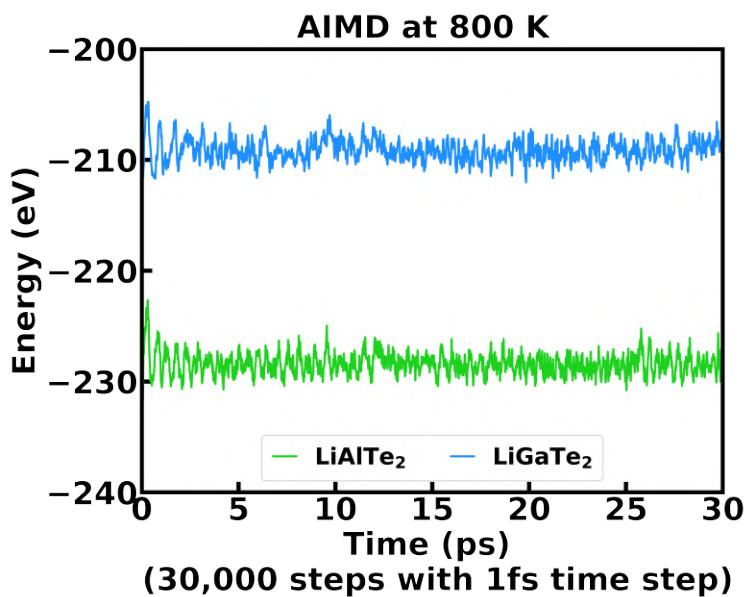


Figure S3: ab initio molecular dynamics simulation at 800 K

S4. Phonon group velocities along q-path

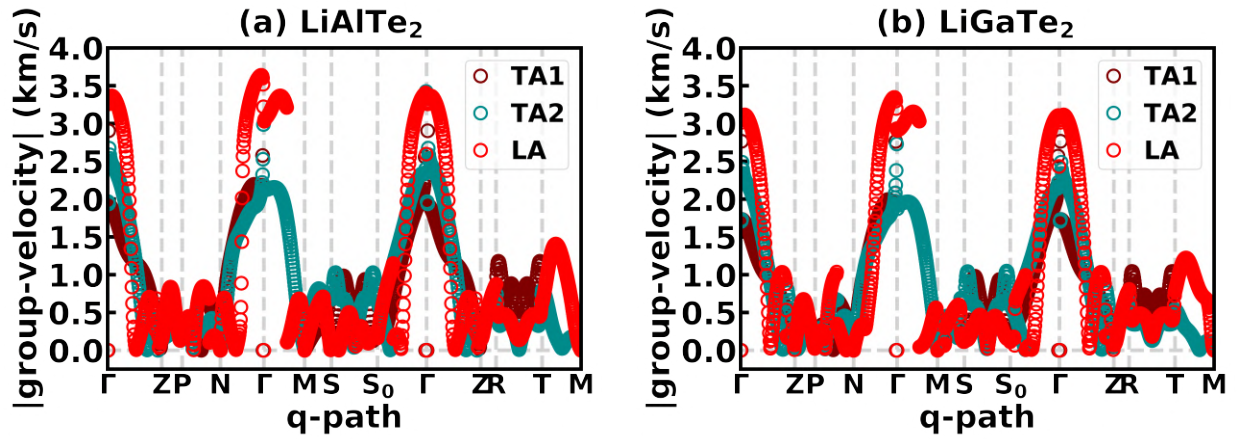


Figure S4: Phonon group velocity along q-path

S5. Phase spaces at 800 K for the three phonon scattering processes

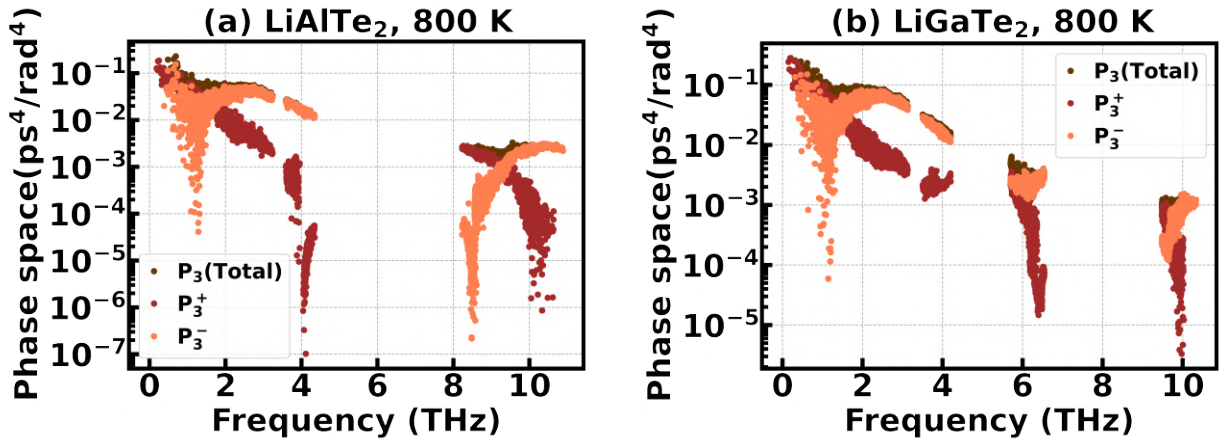


Figure S5: Weighted Phase space at 800 K

S6. Cumulative Lattice Thermal Conductivities at 800 K

K

At 800 K, the acoustic and low-frequency optical branches contributed (64.9, 63.9, 62.4) % and (24.7, 25.1, 25.8) %, respectively, to the lattice thermal conductivities ($\kappa_{l,xx}$, $\kappa_{l,yy}$, $\kappa_{l,zz}$) of LiAlTe₂. In case of LiGaTe₂, contribution to the lattice thermal conductivities ($\kappa_{l,xx}$, $\kappa_{l,yy}$, $\kappa_{l,zz}$) by the acoustic and low-frequency optical branches are (59.2, 53.5, 45.2) % and (25.3, 27.3, 30.2) %, respectively, at 800 K temperature.

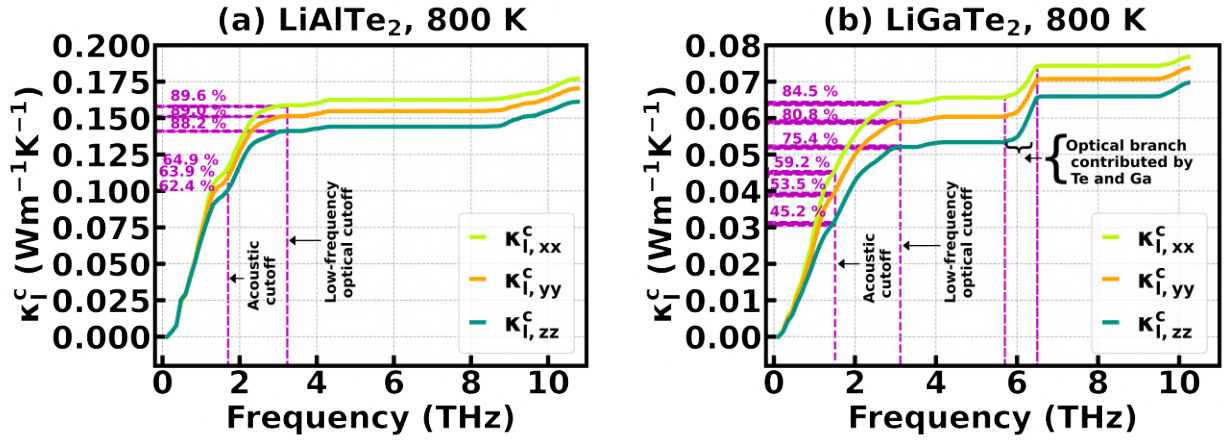


Figure S6: Cumulative lattice thermal conductivities at 800 K

S7. Charge carrier scattering rates at 300 K

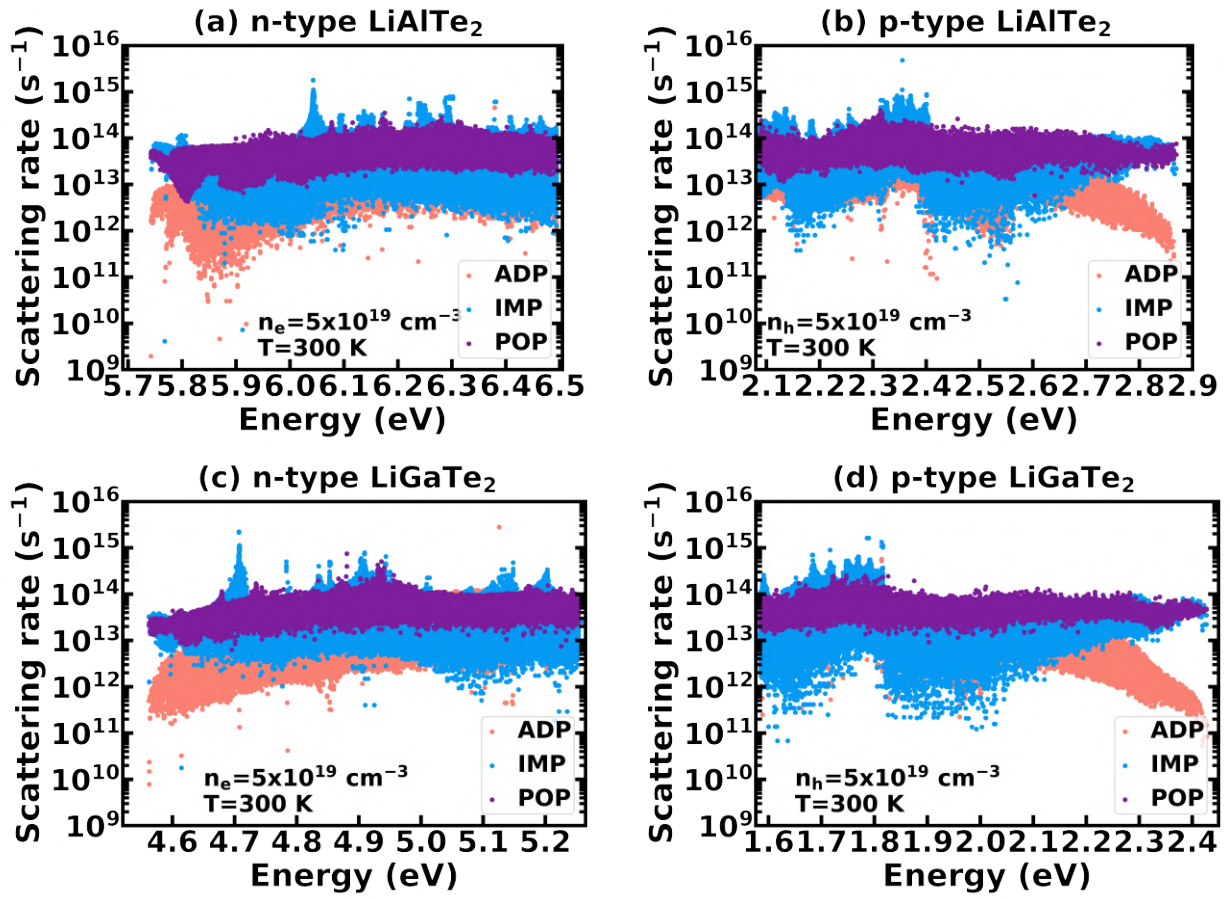


Figure S7: Charge carrier scattering rates at 300 K

S8. Charge carrier scattering rates at 800 K

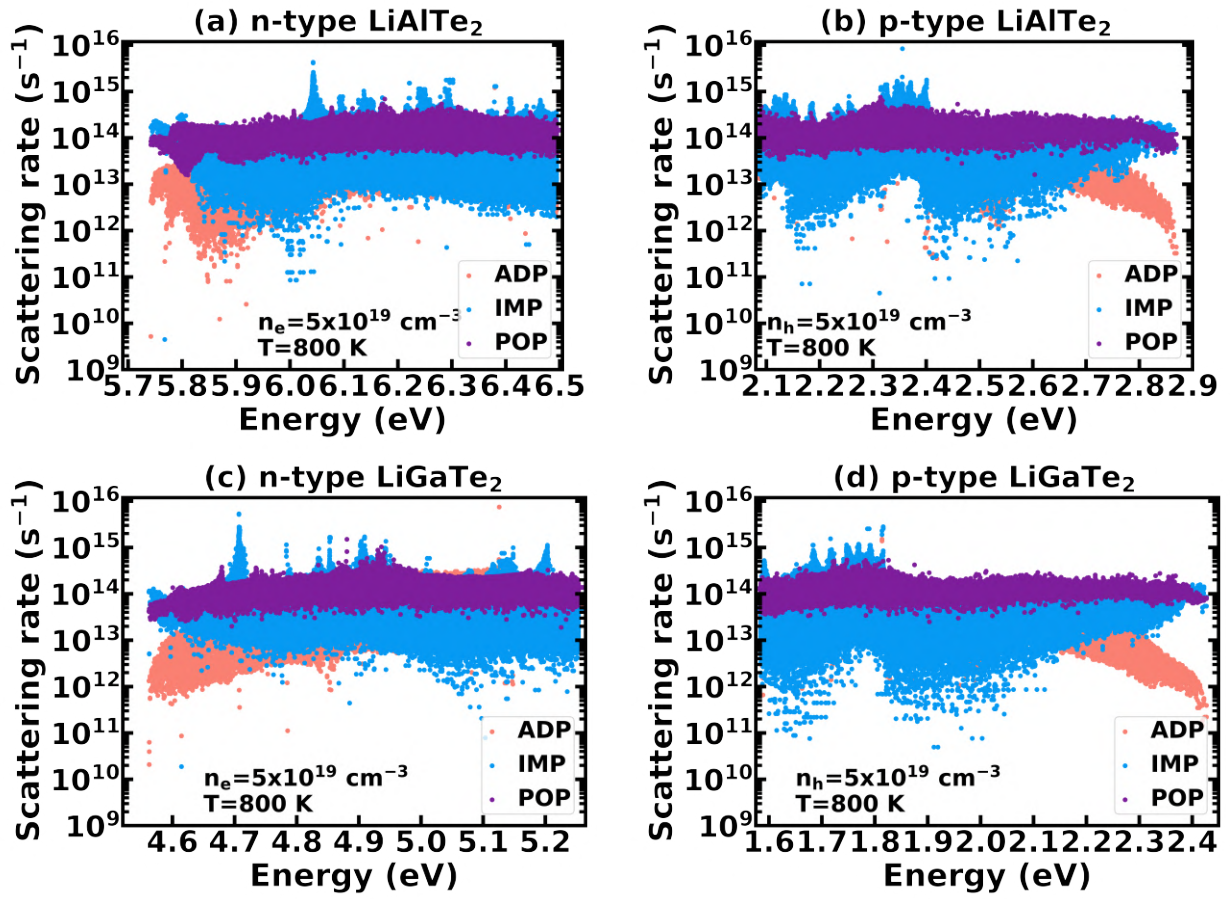


Figure S8: Charge carrier scattering rates at 800 K

S9. Electronic band structures using PBE functional including spin-orbit coupling effect

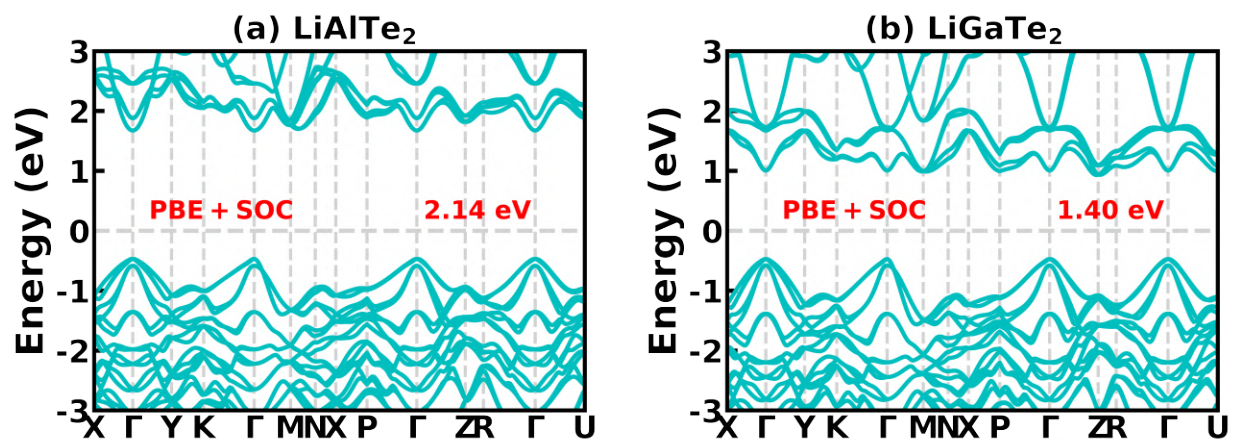


Figure S9: PBE+SOC electronic band structures. Fermi level is set to zero.