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Supplemental information

Unveiling anharmonic scattering in van der Waals semiconductor GaPS₄ through Raman spectroscopy and theoretical calculation

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Table S1 Irreducible representation, calculated and fitted wavenumber of Raman peaks.

Peak	Mode	Wavenumber (cm ⁻¹)		Peak	Mode	Wavenumber (cm ⁻¹)		Peak	Mode	Wavenumber (cm ⁻¹)	
		Cal.	Exp.			Cal.	Exp.			Cal.	Exp.
1	Ag1	60.9	59.7	11	Ag7	141.1	150.2	21	Ag13	337.2	345.3
2	Bg1	63.8	65.6	12	Bg7	150.7	158.0		Bg13	338.2	
3	Ag2	70.5	73.6	13	Ag8	183.4	191.2	22	Ag14	370.7	370.1
	Bg2	77.1			14	Bg8	192.1	200.9	23	Bg14	386.2
4	Ag3	81.8	83.4		Ag9	195.0		24	Bg15	413.4	426.9
	Bg3	85.3		15	Bg9	201.6	208.7		Ag15	414.2	
5	Ag4	89.4	89.3	16	Bg10	248.6	260.9	\	Ag16	504.1	\
6	Bg4	98.2	101.2	17	Ag10	256.8	268.6	25	Bg16	525.1	522.6
7	Ag5	107.6	111.0		Ag11	313.7	309.0	26	Ag17	537.0	544.9
8	Bg5	115.1	120.8	18	Bg11	314.8		27	Bg17	546.7	559.8
9	Ag6	121.1	126.7	19	Bg12	322.1	322.4		Ag18	574.6	
10	Bg6	133.4	138.5	20	Ag12	330.9	335.7	28	Bg18	577.2	594.9

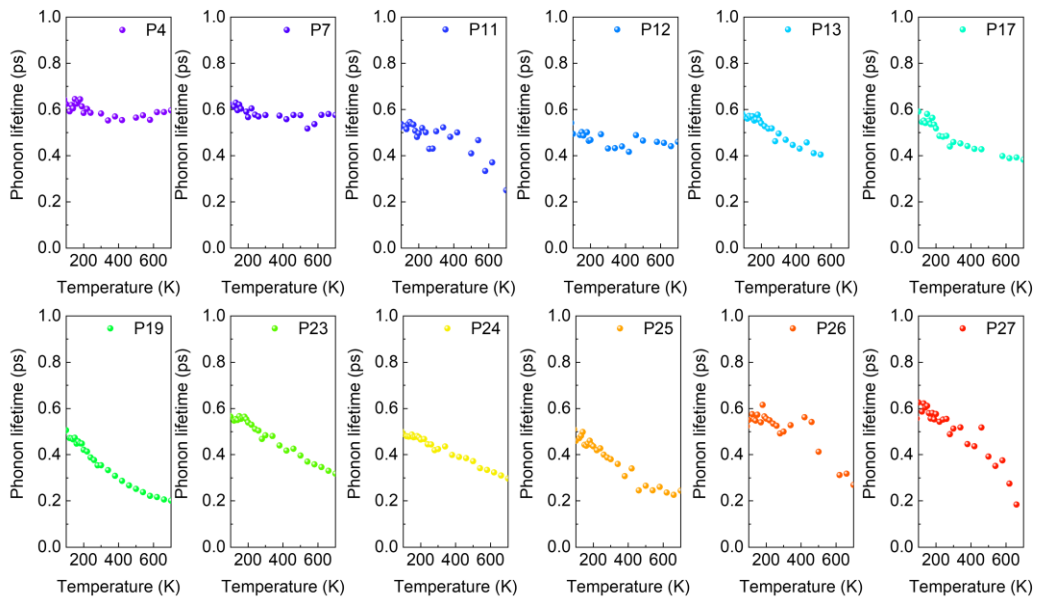


Figure S1 Temperature-dependent phonon lifetimes of GaPS₄, obtaining from the linewidth of Raman spectrum.

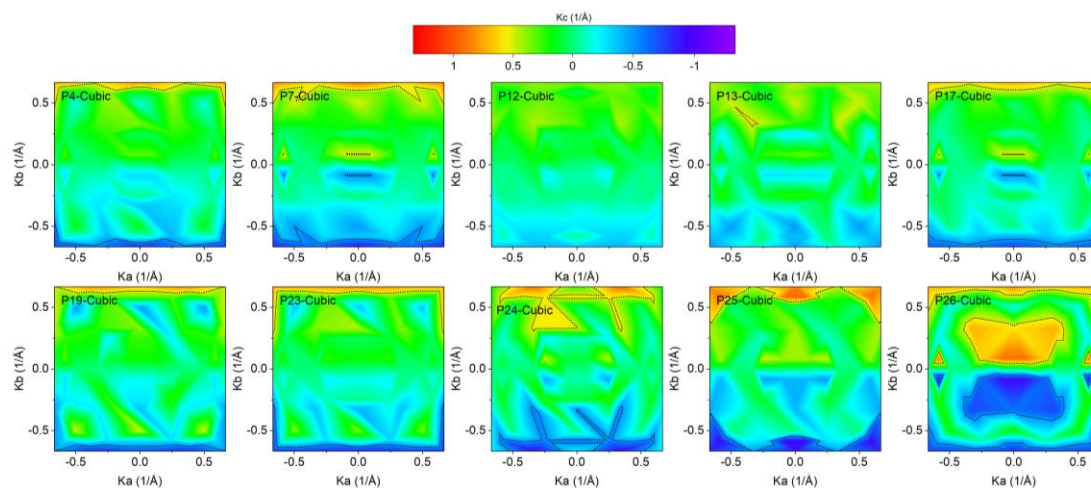


Figure S2 Wavevector of phonons after phonon cubic anharmonic scattering, where the black dashed line represents the edge along the c direction of first Brillouin zone.

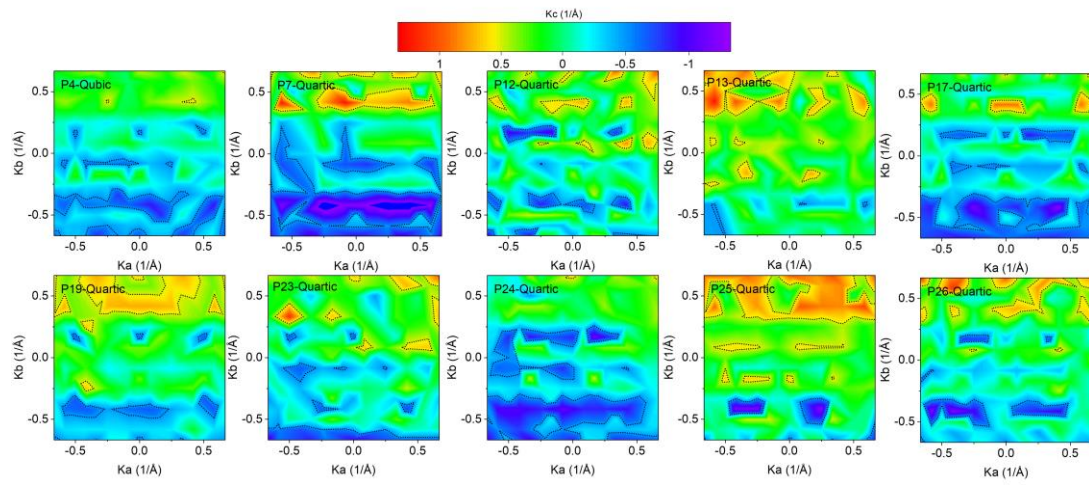


Figure S3 Wavevector of phonons after phonon quartic anharmonic scattering, where the black dashed line represents the edge along the c direction of first Brillouin zone.

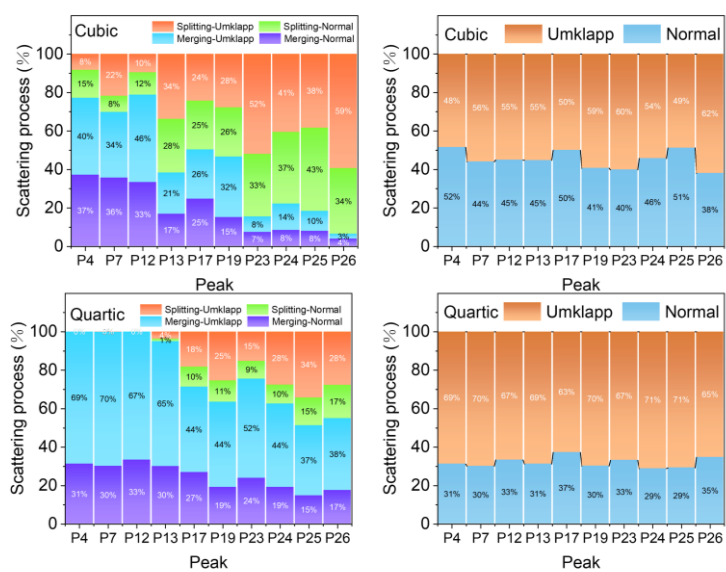


Figure S4 Schematic diagram of the proportion of contributions from different process in phonon scattering.

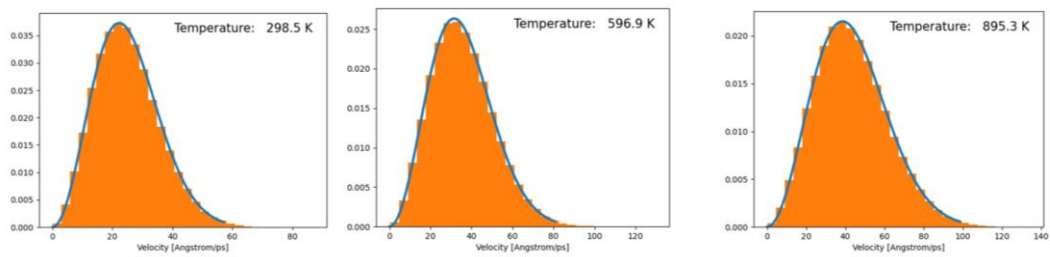


Figure S5 Boltzmann distribution fitting results of the atoms velocity from Molecular Dynamics.

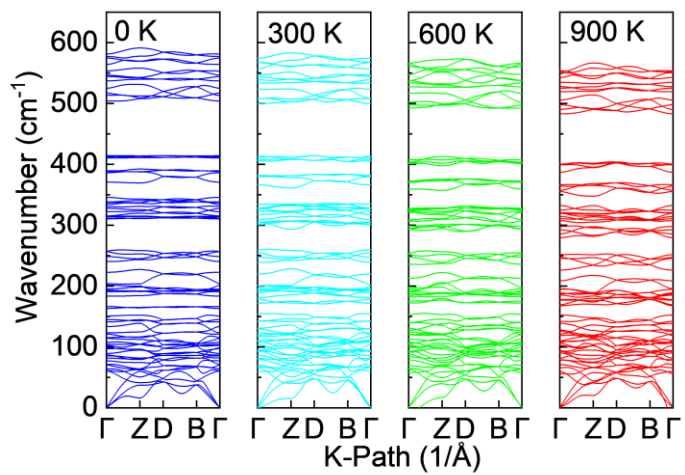


Figure S6 Anharmonic phonon dispersion curves of GaPS₄ at 0K, 300K, 600K and 900K.