

Supporting information for

Lattice Thermal Conductivity of Monolayer AsP from First-Principles Molecular Dynamics

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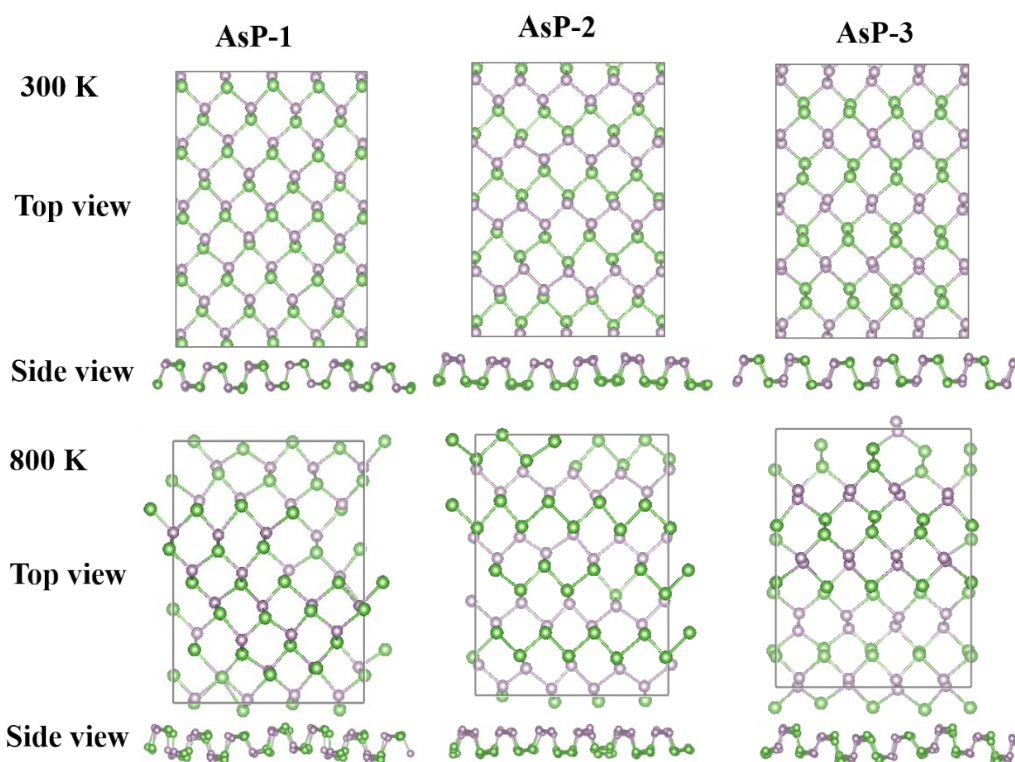


Figure S1. Snapshots of three AsP monolayers taken at the end of 20 ps FPMD simulations at 300 K (upper panel) and 800 K (lower panel), respectively.

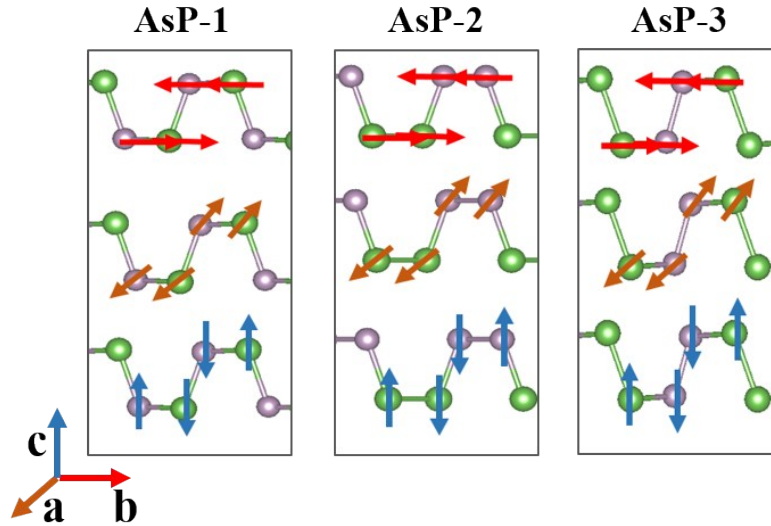


Figure S2. Three low-frequency optical phonon modes in AsP-1, -2, and -3 at the Γ -point. From bottom to top is respectively ZO, TO, and LO mode.

Table S1. The dispersions (in THz) of acoustic (ZA, TA, and LA) modes in AsP and b-P.

Mode	AsP-1	AsP-2	AsP-3	b-P
ZA	2.39	2.37	2.20	3.71
TA	2.42	2.44	2.72	3.81
LA	3.85	3.73	3.78	6.03

Table S2. The average relaxation times and group velocities of each phonon mode in AsP and b-P.

Mode	AsP-1		AsP-2		AsP-3		b-P	
	τ (ps)	v (km/s)	τ (ps)	v (km/s)	τ (ps)	v (km/s)	τ (ps)	v (km/s)
1	13.6	1.38	14.2	1.39	17.2	1.32	21.00	2.12
2	13.1	1.19	26.2	1.25	11.8	1.47	11.74	1.87
3	10.5	1.77	33.9	1.62	13.8	1.73	9.15	2.63
4	9.12	1.56	21.5	1.44	8.86	1.20	9.56	2.45
5	8.06	1.54	12.6	1.81	5.98	1.24	7.18	2.50
6	6.01	0.94	8.04	2.65	5.52	1.00	9.83	1.59
7	11.2	0.76	25.2	0.25	19.5	0.43	6.92	1.25
8	9	0.82	12.96	0.52	21.1	0.49	16.2	1.13
9	10.9	0.37	9.9	0.42	11.6	0.61	14.1	0.58
10	18.5	0.59	22.2	0.91	7.28	0.82	11.5	0.75
11	7.61	0.56	12.6	0.79	2.90	0.77	7.28	0.73
12	4.35	0.56	12.6	1.31	13.1	0.18	5.40	0.73