

“X-AlN ($X = \text{C}, \text{Si}, \text{TC}$)半导体的可见光调控与反常热输运” 补充材料

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Supplementary Material of “Absorption Modulation and Anomalous Thermal Transport in X-AlN(X=C,Si,TC) Semiconductor”

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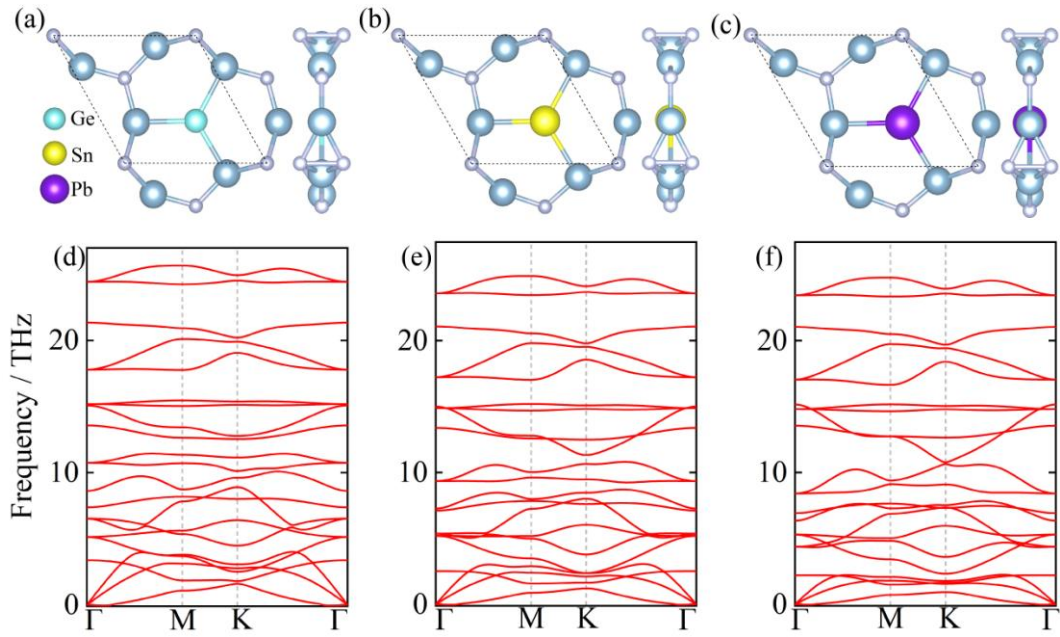


图 S1 稳定的 Ge-, Sn-与 Pb-AIN 结构与其声子谱

Fig. S1. Crystal structures and phonon spectra of stable Ge-, Sn-, and Pb-AIN.

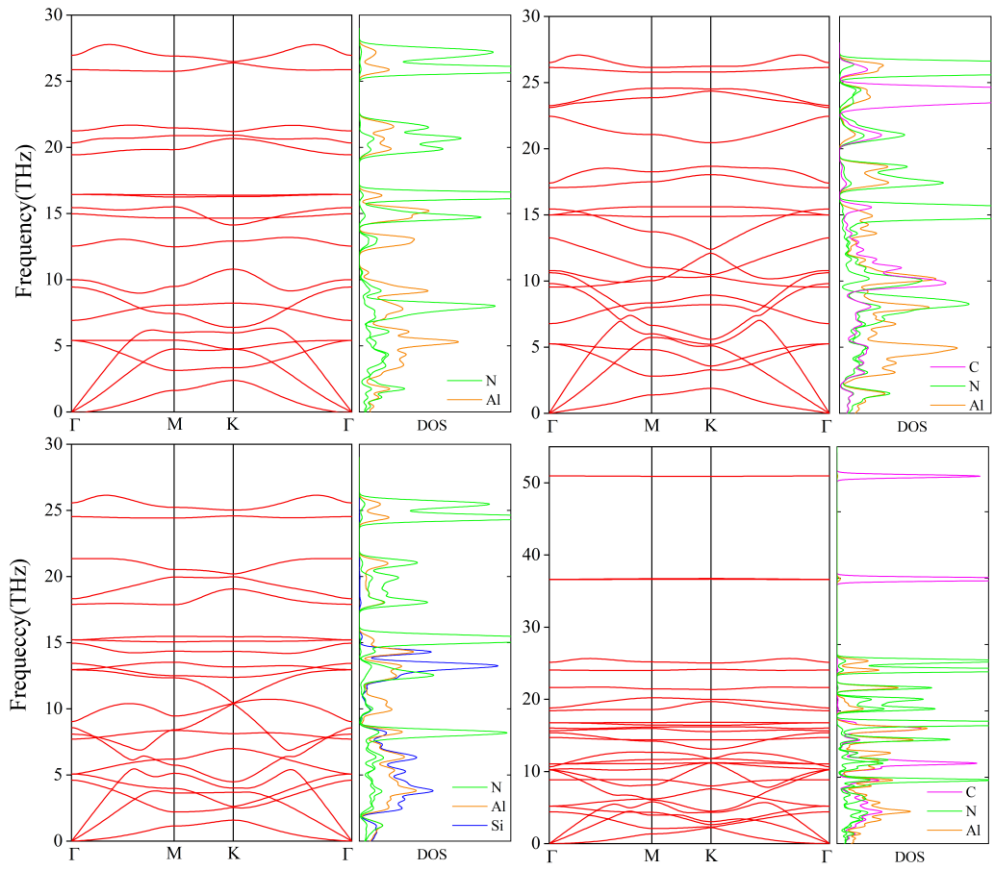


图 S2 孔状皱面 AlN 与 X-AlN (X=C, Si 与 TC)的声子谱及其态密度

Fig. S2. Phonon spectra and its phonon density of states for porous buckled AlN and X-AlN (X=C, Si and TC).

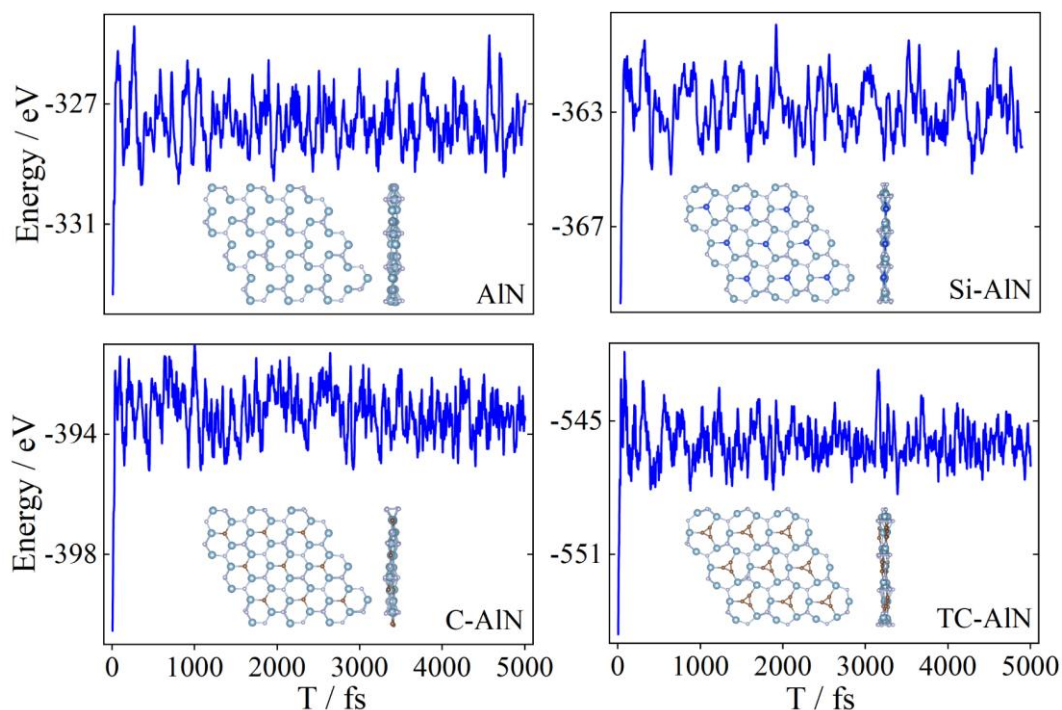


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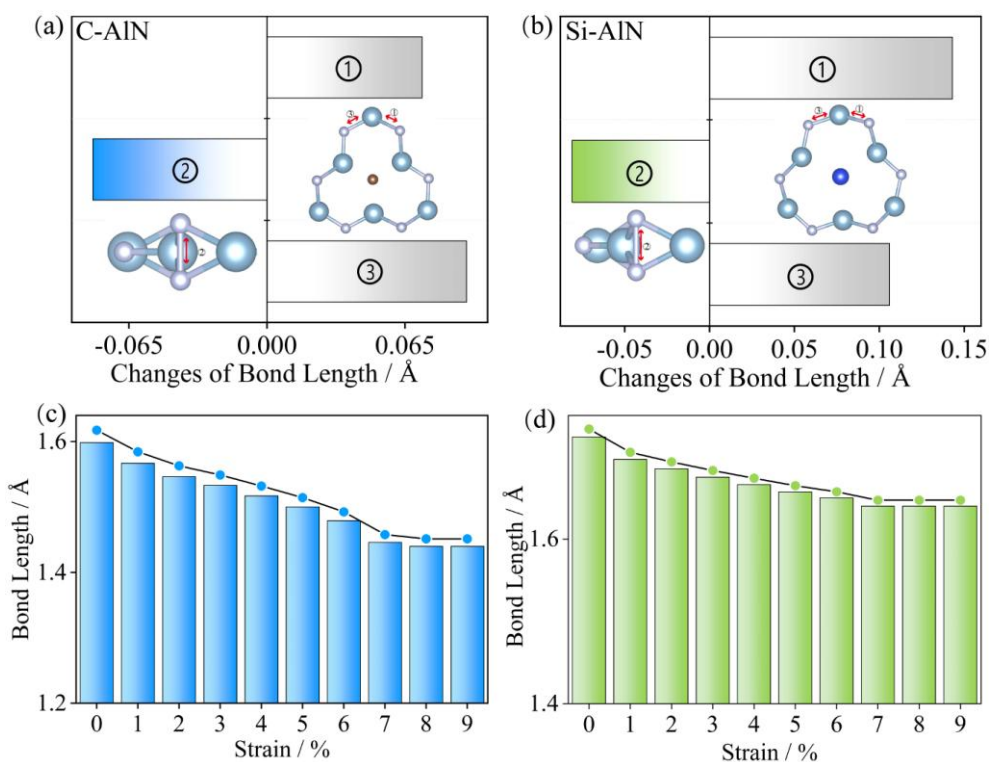


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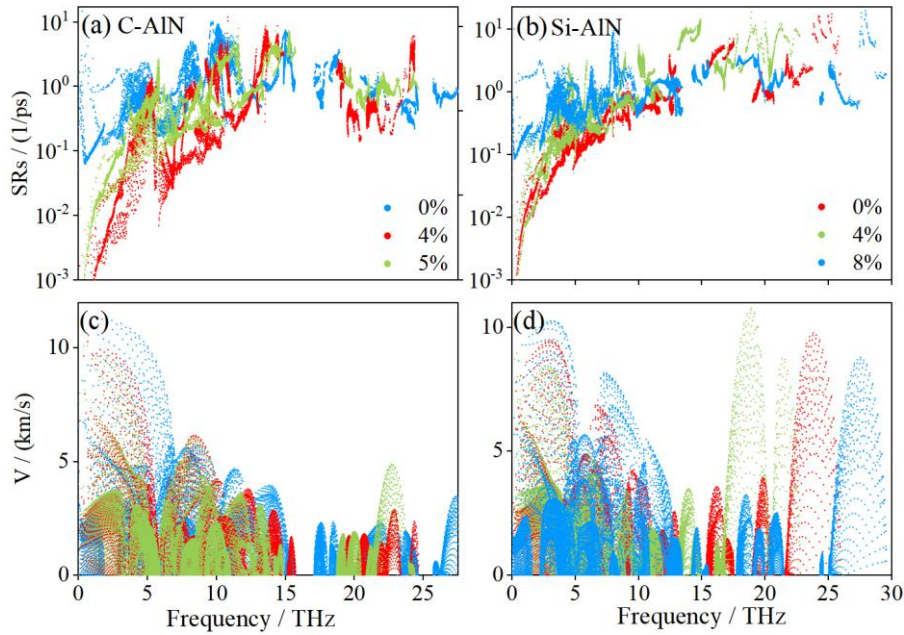


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表 S1 稳定的 Ge-, Sn-与 Pb-AIN 结构的原子序数、原子质量、晶格常数、键角与 X-Al 键长

Table S1. Atomic Number, standard atomic weight, lattice constant, bond angle, and X-Al bond length of stable Ge-, Sn-, and Pb-AIN structures.

	原子序数	原子质量(m^0)	晶格常数(\AA)	键角 α ($^\circ$)	键长(\AA)
Ge-AIN	32	72.63	5.91	139.61	2.48
Sn-AIN	50	118.71	6.05	144.92	2.66
Pb-AIN	82	207.20	6.08	146.67	2.72

表 S2 X-AIN (X=C, Si 与 TC) 在 0%, 4% 与 5%/8% 拉伸应变下 4 个键 (见图 6 与图 S1) 的键长(L)与键强(S)

Table S2. Bond length (L) and bond strength (S) for four bonds (see Figure 6 and Figure S1) at 0%, 4%, and 5%/8% tensile strain in X-AIN (X=C, Si and TC).

	C-AIN				Si-AIN				TC-AIN				
	1	2	3		1	2	3		1	2	3		4
	L	L	L	S	L	L	L	S	L	L	L	S	L
0%	1.80	1.95	1.60	1.78	1.82	1.93	1.72	1.51	1.84	1.92	1.75	1.20	1.39
4%	1.86	2.02	1.53	2.13	1.89	1.98	1.68	1.57	1.93	1.98	1.69	1.25	1.40
8% (5%)	1.88	2.04	1.52	2.29	1.97	2.03	1.64	1.59	2.03	2.04	1.67	1.26	1.41