Supplementary Information (SI) for Nanoscale.
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Supplementary Information for

The effect originated from atomic vibration on thermal transport in diatomic semiconductors via *ab initio* molecular dynamics

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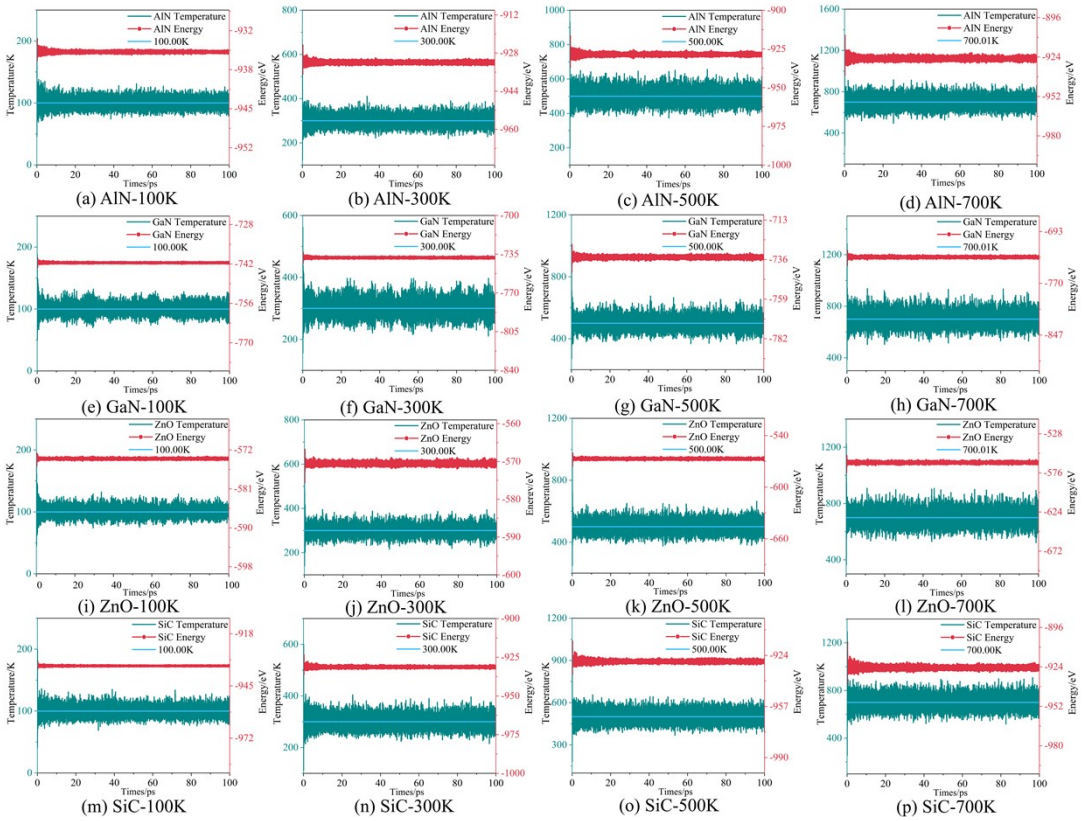
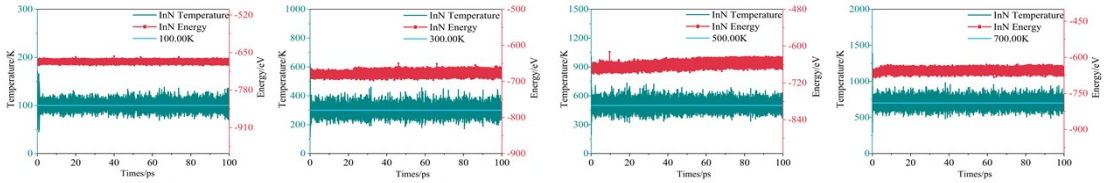
1. Thermodynamic stability of semiconductors



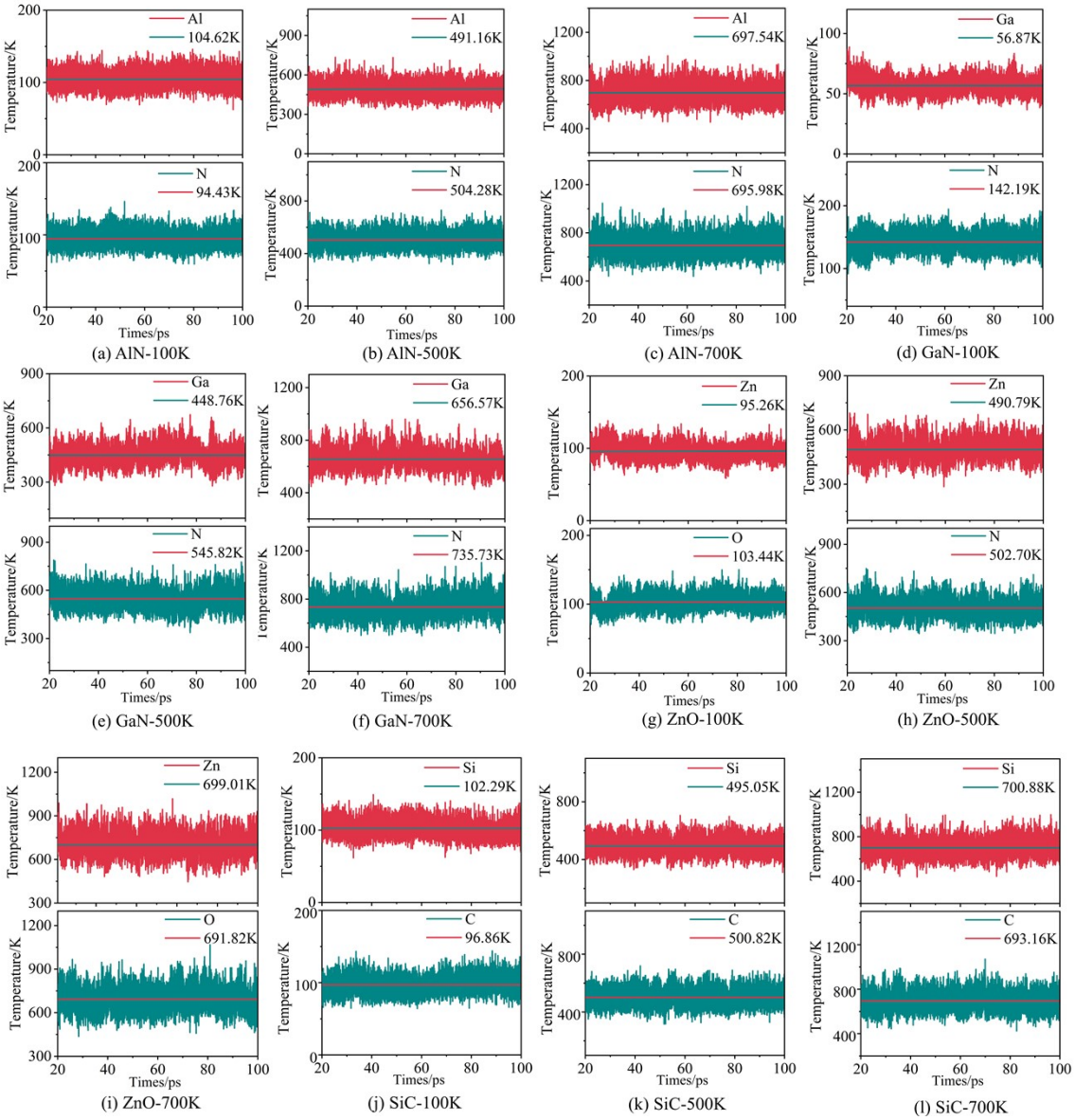


(q) InN-100K (r) InN-300K (s) InN-500K (t) InN-700K

Figure S1. Temperature fluctuations and total energy fluctuations of (a)(b)(c)(d) AlN, (e)(f)(g)(h) GaN, (i)(j)(k)(l) ZnO, and (m)(n)(o)(p) SiC, (q)(r)(s)(t) InN for 100 ps at 100, 300, 500, and 700 K.

2. Temperature fluctuations of heavy and light atoms

The temperature fluctuations of Al and N in AlN, Ga and N in GaN, Zn and O in ZnO, Si and C in SiC, and In and N in InN at 100, 500, and 700 K are shown in Figure S2a-o.



(a) AlN-100K (b) AlN-500K (c) AlN-700K (d) GaN-100K

(e) GaN-500K (f) GaN-700K (g) ZnO-100K (h) ZnO-500K

(i) ZnO-700K (j) SiC-100K (k) SiC-500K (l) SiC-700K

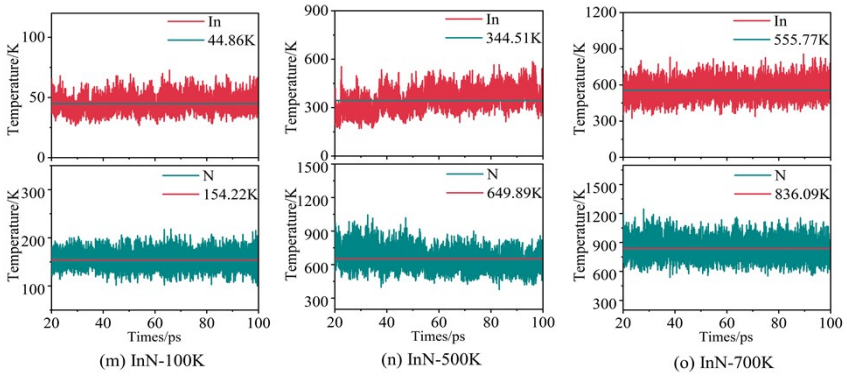


Figure S2. Temperature fluctuations of (a)(b)(c) Al and N atoms in AlN, (d)(e)(f) Ga and N atoms in GaN, (g)(h)(i) Zn and O atoms in ZnO, (j)(k)(l) Si and C atoms in SiC and (m)(n)(o) In and N atoms in InN at 100, 500, and 700 K . (Average temperatures of atoms are labeled.)

3. Atomic lattice vibrations and EPO

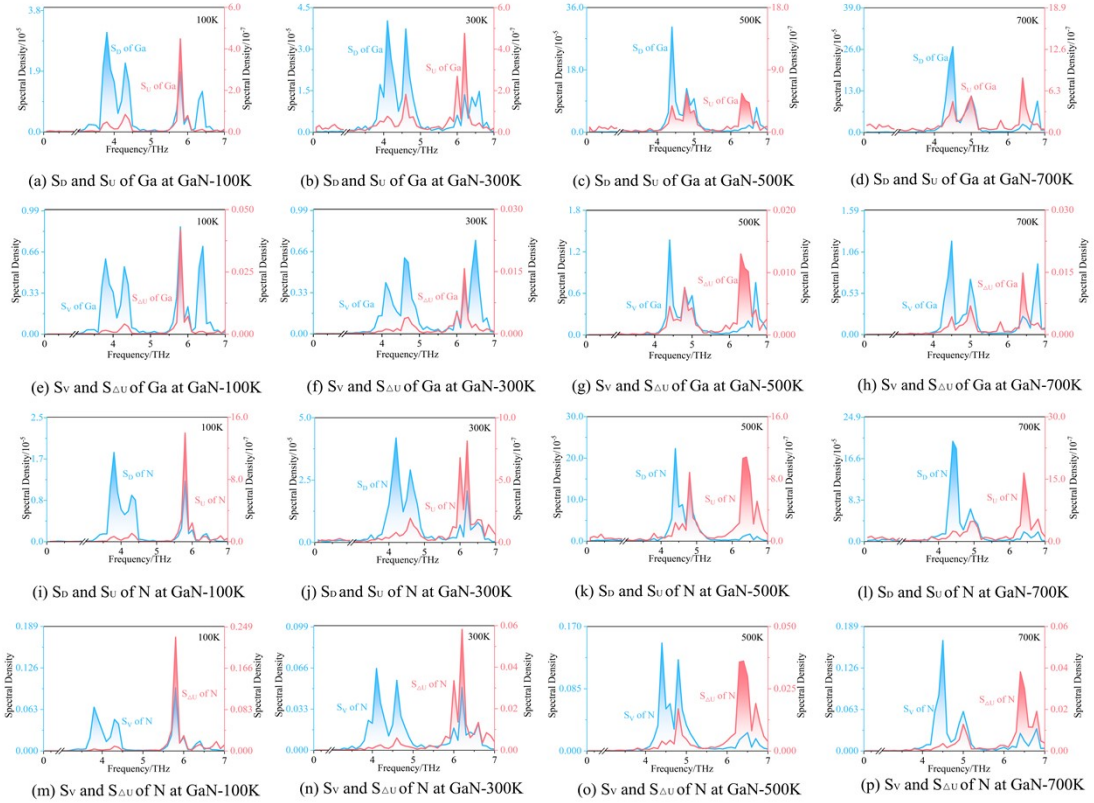


Figure S3. S_D and S_U of Ga atoms in GaN at (a) 100, (b) 300, (c) 500, and (d) 700 K. S_V and $S_{\Delta U}$ of Ga atoms in GaN at (e) 100, (f) 300, (g) 500, and (h) 700 K. S_D and S_U of N atoms in GaN at (i) 100, (j) 300, (k) 500, and (l) 700 K. S_V and $S_{\Delta U}$ of N atoms in GaN at (m) 100, (n) 300, (o) 500, and (p) 700 K.

4. Strength and velocity of EPO changes at high and low temperatures

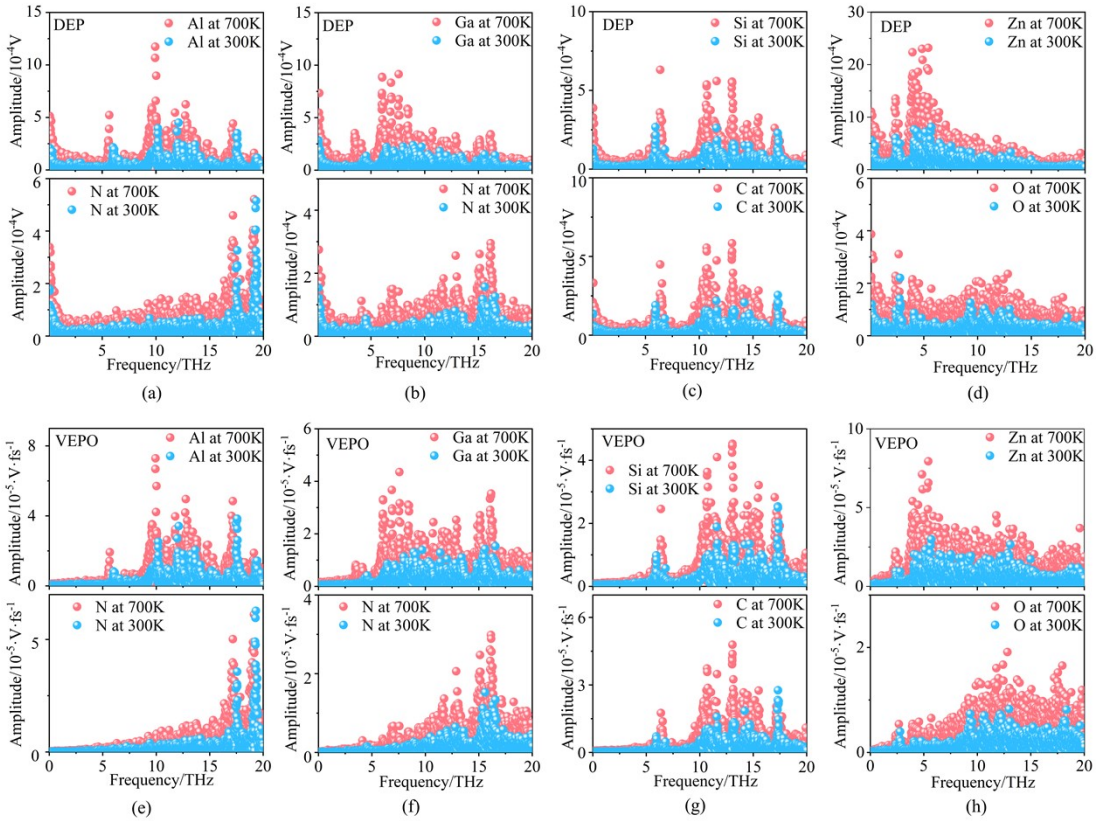


Figure S4. FFT amplitudes of DEP at ion cores of (a) Al and N atoms in AlN, (b) Ga and N atoms in GaN, (c) Si and C atoms in SiC, (d) Zn and O atoms in ZnO at 300 and 700 K. FFT amplitudes of VEPO at ion cores of (e) Al and N atoms in AlN, (f) Ga and N atoms in GaN, (g) Si and C atoms in SiC, (h) Zn and O atoms in ZnO at 300 and 700 K.

5. Convergence test

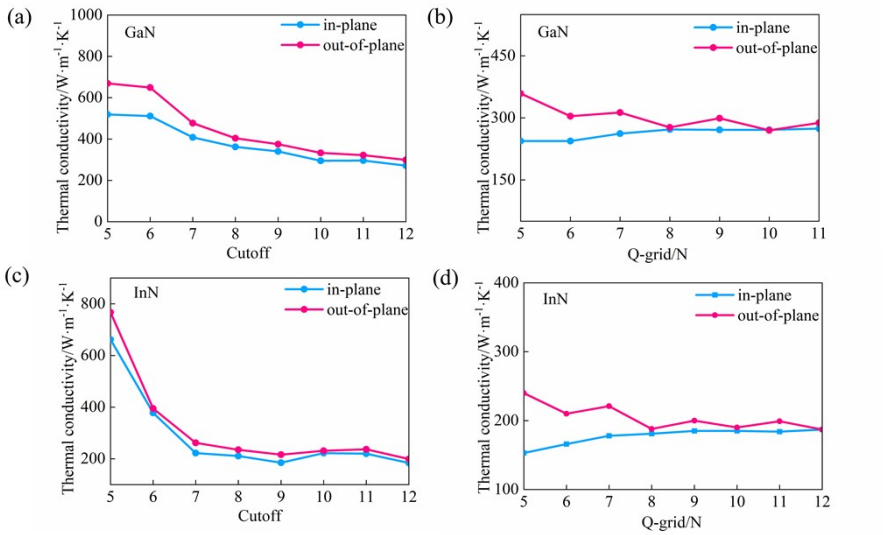


Figure S5. Convergence test results of the thermal conductivity with respect to the nearest neighbors (a) and mesh size (b) in GaN at 300 K, and with respect to the nearest neighbors (c) and mesh size (d) in InN at 300 K.

6. Entropy of canonical ensemble

When the temperature is from 100 to 700 K, the EP, VEP, atomic velocity, and atomic temperature distribution of Al and N atoms in AlN, Ga and N atoms in GaN, Si and C atoms in SiC, Zn and O atoms in ZnO goes from a centralized distribution to a dispersed distribution as shown in Figures S6, 7. The p_i on two sides of the distribution increase, and its H_{EPO}, H_{VEPO}, H_{V} and H_{T} increase.

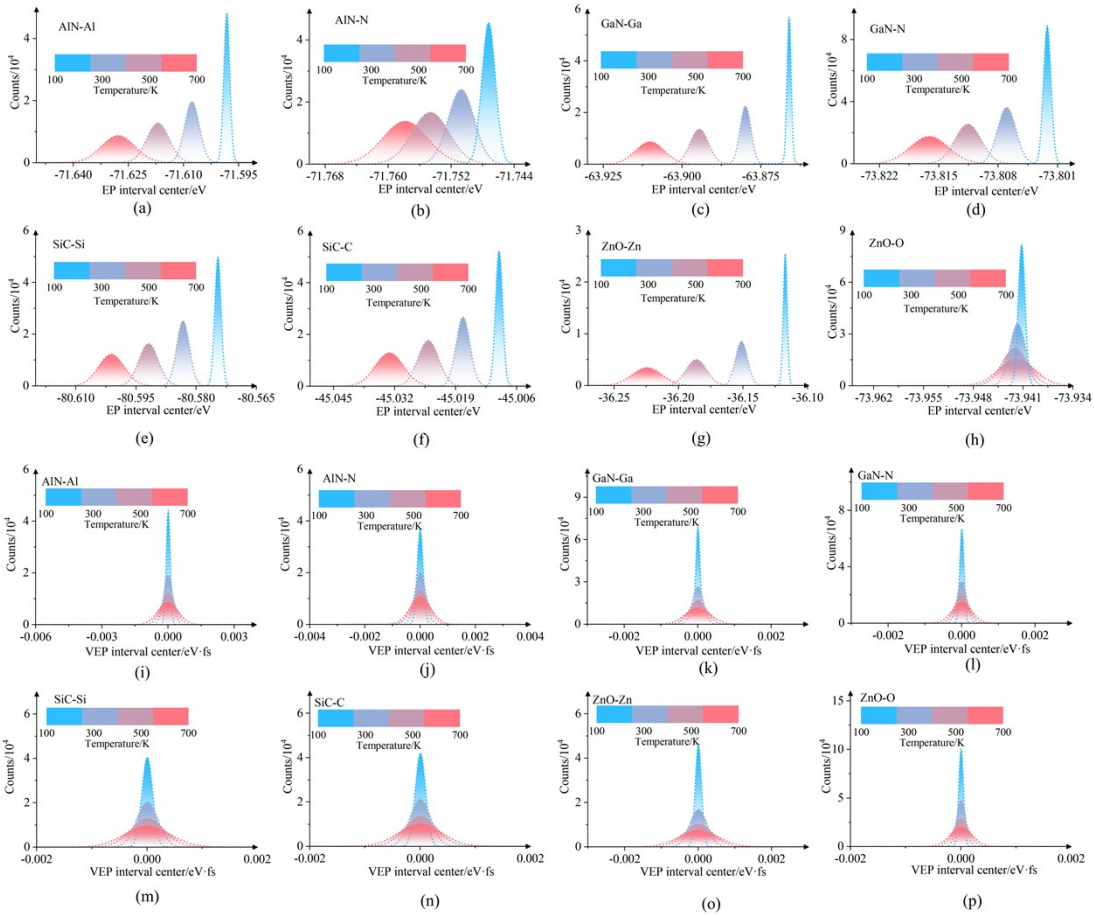


Figure S6. Gaussian fitting of EP distributions of (a) Al atoms in AlN, (b) N atoms in AlN, (c) Ga atoms in GaN, (d) N atoms in GaN, (e) Si atoms in SiC, (f) C atoms in SiC, (g) Zn atoms in ZnO, (h) O atoms in ZnO, at 100, 300, 500, and 700 K. Gaussian fitting of VEP distributions of (i) Al atoms in AlN, (j) N atoms in AlN, (k) Ga atoms in GaN, (l) N atoms in GaN, (m) Si atoms in SiC, (n) C atoms in SiC, (o) Zn atoms in ZnO, (p) O atoms in ZnO, at 100, 300, 500, and 700 K.

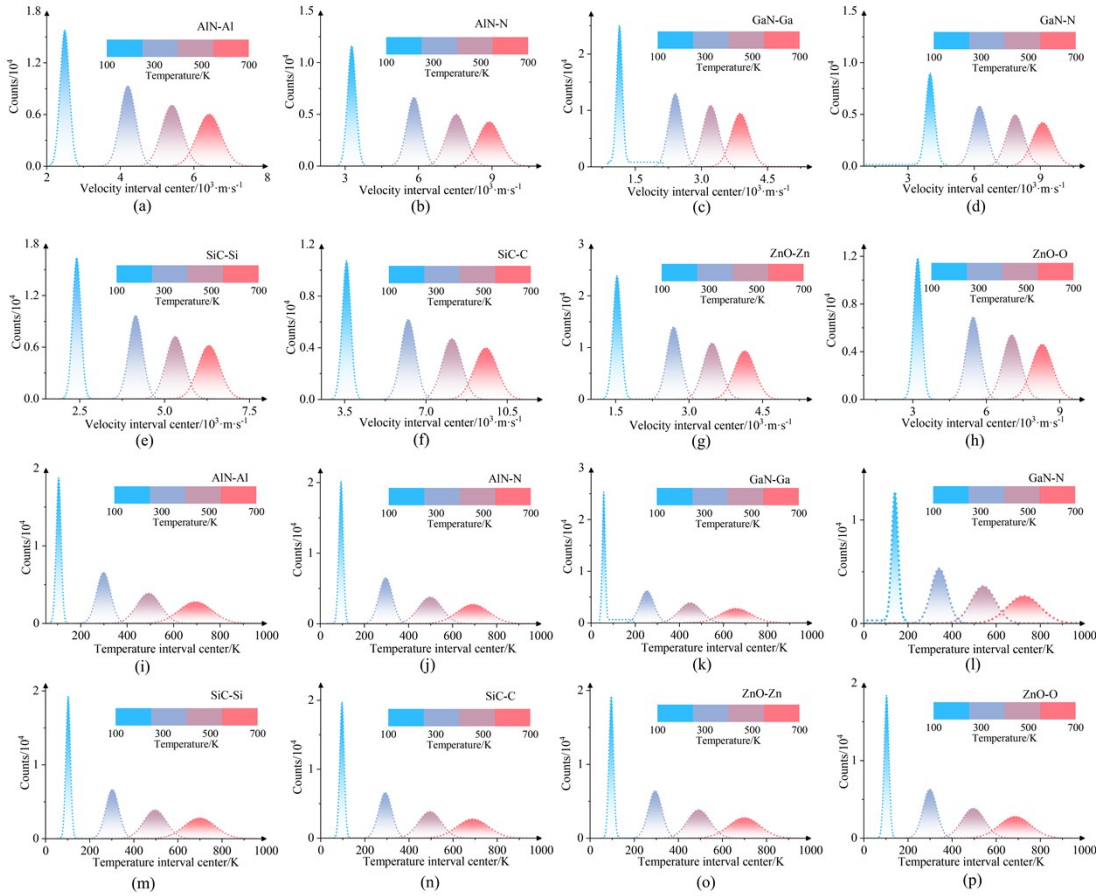


Figure S7. Gaussian fitting of atomic velocity distributions of (a) Al atoms in AlN, (b) N atoms in AlN, (c) Ga atoms in GaN, (d) N atoms in GaN, (e) Si atoms in SiC, (f) C atoms in SiC, (g) Zn atoms in ZnO, (h) O atoms in ZnO, at 100, 300, 500, and 700 K. Gaussian fitting of atomic temperature distributions of (i) Al atoms in AlN, (j) N atoms in AlN, (k) Ga atoms in GaN, (l) N atoms in GaN, (m) Si atoms in SiC, (n) C atoms in SiC, (o) Zn atoms in ZnO, (p) O atoms in ZnO, at 100, 300, 500, and 700 K.