

Supporting Information

Super strain enhanced thermal conductivity of monolayer aluminum/gallium nitride ($\text{Al}_x\text{Ga}_{1-x}\text{N}$) alloys

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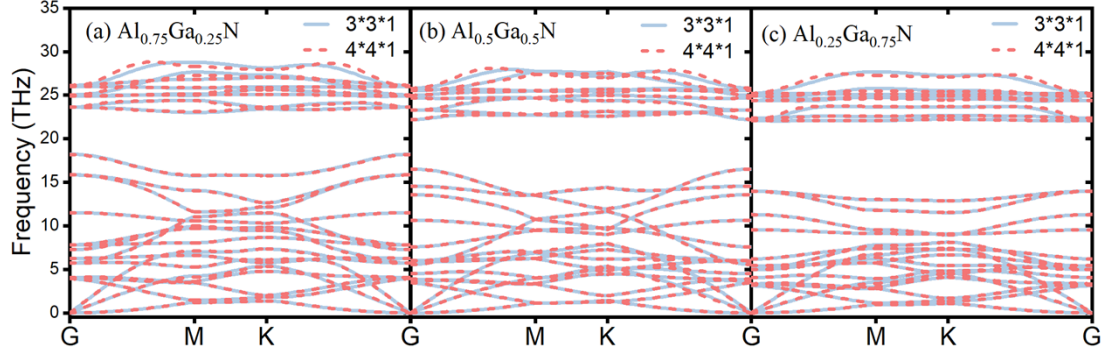


Fig. S1. Phonon dispersion convergence tests for $3\times3\times1$ and $4\times4\times1$ expanded supercells of (a) $\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}$, (b) $\text{Al}_{0.5}\text{Ga}_{0.5}\text{N}$, and (c) $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$.

As shown in Fig. S1, we calculated the phonon dispersion based on $3\times3\times1$ and $4\times4\times1$ supercells. The difference between the results is very small and is sufficient to ensure convergence under the $3\times3\times1$ supercell strategy.

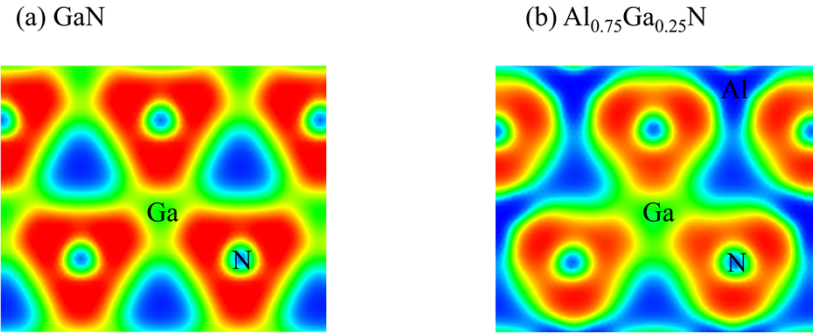


Fig. S2. The electron localization function (ELF) for (a) GaN and (b) $\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}$.