

Supplementary Information for
Tensile strains give rise to strong size effects for thermal conductivities
of silicene, germanene and stanene

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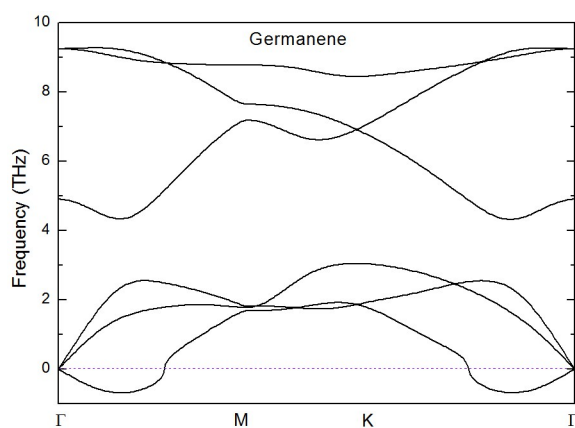


Figure S1. Calculated phonon dispersion of unstrained germanene (*d*-electron included in valence). The ground state was determined by full geometrical optimization based on

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the following setup: plane wave cutoff 560 eV, 28×28 k-mesh, energy convergence tolerance of 1.0×10^{-9} , force convergence precision 1.0×10^{-6} eV/Å and a vacuum layer thickness 1.6 nm using the VASP package. We obtain an equilibrium lattice constant of 3.954 Å and a buckling height of 0.638 Å. The harmonic IFCs are calculated using a 7×7 supercell without additional neighbor cutoff, a 4×4 k-mesh and the same plane wave cutoff, energy convergence tolerance and vacuum layer thickness as those used for the optimization. Note the soft (imaginary) out-of-plane acoustic modes at low frequency.

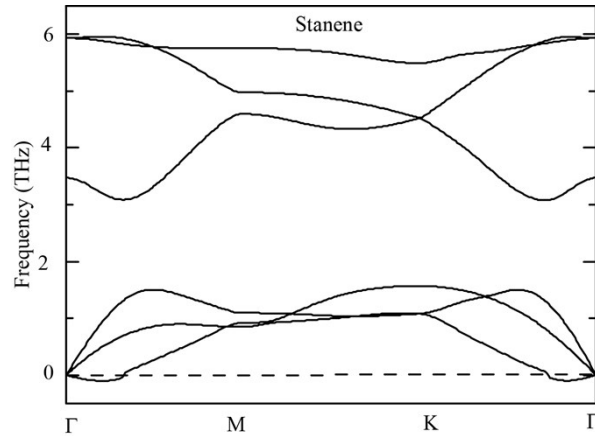


Figure S2. Phonon dispersion of unstrained stanene based on the setups of fast Fourier transformations (FFT) grid densities $NGX=360$ and $NGY=360$ respectively for two vertical in-plane directions and $NGZ=90$ for the out-of-plane direction. In the manuscript the phonon dispersion of unstrained stanene (Figure 1c), the corresponding FFT grid densities are $NGX=180$, $NGY=180$ and $NGZ=90$. No significant difference in the ZA phonon dispersion is seen with increasing FFT grid density.

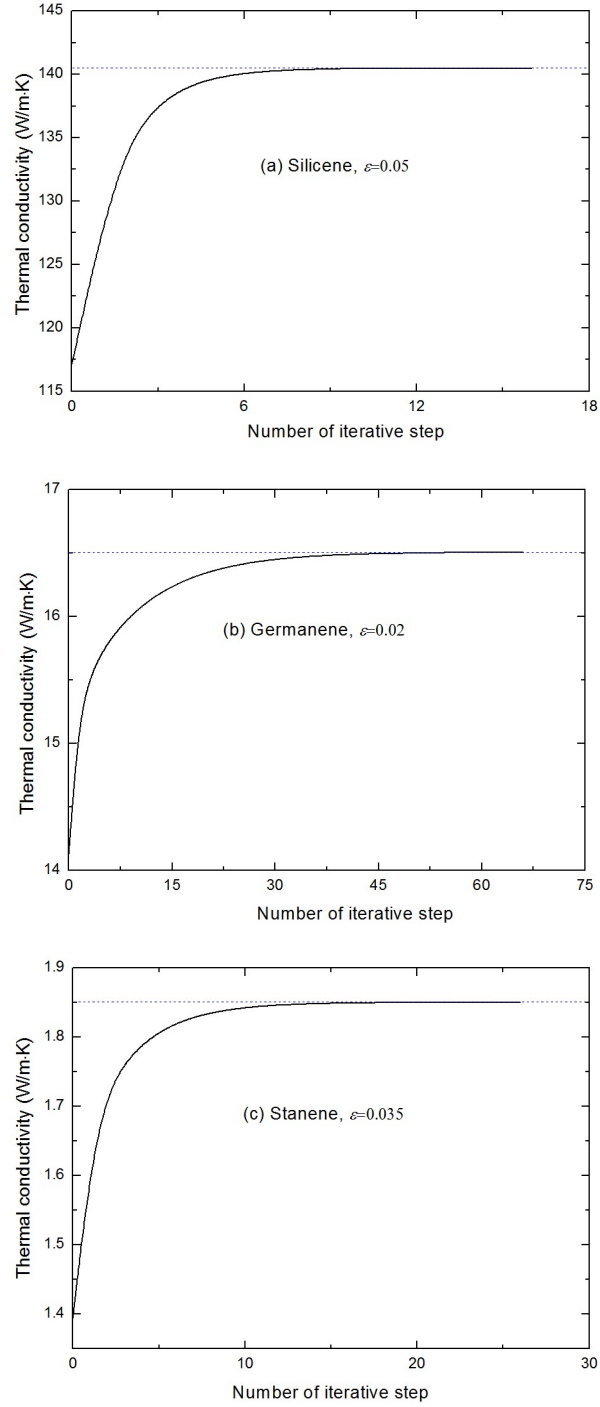


Figure S3. The thermal conductivity as a function of iterative step for silicene at $\varepsilon=0.05$, germanene at $\varepsilon=0.02$ and stanene at $\varepsilon=0.035$ corresponding to q -point grid density $N_1=301$. Good convergence is achieved after 16, 64 and 27 iterations using convergence precision 1×10^{-5} for silicene, germanene and stanene, respectively.