

Supplementary Information for

Phonon Transport in Ground State of Two-dimensional Silicon and Germanium

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SI-1. Density of K grid $N_K \times N_K$ for solving BTE

The convergence of κ with respect to the BZ sampling density of K grid $N_K \times N_K$ for solving BTE is tested. The κ values obtained for the LHD silicene/germanene are shown in **Fig. S1**, from which we can see that κ values of the both structures are stable as long as the density of K grid $N_K \times N_K$ is larger than 19×19 . The largest tested density of K grid is $N_K \times N_K = 83 \times 83$, where κ values obtained for LHD silicene/germanene are 5.9 and 1.6 W/mK, respectively. All analysis in our work is based on this largest density ($N_K \times N_K = 83 \times 83$).

SI-2. Cutoff radius for third-order calculations

Our method involves discarding all interactions between atomic triplets at distances larger than a cutoff radius N_{cutoff} . Naturally, a satisfactory result demands that this radius exceeds the range of physically relevant anharmonic interactions in the crystal. To select a value of N_{cutoff} we analyzed the convergence of our computed κ at $T = 300$ K. We started by considering interactions up to $N_{\text{cutoff}} = 3^{\text{rd}}$ nearest neighbors and we progressively included more coordination shells. The results are shown in **Fig. S2**. We found that $N_{\text{cutoff}} = 4^{\text{th}}$ for the LHD silicene/germanene yield satisfactorily converged values.

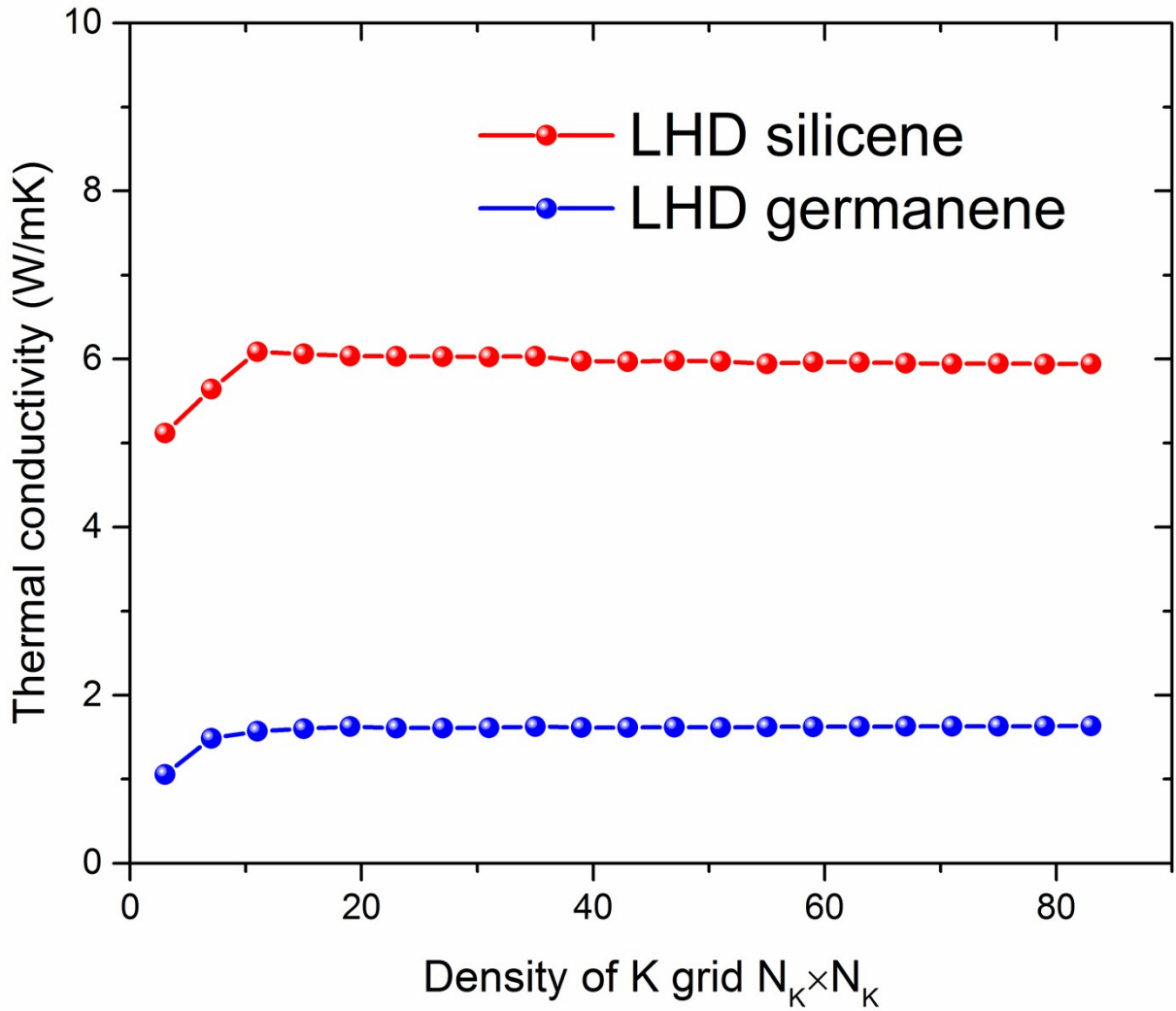


Figure S1. Convergence test of κ for the LHD silicene/germanene at $T = 300$ K with respect to the density of K grid $N_K \times N_K$ employed in solving BTE (all κ are obtained at the selected $N_{\text{cutoff}} = 4$ which is employed in the 3rd IFC calculations).

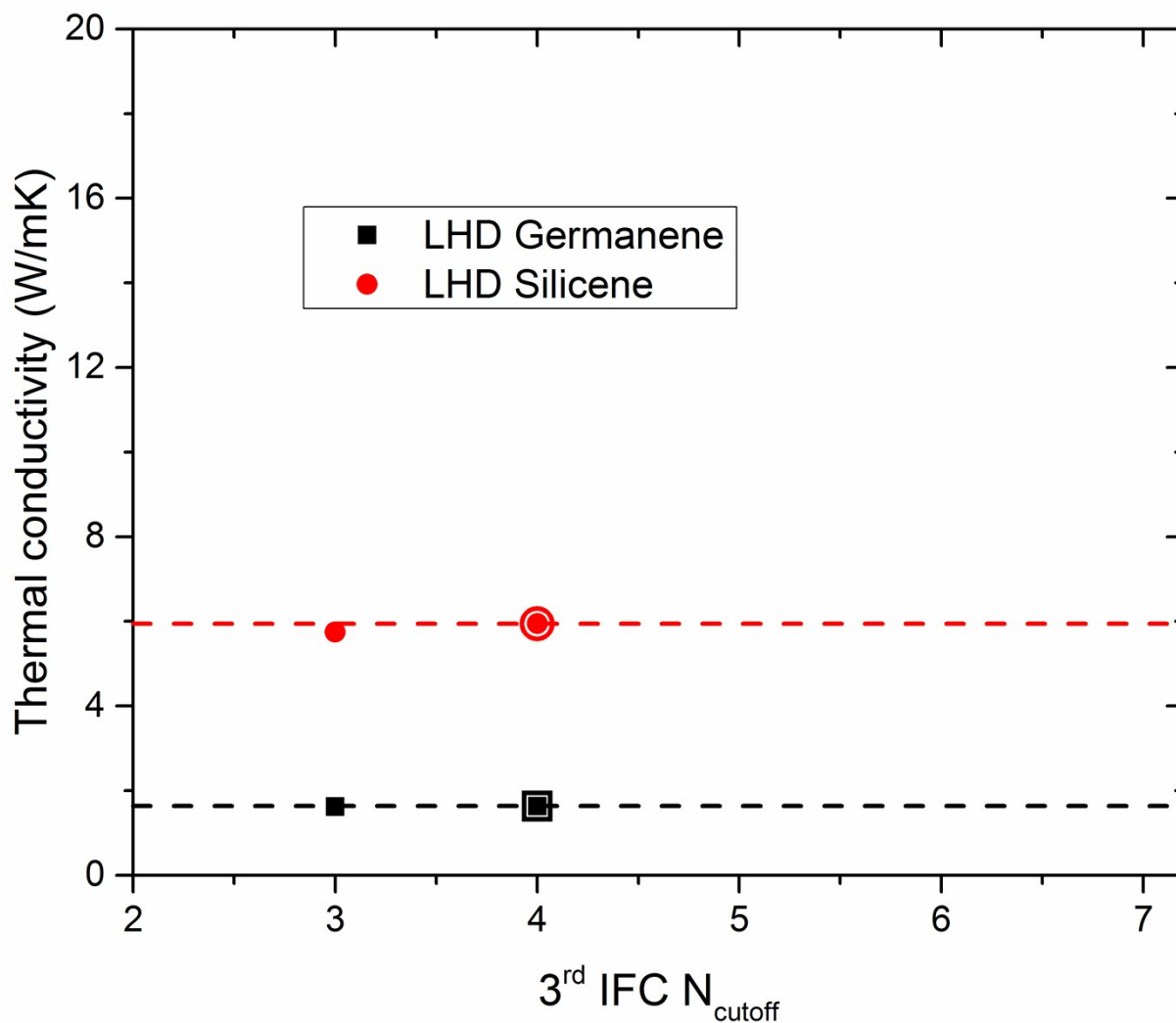


Figure S2. Convergence test of κ for the LHD silicene/germanene at $T = 300$ K with respect to the N_{cutoff} employed in the 3rd IFC calculations (all κ are obtained at the density of K grid $N_K=83$). The selected N_{cutoff} values of the 4th for LHD silicene/germanene are highlighted by black hollow square and red hollow circle, respectively.