Title: A Formalism for Calculating the Modal Contributions to Thermal Interface Conductance

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Figure S1. (a) Heat flux auto-correlation function (HFACF) for total heat flux, and heat flux cross correlation functions (HFCCF) between total heat flux and (b) a low frequency
(f = 0.19 THz), (c) a mid-frequency (f = 0.98 THz), and (d) a high frequency (f = 2.01 THz) eigen mode of vibration. (e) Integrated value of the total interface thermal conductance. The convergence time for the total interface thermal conductance is calculated based on the first avalanche technique\(^1\), and the same time is used to calculate the values of the modal interface thermal conductance. The data is shown for a system size of 3x3x60 FCC unit cells and a simulation temperature of 60K.

References
1 Chen, J., Zhang, G. & Li, B. How to improve the accuracy of equilibrium molecular dynamics for computation of thermal conductivity? *Physics Letters A* **374**, 2392-2396 (2010).