

Effect of silicon surface reconstruction on thermal conductance across vacuum nanogaps

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Heat transport in nanostructured systems may exhibit non-diffusive behavior when the characteristic dimensions become comparable to the relevant phonon transport lengths. In this context, configurations consisting of silicon ultra-thin membranes separated by nanometer-scale vacuum gaps provide a suitable platform to investigate vibrational coupling mechanisms across the vacuum.

In this work, the interaction between two nanomembranes with reconstructed surfaces is studied using a Density Functional Tight Binding (DFTB) approach. Based on an atomistic effective harmonic model, the vibrational modes and the characteristic energy exchange times are calculated, allowing for the estimation of the effective thermal conductance between the membranes.

It is found that both surface reconstruction and the relative orientation of dimers on the facing surfaces significantly modify the coupling between vibrational modes, leading to variations in thermal conductance. These results highlight the role of structural details in phonon-mediated heat transport across nanogaps.

Despite the limitations of the harmonic model, the observed trends are consistent with previous studies, supporting its validity as an efficient computational approach for analyzing thermal transport at the nanoscale.