Tuning phonon thermal transport through graphene by using ensembles of molecular antiresonances

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We propose a scheme for engineering thermal transport properties of low dimensional materials. The method consists of three main ingredients. First, we introduce antiresonance lineshapes in phonon transmission spectrum by molecular functionalization. Even though different molecular species give rise to diverse transmission spectra, thermal resistances due to different species are quite similar, because of the bosonic character of phonons. The bosonic character gives rise to another important feature, which is the second ingredient of the proposed scheme. Combinations of series of phononic thermal resistances are not additive, in general. The more different the transmission spectra of individual scatterers are, the larger total thermal resistance becomes. The third ingredient of the scheme is optimization of the thermal conductance by constructing suitable combinations of scatterers. We use combinatorics principles to show that it is possible to obtain large variances in thermal resistance. We show that a wide range of thermal conductance values are possible, where the range to the average ratios as high as 0.66 are predicted at room temperature, while it can be as high as 1.46 at low temperatures. These figures demonstrate the tunability of thermal transport using the proposed scheme.

Figures

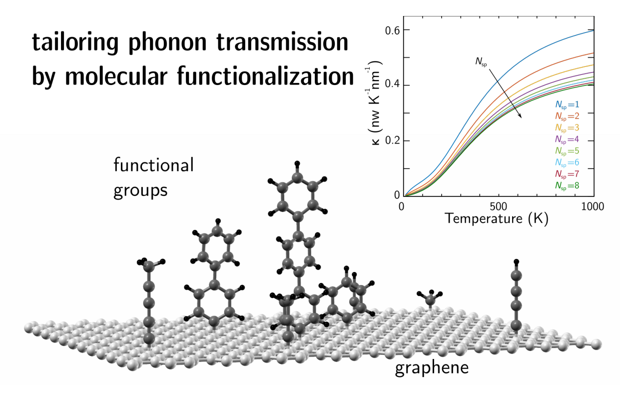

Figure 1: Tailoring phonon transport by chemical functionalization

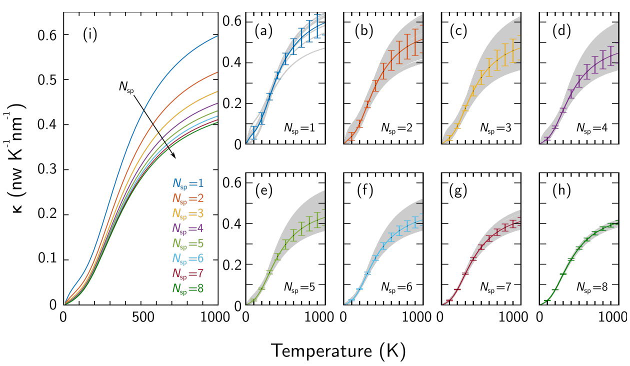

Figure 2: Thermal conductance for ensembles containing 100 molecular adsorbants distributed over different number of species, N_{sp}.