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Ab Initio Studies on Strain-Dependant Thermal Transport Properties of Graphene

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Abstract : In this work, we present a comprehensive investigation of graphene's thermal conductivity (κ) using first-principles density functional perturbation theory calculations, with a focus on the phonon and lattice vibrational properties underlying its superior heat transport capabilities. The study highlights the role of phonon frequencies, lifetimes, and mode-resolved contributions in determining graphene's thermal performance, emphasizing its high phonon group velocities and long mean free paths that contribute to thermal conductivity exceeding 3000 W/mK at room temperature. The results are compared with other two-dimensional materials like silicene (κ < 10 W/mK) and MoS_2 (κ ≈ 83 W/mK) to underline graphene's advantages in nanoscale applications. Here, we report the concept of "velocity-lifetime trade-off" and use it to explain graphene's excellent invariance to high tensile and compressive strains as it exhibits minimal variation in thermal conductivity, making it an ideal material for applications requiring stability in environments with strain variability and deformation. This study establishes graphene as a benchmark material for thermal transport in next-generation 2D channel FET devices and offers a roadmap for its optimization in practical applications.

Keywords : phonons, thermal conductivity, transport, strain, vibrational analysis
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