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Phonon hydrodynamics in two-dimensional materials[1]

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The conduction of heat in two dimensions displays a wealth of fascinating phenomena of key relevance to the scientific and technological applications of novel layered materials. Here, we use third order density-functional perturbation theory and an exact, variational solution of the Boltzmann transport equation to study fully from first-principles phonon transport and heat conductivity in graphene and related materials (boron nitride, functionalized derivatives, transition-metal dichalcogenides...). Very good agreement is obtained with experimental data, where available, together with a microscopic understanding of the collective character of heat-carrying excitations, and the unusual length scales involved. Last, and at variance with typical three-dimensional solids, normal processes dominate over Umklapp scattering well above cryogenic conditions, extending to room temperature and more. As a result, novel hydrodynamics regimes, hitherto typically confined to ultra-low temperatures, become readily apparent.

[1]Work done in collaboration with Andrea Cepellotti, Giorgia Fugallo, Lorenzo Paulatto, Michele Lazzeri, and Francesco Mauri.