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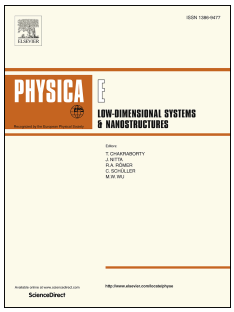

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First-principles study of intrinsic phononic thermal transport in monolayer C_3N

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Very recently, a new graphene-like crystalline, hole-free, 2D-single-layer carbon nitride C_3N, has been fabricated by polymerization of 2,3-diaminophenazine and used to fabricate a field-effect transistor device with an on-off current ratio reaching 5.5×10^{10} (Adv. Mater. 2017, 1605625). Heat dissipation plays a vital role in its practical applications, and therefore the thermal transport properties need to be explored urgently. In this paper, we perform first-principles calculations combined with phonon Boltzmann transport equation to investigate the phononic thermal transport properties of monolayer C_3N, and meanwhile, a comparison with graphene is given. Our calculated intrinsic lattice thermal conductivity of C_3N is 380 W/mK at room temperature, which is one order of magnitude lower than that of graphene (3550 W/mK at 300 K), but is greatly higher than many other typical 2D materials. The underlying mechanisms governing the thermal transport were thoroughly discussed and compared to graphene, including group velocities, phonon relax time, the contribution from phonon branches, phonon anharmonicity and size effect. The fundamental physics understood from this study may shed light on further studies of the newly fabricated 2D crystalline C_3N sheets.