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Atomistic simulations of water flow in graphene channels driven by imposed thermal gradients

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Body:

Nanofluidics has become interesting as the basis for further device miniaturization. Different from macro and microfluidics, nanoconfined flows are significantly influenced by fluid-wall interaction. In this context, recent studies have reported the potential exploitation of imposed thermal gradients as mechanism to transport water in nanoconduits. Moreover, graphene-based materials have attracted increasing attention in nanofluidic applications due to their unique thermal, structural and hydrodynamic properties. Here, we conduct atomistic simulations to investigate water transport in graphene nanoslit channels driven by thermal gradients. The study is focused in understanding the relation between phonon currents induced in the walls by imposed thermal gradients and the corresponding measured flow rates. Furthermore, a comprehensive analysis of the influence of wettability, multi-layer graphene in the walls and geometrical asymmetries is performed. Our results provide valuable information for the design of thermal graphene-based nanopumps and contribute to the understanding of suitable driving mechanisms for liquids in nanoconduits.

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