Water transport in graphene nano-channels

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Water transport in graphene nano-channels[1] ENRIQUE WAGEMANN, ELTON OYARZUA, University of Concepcion, J. H. WALTHER, Technical University of Denmark, HARVEY ZAMBRANO, University of Concepcion — The transport of water in nanopores is of both fundamental and practical interest. Graphene Channels (GCs) are potential building blocks for nanofluidic devices due to their molecularly smooth walls and exceptional mechanical properties. Numerous studies have found a significant flow rate enhancement, defined as the ratio of the computed flow rate to that predicted from the classical Poiseuille model. Moreover, these studies point to the fact that the flow enhancement is a function of channel height and the fluid-wall physical-chemistry. In spite of the intensive research, an explicit relation between the chirality of the graphene walls and the slip length has not been established. In this study, we perform non-equilibrium molecular dynamics simulations of water flow in single- and multi-walled GCs. We examine the influence on the flow rates of dissipating the viscous heat produced by connecting the thermostat to the water molecules, the CNT wall atoms or both of them. From the atomic trajectories, we compute the fluid flow rates in GCs with zig-zag and armchair walls, heights from 1 to 4 nm and different number of graphene layers on the walls. A relation between the chirality, slip length, and flow enhancement is found.

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