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Wagemann, Enrique; Walther, Jens Honore; Zambrano, Harvey

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Drag reduction in silica nanochannels induced by graphitic wall coatings.¹ ENRIQUE WAGEMANN, Universidad de Concepcion, J. H. WALTHER, Technical University of Denmark, HARVEY A. ZAMBRANO, Universidad de Concepcion — Transport of water in hydrophilic nanopores is of significant technological and scientific interest. Water flow through hydrophilic nanochannels is known to experience enormous hydraulic resistance. Therefore, drag reduction is essential for the development of highly efficient nanofluidic devices. In this work, we propose the use of graphitic materials as wall coatings in hydrophilic silica nanopores. Specifically, by conducting atomistic simulations, we investigate the flow inside slit and cylindrical silica channels with walls coated with graphene (GE) layers and carbon nanotubes (CNTs), respectively. We develop realistic force fields to simulate the systems of interest and systematically, compare flow rates in coated and uncoated nanochannels under different pressure gradients. Moreover, we assess the effect that GE and CNT translucencies to wettability have on water hydrodynamics in the nanochannels. The influence of channel size is investigated by systematically varying channel heights and nanopore diameters. In particular, we present the computed water density and velocity profiles, volumetric flow rates, slip lengths and flow enhancements, to clearly demonstrate the drag reduction capabilities of graphitic wall coatings.

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Enrique Wagemann
Universidad de Concepcion

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