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Hydrodynamics in a Polymeric Nanoslit Pore with Graphene and Hexagonal Boron Nitride Wall Coatings: An Atomistic Study[1] DIEGO BECERRA, ANDRES CORDOBA, Universidad de Concepcion, JENS HONORE WALTHER, Technical University of Denmark, HARVEY A. ZAMBRANO, Universidad Tecnica Federico Santa Maria — Design of efficient nanofluidic platforms requires effective reduction of flow resistance within the channel network. With this purpose, 2D-materials can be deposited on polymeric substrates increasing the transport efficiency of water solutions through nanopores. In the present work, we show that significant drag reduction can be achieved in a polyamide nanoslit pore by using graphene and boron nitride as wall coatings. Here, Molecular Dynamics simulations are performed to study water flow through uncoated and coated polyamide nanoslit pores. From atomistic trajectories, we investigate interfacial properties and evaluate the effect that the polymeric matrix has on water structure inside the pores. Furthermore, we compute density and temperature profiles, molecular orientations, friction coefficient and velocity profiles. Using these observables, we analyze the correlation between local water structure, flow enhancement and slip length. Our results indicate that in coated pores the interactions between water molecules and the underlying polyamide substrate have a significant influence on the flow rates. The insights reported in this work may assist the design of strategies to achieve low friction water transport in nanostructured pores.

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Diego Becerra
Universidad de Concepcion

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