“High-throughput simulations for Nanofuidics”

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Abstract:

We explore the dynamics of water transport in carbon-based materials for nanofluidics with high-throughput Molecular Dynamics (MD) simulations. We examine the efficiency of water permeability and the transport of water/ion solutions in carbon capillaries or on graphene. We study interfacial phenomena and quantify uncertainties of MD simulation conditions that affect the evaluated water transport through nano-capillaries. We provide insights for the underlining physics of nanoscale systems of fluidic transport for applications that include membrane filtration, water purification and drug delivery.