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Labyrinthine flows across multilayer graphene-based membranes[1]

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Graphene-based materials have recently found extremely wide applications for fluidic purposes thanks to remarkable developments in micro-/nano-fabrication techniques. In particular, high permeability and specific selectivity have been reported for these graphene-based membranes, such as the graphene-oxide membranes, with however controversial experimental results. There is therefore an urgent need to propose a theoretical framework of fluid transport in these architectures in order to rationalize the experimental results.

In this presentation, we report a theoretical study of mass transport across multilayer graphene based membranes, which we benchmark by atomic-scale molecular dynamics. Specifically, we consider the water flow across multiple graphene layers with an inter-layer distance ranging from sub-nanometer to a few nanometers. The graphene layers have nanoslits aligned in a staggered fashion, and thus the water flows involve multiple twists and turns. We compare the continuum model predictions for the permeability with the lattice Boltzmann calculations and molecular dynamics simulations. The highlight is that, in spite of extreme confinement, the permeability across the graphene-based membrane is quantitatively predicted on the basis of a properly designed continuum model [1]. The framework of this study constitutes a benchmark to which we compare favourably published experimental data.

In addition, flow properties of a water-ethanol mixture are presented, demonstrating the possibility of a novel separation technique. While the membrane is permeable to both pure liquids, it exhibits a counter-intuitive "self-semi-permeability" to water in the presence of the mixture. This suggests a robust and versatile membrane-based separation method built on a pressure-driven reverse-osmosis process, which is considerably less energy consuming than distillation processes [2].

References:

[1] "Labyrinthine water flows across multilayer graphene-based membranes: molecular dynamics versus continuum predictions," H. Yoshida and L. Bocquet, J. Chem. Phys. 144, 234701 (2016).

[2] "Carbon membranes for efficient water-ethanol separation," S. Gravelle, H. Yoshida, L. Joly, C. Ybert, L. Bocquet, J. Chem. Phys. 145, 124708 (2016).

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