2D water: How does it flow?

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Two-dimensional (2D) water, confined by atomically flat layered materials, may transit into various ordered phases even at room temperature [1]. However, the transport of such water is still not well understood. The problem is that conventional hydrodynamic approach in terms of the slip length requires a well-developed out-of-plane flow velocity profile absent in the truly 2D limit. Here, we consider the Navier-Stokes equation in the 2D limit assuming no vorticity (rot **v** = 0) but a certain compressibility (div **v** ≠ 0), where **v** is the flow velocity [2]. The first and second viscosity coefficients deduced from the viscous stress tensor then acquire the physical meanings of the effective interfacial and dilatational viscosities, respectively. At the same time, we perform molecular dynamic (MD) simulations and fit the resulting flow velocity using the effective viscosity coefficients. **Figure 1** demonstrates how the effective viscosity coefficients are influenced by the channel's material and height. The result opens an interesting opportunity to obtain various nanofluids out of the same water molecules just by using alternate materials to fabricate the 2D channels.

References

[1] S. Negi, A. Carvalho, M. Trushin, A. H. Castro Neto, The Journal of Physical Chemistry C, 37 (2022) 16006.
[2] M. Trushin, A. Carvalho, A. H. Castro Neto, unpublished.

Figures

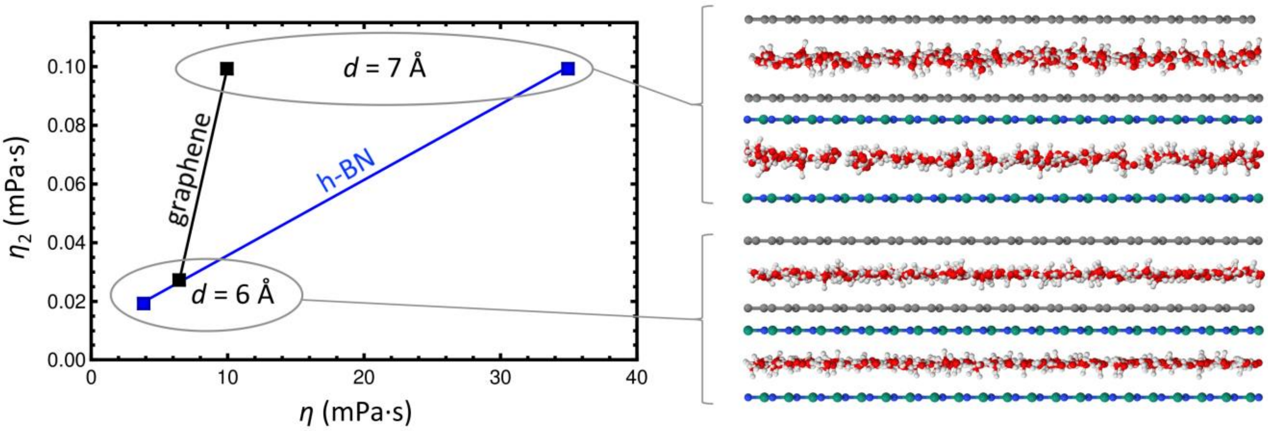

Figure 1: Changing the channel's height and material strongly influences the effective viscosity coefficients obtained by fitting our MD simulations. The snapshots on the right show that while all oxygen atoms are nearly aligned in one plane in narrow channels (6 Angstrom), they acquire an out-of-plane staggering pattern in wider channels (7 Angstrom) leading to stronger interactions with the channel walls. The water layer remains 2D in all cases (monolayer). The staggering pattern is more pronounced in the h-BN channel, which is reflected in the higher viscosity coefficients. Here, O, H, C, B and N atoms are represented in red, white, grey, green and blue, respectively.