On slip and diffusion of water confined between two-dimensional materials from ab initio molecular dynamics

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Water slip under confinement has received increased attention in the recent years, driven by the interest to develop efficient desalination membranes, as well as nanoscale osmotic power generators [1,2]. The electronic and chemical nature of materials has been suggested to be highly relevant to slip [3,4]. In this work, we present results on the structure and collective dynamics (i.e. the friction and the diffusion coefficient of the fluid) of liquid water confined between graphene, hBN, and MoS_2 sheets from ab initio molecular dynamics simulations. We find that the friction coefficient changes dramatically between the three materials, due to their strikingly different underlying energy landscape. We also report on an intriguing mechanism driving slip under confinement, where stronger confinement regimes give rise to an enhanced slip, due to a reduced friction decorrelation time. Finally, we find that the mean square displacement of the liquid under confinement m ay not be linear with time (as it is instead in Brownian motion), and instead its exponent may depend on the confining material.

[1] Siria A, Bocquet ML, Bocquet L. , *Nature Reviews Chemistry* **1**, 11 (2017).
[2] Abraham J, Vasu KS, Williams CD, Gopinadhan K, Su Y, et al. , *Nature Nanotechnology* **12**, 546 (2017).
[3] Tocci G, Joly L, Michaelides A., *Nano Letters* **14**, 6872 (2014).
[4] Secchi E, Marbach S, Nigues A, Stein D, Siria A, Bocquet L., *Nature* **537**, 210 (2016).