Fluctuation-induced quantum friction in nanoscale water flows

The flow of water in carbon nanochannels has defied understanding thus far, with accumulating experimental evidence for ultra-low friction, exceptionally high water flow rates and curvature-dependent hydrodynamic slippage. In particular, the mechanism of water–carbon friction remains unknown, with neither current theories nor classical or ab initio molecular dynamics simulations providing satisfactory rationalization for its singular behaviour. Here we develop a quantum theory of the solid–liquid interface, which reveals a new contribution to friction, due to the coupling of charge fluctuations in the liquid to electronic excitations in the solid. We expect that this quantum friction, which is absent in Born–Oppenheimer molecular dynamics, is the dominant friction mechanism for water on carbon-based materials. As a key result, we demonstrate a marked difference in quantum friction between the water–graphene and water–graphite interface, due to the coupling of water Debye collective modes with a thermally excited plasmon specific to graphite. This suggests an explanation for the radius-dependent slippage of water in carbon nanotubes, in terms of the electronic excitations of the nanotubes. Our findings open the way for quantum engineering of hydrodynamic flows through the electronic properties of the confining wall.

Even though the liquid flow rate through a macroscopic channel is determined solely by its geometry, the permeability of nanoscale channels depends strongly on the amount of liquid friction at the channel walls. Current theories of the solid–liquid interface picture the solid as a static external potential that acts on the fluid molecules, with the friction resulting from the surface roughness of the solid. This approach involves a high degree of arbitrariness when applied to atomically smooth surfaces, through the choice of the molecular force fields. There is, for instance, a three orders of magnitude spread in the reported molecular dynamics (MD) simulation results for the water friction coefficient inside sub-10 nm carbon nanotubes (CNTs). On the experimental side, water–carbon friction presents a particularly puzzling picture: friction is found to be much stronger on graphite than on monolayer graphene, and in carbon nanotubes, in terms of the electronic excitations of the nanotubes. Our findings open the way for quantum engineering of hydrodynamic flows through the electronic properties of the confining wall.

Single-particle friction

We first consider a single point charge $e$ moving at a height $h$ parallel to a solid surface lying in the $(x, y)$ plane. Taking electronic degrees of freedom into account gives rise to a polarization charge within the solid and dissipation through the polarization charge dynamics. We formalize this mechanism by introducing the solid surface response function $g_e(q, \omega)$, defined in terms of the density–density response function $\chi_e$:

$$
\chi_e(q, \omega) = \frac{-e^2}{4\pi \epsilon_0} \int_{-\infty}^{0} dz dz' e^{i (q^2 + q') z} \chi_e(q, z, z', \omega),
$$

with the wavevector $q$ lying in the plane of the interface. Physically, $g_e(q, \omega)$ relates the external potential applied to the solid in the half-space $z < 0$ to the induced potential in the half-space $z > 0$ (Supplementary Section 3.1). The friction force on the charge moving at velocity $v$ is then written as (Supplementary Section 1):

$$
f = \frac{-e^2}{8\pi \epsilon_0} \int dq \frac{q}{q} e^{-2\pi h} \text{Im} \, g_e(q, q \cdot v).
$$

Equation (2) accounts for electronic friction, that is, friction through the generation of electronic excitations within the solid. This phenomenon has been invoked in various situations in which classical nuclear degrees of freedom are coupled to an electron bath. The mechanism

---

Nikita Kavokine1,2✉, Marie-Laure Bocquet3 & Lydéric Bocquet1,2✉

1Laboratoire de Physique de l’Ecole Normale Supérieure, ENS, Université PSL, CNRS, Sorbonne Université, Université Paris-Diderot, Sorbonne Paris Cité, Paris, France. 2Center for Computational Quantum Physics, Flatiron Institute, New York, NY, USA. 3PASTEUR, Département de Chimie, École Normale Supérieure, PSL University, Sorbonne Universités, CNRS, Paris, France.

✉e-mail: nikita.kavokine@ens.fr; lyderic.bocquet@ens.fr

Published online: 2 February 2022

Received: 7 May 2021

Accepted: 25 November 2021

https://doi.org/10.1038/s41586-021-04284-7

Check for updates

84 | Nature | Vol 602 | 3 February 2022
Here $V$ is the Coulomb potential, $n_{e}$ is the instantaneous charge density of water, $\hat{n}$ is the electron density operator and $\nabla$ represents the gradient with respect to the position $r$ in the direction parallel to the interface; the average is over all thermal and quantum fluctuations of the system. The dynamics of water are well described within classical mechanics even at the molecular scale. Nevertheless, to ensure formal consistency, we represent the water charge density by a Gaussian quantum field $\hat{n}_{w}$ with prescribed correlation functions, as is done, for example, in the theory of solvation. The average in equation (3) is then computed in the framework of many-body perturbation theory, with respect to the interaction Hamiltonian that comprises both the electron–water and electron–electron Coulomb interactions:

$$\hat{H}_{int} = \int dr dr' \hat{n}_{w}(r', t) V(r-r') \hat{n}_{w}(r, t) + \frac{1}{2} \int dr dr' \hat{n}_{e}(r', t) V(r-r') \hat{n}_{e}(r, t).$$

As the system is out of equilibrium in the presence of water flow, we treat the perturbative expansion in the Schwinger–Keldysh framework. After a computation reported in Supplementary Section 2, our most general result is a Dyson equation relating the water–electron, water–water and electron–electron density correlation functions, whose Feynman diagram representation is given in Fig. 1d. The friction force may then be expressed in terms of the Keldysh component of the water–electron correlation function.

The formal Dyson equation can be simplified if the water and electron densities are no longer allowed to interpenetrate each other. This is a reasonable approximation as long as there is no chemisorption of water on the solid surface. The short-range Pauli repulsion effectively acts as an infinite potential barrier between the water and the electrons, as confirmed by density functional calculations of the water–graphene interface. The hydrodynamic flow profile above the solid surface is assumed to be uniform and equal to the interfacial velocity $v$, which is justified as long as the typical range of the solid–liquid interactions is smaller than the slip length. Then, expanding the Dyson equation to linear order in $v$, we obtain a closed expression of the form $\langle F \rangle / A = -\lambda v$, where $A$ is the surface area and $\lambda$ is the solid–liquid friction coefficient. The coefficient $\lambda$ separates into two terms, $\lambda = \lambda_{cl} + \lambda_{Q}$, with

$$\lambda_{cl} = \frac{1}{4\pi^{2}k_{B}T} \int dq \langle (q) \rangle^{2} \int_{0}^{\infty} dr \ S_{w}(\mathbf{q}, t)$$

and

$$\lambda_{Q} = \frac{1}{8\pi} \int \int_{0}^{\infty} dq d(\hbar q) \frac{d(\hbar q)}{k_{B}T} \frac{qu}{\sinh^{2}\left(\frac{\hbar q}{2k_{B}T}\right)} \right|_{1 - g_{w}(\mathbf{q}, \omega) g_{w}(\mathbf{q}, \omega)}^{0}.$$
As it is accessible through MD simulations, the classical contribution has been well studied for numerous solid–liquid systems\(^2\). We will therefore discuss in detail only the quantum contribution in equation (6), which has not been considered previously. The structure of equation (6) can be understood in terms of quasiparticle tunnelling between the surface fluctuation modes of the two media, as detailed in Supplementary Section 2.8. In brief, the quantum friction force \(\mathbf{\nu} \times \boldsymbol{\xi}_0\) decomposes into a (continuous) sum over the wavevectors \(q\) of surface modes: \(\mathbf{\nu} \times \boldsymbol{\xi}_0 = (1/4\pi) \int dq f_q\). The elementary friction force \(f_q\) is given by the elementary momentum \(h\kappa\) multiplied by an integral over the frequencies \(\omega\). The frequency integral corresponds to the quasiparticle tunnelling rate between modes at wavevector \(q\). This rate is non-zero only in the presence of a water flow, which effectively increases the occupation of the liquid modes with respect to the solid modes (Fig. 1c). We note that the contribution in equation (6) requires thermal fluctuations, as it vanishes at a temperature of 0 K. A purely quantum contribution to non-contact friction, that survives at 0 K, may be derived\(^2\), but it scales as \(q^3\) and is hence negligible for our purposes.

The quantitative evaluation of water–solid quantum friction coefficients requires both surface excitation spectra, \(\text{Im} g_q(q, \omega)\) and \(\text{Im} g_{\text{w}}(q, \omega)\), as inputs. We focus on excitations at low energy, typically around 100 meV. It results from the collective relaxation of molecular dipoles and it is a general feature of polar liquids\(^24,25\). Hence, our subsequent discussion, although focussed on water, applies qualitatively to quantum friction in other polar liquids as well. The sharp peak at around 100 meV corresponds to the librational modes of the water molecule.

The water surface response function shows little dispersion as the momentum \(q\) is increased (Fig. 2c and Supplementary Fig. 1), and only small variations are found between the two models for the graphite surfaces. At large momenta \((q \gtrsim 1 \text{ Å}^{-1})\), the surface response function shows an exponential decrease, which we attribute to the depletion of water near the hydrophobic surface. For the purposes of calculation, \(g_{\text{w}}(q, \omega)\) is well represented by the sum of two Debye peaks at \(\omega_{D,1} = 1.5\text{ meV}\) and \(\omega_{D,2} = 20\text{ meV}\), with momentum-dependent oscillator strengths:

\[
g_{\text{w}}(q, \omega) = \frac{f_1(q)}{1 - \text{i} \omega/\omega_{D,1}} + \frac{f_2(q)}{1 - \text{i} \omega/\omega_{D,2}},
\]

Analytical expressions for \(f_1(q)\) and \(f_2(q)\) are given in Supplementary Section 4.3; at large \(q\), \(f_1(q) + f_2(q) = e^{-2qd}\), with \(d = 0.95\text{ Å}\). Further MD simulations show that the features of the water surface response relevant for quantum friction are largely unaffected by planar confinement down to 1 nm (Supplementary Section 4.4), so that the expression in equation (8), determined for a semi-infinite liquid, can be safely applied to nanoconfined geometries.

### Electronic excitations and the jellium model

A solid has low-energy electronic excitations if it contains free charge carriers, but the precise location of these excitations in energy–momentum space depends strongly on the exact band structure. The simplest way to account for this dependence is in the framework of the jellium model. The nuclei and core electrons are assimilated to a semi-infinite positive background, whereas the conduction electrons behave as free...
electrons (Fig. 3a). They occupy a parabolic band, \( E(k) = \hbar^2 k^2/(2m') \): the electronic structure is then completely determined by the effective mass \( m' \) and the Fermi energy \( E_F \). In general, in the jellium model, electrons are allowed to spill over the positive background edge. However, in the presence of water, the spillover is limited by the Pauli repulsion between the water and the surface electrons (Fig. 1b), so that the infinite barrier jellium model seems better suited to describing the electronic system under scrutiny. The model may then be treated within the specular reflection approximation—expressing the surface response in terms of the bulk dielectric response—with only small quantitative differences with respect to the exact semi-infinite computation (Supplementary Sections 3.2 and 5.1). A typical result for the jellium surface response function \( g_\omega (q, \omega) \) in the specular reflection approximation is shown in Fig. 3b. It presents two types of features: incoherent particle–hole excitations and a collective surface plasmon mode. We then compute the quantum friction coefficient \( \lambda_Q \) of water on the jellium surface according to equation (6), for a range of Fermi energy and effective mass values (Fig. 3c). Note that in terms of the slip length \( b = \eta/\lambda \) (with \( \eta \) the fluid viscosity), \( \lambda = 10^3 \text{ N s m}^{-3} \) corresponds to a slip length \( b = 10 \text{ nm} \) for water.

We find the quantum contribution to friction to be very small for water on semiconductor surfaces, which, for our purpose, can be described by a jellium model with low Fermi energy and effective mass. In such systems, electronic excitations are restricted to very small momenta, and we expect the hydrodynamic friction to be dominated either by the classical roughness term or by the optical phonon contribution (Supplementary Section 5.3). On metal surfaces, with high Fermi energy (1–10 eV) and effective mass close to unity, we find \( \lambda_Q = 10^2 \text{ N s m}^{-3} \), which is two orders of magnitude lower than typical hydrodynamic friction coefficients, and probably smaller than the roughness-based contribution. We note that our theory does not address reactive (typically non-close-packed) metal surfaces, on which chemical bonding with water occurs. The highest values of \( \lambda_Q \) are obtained in the region of low Fermi energy and high effective mass. The electronic surface plasmon mode is then at low enough energy (around 10 meV) and high enough momenta (around 0.5 Å\(^{-1})\), to couple with the Debye peak of water, yielding a particular friction enhancement (Fig. 3c and Supplementary Fig. 3).

**The odd water–carbon interface**

The classical contribution to water–carbon friction has been extensively studied in the framework of MD simulations. On flat graphite surfaces, simulated friction coefficient values \( \lambda_{Cl} = 10^4 \text{ N s m}^{-3} \) have been reported, depending on the chosen force field. In CNTs, these values were found to be unaffected by wall curvature for tube radii larger than 10 nm (refs. 8,9). This strongly suggests that the radius dependence of water slippage observed experimentally in CNTs with radii between 15 and 50 nm (ref. 4) cannot be explained by the classical contribution to friction alone. The experiments in ref. 4 then set an upper bound for the water–carbon classical friction at the lowest total friction coefficient measured in large radius nanotubes, that is, \( \lambda_{Cl}^{\text{max}} = 3 \times 10^3 \text{ N s m}^{-3} \). Hence, MD simulations probably overestimate the water–graphite friction coefficient by at least a factor of 3, which is typical in simulations of other water–solid systems.

We now consider quantum friction in various water–carbon systems. For a single graphene sheet, the surface response function can be calculated analytically (Supplementary Section 6.1). The result is plotted in Fig. 4a, with a doping level \( E_F = 0.1 \text{ eV} \). Graphene is found to have low-energy excitations (\( \omega < 100 \text{ meV} \)) only at very small momenta (\( q < 0.05 \text{ Å}^{-1})\). An intralayer plasmon mode is present, but it displays a steep square-root dispersion at small momenta. The quantum contribution to the water friction coefficient, evaluated with equation (6), is accordingly found to be very small, below \( 10^{-6} \text{ N s m}^{-3} \), regardless of doping level. We conclude that hydrodynamic friction on monolayer graphene is dominated by the classical contribution and should therefore be very small (\( \lambda = \lambda_{Cl}^{\text{max}} \)). This is in line with recent measurements of water slippage on silica-supported graphene, which yielded friction coefficients as small as \( 4.5 \times 10^{-5} \text{ N s m}^{-1} \) (slip length \( b = 200 \text{ nm} \)).

The situation must be different for water on multilayer graphite, which was found experimentally to exhibit much higher hydrodynamic friction: \( \lambda = 2 \times 10^4 \text{ N s m}^{-3} \) on flat graphite surfaces and \( \lambda = 3 \times 10^4 \text{ N s m}^{-3} \) in multilayer CNTs with large (50 nm) radii. Indeed, in a staggered stack of graphene sheets (Fig. 4b), electrons acquire an extra degree of freedom compared to monolayer graphene, as they may tunnel between the sheets. In particular, the coupling between second nearest layers is associated with a bandwidth \( \gamma_{Plas} = 40 \text{ meV} \) (with \( \gamma_P \) an interlayer coupling parameter, see Fig. 4b), resulting in a markedly different low-energy excitation spectrum. In electron energy loss spectroscopy, graphite was found to show a surface plasmon mode, polarized perpendicularly to the layers, at a frequency \( \omega_P = 50 \text{ meV} \) (at 300 K), with a very flat dispersion in the measured momentum range, which was up to \( \omega_{\max} = 0.2 \text{ Å}^{-1} \) at 300 K (ref. 20) and \( \omega_{\max} = 0.4 \text{ Å}^{-1} \) at 600 K (ref. 20) (Fig. 4a). We expect this low-energy plasmon of graphite to strongly interact with the water Debye mode, resulting in an enhancement of the quantum friction. As a first approximation, we describe the plasmon contribution to the graphite surface response in terms of a Drude model, which is based on the semiclassical treatment of free electron dynamics:

\[
g_{sc}(q, \omega) = \frac{\omega_p^2}{\omega_p^2 - \omega^2 - 2i\omega \gamma_P(q_{\max} - q)},
\]

where \( \omega_P = 40 \text{ meV} \) and \( \gamma_P = 40 \text{ meV} \) (ref. 20). We note that the quantum contribution to friction is then small in the region of low momenta, where the Drude mode is dominant, and large for large momenta, where it is negligible.

**Surface response function for a semi-infinite barrier jellium model: the water and solid electrons are separated by an infinite potential barrier.** a, b, Surface response function for a semi-infinite barrier jellium model: the water and solid electrons are separated by an infinite potential barrier. b, Surface response function for a semi-infinite barrier jellium model: the water and solid electrons are separated by an infinite potential barrier. c, Quantum friction coefficient for water on a jellium surface, as a function of the jellium Fermi energy and effective mass (in units of electron mass).
For graphite, the friction coefficient is determined from the one-dimensional density. For graphene, the carrier density is determined by the doping level. A microscopic model is needed to extract the essential physics at play. Our starting point is that the free charge carriers contributing to the low-energy plasmon are located mainly on the B sublattice (Fig. 4b). We then compute the local density response of the topmost (surface) atoms. We then compute the local density response of the topmost atom of a one-dimensional chain $\delta n_q(\omega) = X_0(\omega) \phi_0(\omega)$, where $\phi_0$ is the potential acting on atom $a$ (Supplementary Section 6.2). Then, treating the Coulomb interactions between the chains in the random phase approximation, we obtain the graphite surface response function as

$$g_0(q, \omega) = \frac{n_s \nu_q X_0(q, \omega)}{n_s \nu_q X_0(q, \omega) - 1}. \quad (10)$$

where $\nu_q = \frac{e^2}{4 \pi \varepsilon_0} \frac{2n}{q}$ is the free charge carrier density in bulk graphite at $300\, \text{K}$ ($n_s = 2.3 \times 10^{12}\, \text{cm}^{-2}$; see Supplementary section 6.2); this yields a friction coefficient $\lambda_q = 1.8 \times 10^{-4}\, \text{N s m}^{-2}$, which is slightly larger than the Drude model estimates and within the range of experimentally measured water friction coefficients on graphite (Fig. 4d). Ultimately, the value of $n_s$ depends on the details of the electronic structure at the graphite surface, which undergoes renormalization in the presence of water. An increase in the density of states at low energy and high momenta with $\nu = 25\, \text{meV}$ the surface plasmon width and $\theta$ the Heaviside step function. Using this expression in equation (6), we obtain a water friction coefficient $\lambda_q = 0.4 \times 10^{-3}\, \text{N s m}^{-2}$ for $q_{\text{max}} = 0.2\, \text{Å}^{-1}$ and $\lambda_q = 5 \times 10^{-3}\, \text{N s m}^{-2}$ for $q_{\text{max}} = 0.4\, \text{Å}^{-1}$. This is orders of magnitude larger than the expected value for graphite (Fig. 4c) and comparable to the upper bound for the classical contribution $\lambda_{\text{bulk}}$. Hence, the Drude model estimate suggests that the quantum contribution may account for the difference in hydrodynamic slippage between monolayer graphene and multilayer graphite.

Going beyond a phenomenological treatment for the water–graphite quantum friction is particularly challenging, due to the very large unit cell required for a numerical investigation of low-energy and high-momentum surface excitations. We propose here a simplified microscopic model to extract the essential physics at play. Our starting point is that the free charge carriers contributing to the low-energy plasmon are located mainly on the B sublattice (Fig. 4b). The flat plasmon dispersion has been attributed to the shape of the bands containing those free carriers. As a consequence of interlayer coupling, these are nearly flat up to parallel momentum $k = \gamma_1 / \nu_1 = 0.06 - 0.11\, \text{Å}^{-1}$, with $\gamma_1$ the nearest-neighbour interlayer coupling parameter (Fig. 4b) and $\nu_1$ the graphene Fermi velocity. Then, from the perspective of low-energy excitations, graphite may be pictured as an array of independent one-dimensional chains extending perpendicular to the layers, at least within a certain momentum range. This assembly of localized oscillators is then expected to have excitations whose energy does not depend on the wavevector, as is observed experimentally.
due to electron scattering on water fluctuations may lead to a higher apparent $n_1$, (the upper limit being the total electron density on the B sublattice. $4.3 \times 10^{14}$ cm$^{-2}$) and to a further increase in the expected value for the quantum friction coefficient (Fig. 4c).

Overall, our theory predicts a strong difference in quantum friction between monolayer and multilayer carbon structures, explaining how water can exhibit larger slippage on monolayer graphene than on multilayer graphite$^{31,32}$. This further suggests an explanation for the radius-dependent water slippage in multilayer CNTs$^8$. In these quite large nanotubes (with 15–50 nm radii), although the water surface response is unaffected by confinement (Supplementary Section 4), the interlayer coupling is known to strongly depend on radius. It was observed that a 50-nm-radius tube locally has a graphite-like structure, whereas in a 10-nm-radius tube the shells are completely decoupled$^{34}$. Therefore, in large radius nanotubes, water is subject to graphite-like high quantum friction, whereas in smaller radius nanotubes water experiences graphene-like low friction, probably dominated by the classical contribution.

The quantitative relevance of this argument can be checked, at the simplest level, in the framework of the Franklin model$^{35,36}$, which relates the probability $p$ of two layers being misaligned in a graphite structure to the average interlayer spacing $d$: $d = 3.44 - 0.086 \times (1 - p^2) (\AA)$. The dependence of $d$ on the inner radius $R$ for a multiwall nanotube can be inferred from experiment$^{38}$ (Supplementary Section 6.4). We may then assume that the electron density $n_1$ in equation (10) scales according to $n_1(R) = n_1(1 - p(R))$, and we choose $n_1 = 10^{12}$ cm$^{-2}$ so that $\lambda(R \rightarrow \infty) = 4.4 \times 10^4$ N m$^{-1}$. The resulting prediction for the slip length is shown in Fig. 4d and it is found to be in good agreement with the experimental data. We note that if the inner shell tubes are semiconducting, then the radius-dependent band gap $E_\text{F}(R) = (2/3) \varepsilon_0 R(\text{ref. } 35)$ may also reduce the number of charge carriers contributing to low-energy excitations; we then expect a scaling $n_1(R) = n_1 \varepsilon_0 E_\text{F}(R)/\hbar^2$, which also provides reasonable agreement with the data (Fig. 4d).

Although the details of electronic excitations in multilayer CNTs are hard to investigate theoretically, our theory strongly suggests that quantum friction is a key ingredient for determining the water slip length in these systems.

Perspectives
Our theory predicts quantum effects in the dynamics of the solid–liquid interface. We show that hydrodynamic friction results not only from the static roughness of the solid surface, but also from the coupling of water fluctuations to electronic excitations within the solid. Such ‘quantum friction’ is uniquely revealed at the water–carbon interface. Water friction is not anomalously low on graphene, but instead it is anomalously high on graphite, due to the quantum contribution resulting from a graphite-specific terahertz plasmon mode. This finding enables us to rationalize the peculiar friction properties of water on carbon surfaces, and in particular the radius dependence of slippage in CNTs. More generally, quantum friction may be an important contribution to hydrodynamic friction on atomically smooth surfaces, provided that these have electronic excitations at low energy ($\omega \leq 100$ meV) and high momenta ($q \approx 0.5$ Å$^{-1}$), which may couple to the Debye mode of water. However, true atomic smoothness cannot be achieved for any material, because many surfaces become oxidized or charged in water. For instance, the negligible water slippage observed on hexagonal boron nitride surfaces$^8$ can be attributed to the chemical–isolation of charged species$^{31,38}$. We stress that quantum friction is an effect beyond the Born–Oppenheimer approximation. Although it can be overcome in the numerical treatment of single molecules on surfaces$^{39}$, the Born–Oppenheimer approximation remains a fundamental limitation in simulations of solid–liquid interfaces. Our results call for the development of new methods for simulating such complex interfacial systems$^{39}$.

Online content
Any methods, additional references, Nature Research reporting summaries, source data, extended data, supplementary information, acknowledgements, peer review information; details of author contributions and competing interests; and statements of data and code availability are available at https://doi.org/10.1038/s41586-021-04284-7.

1. Bocquet, L. Nanofluidics coming of age. Nat. Mater. 19, 254–256 (2020).
2. Holt, J. K. et al. Fast mass transport through sub-2-nanometer carbon nanotubes. Science 312, 1034–1037 (2006).
3. Whitby, M., Cagnon, L., Thanou, M. & Quirke, N. Enhanced fluid flow through nanoconfined carbon pipes. Nano Lett. 8, 2632–2637 (2008).
4. Secchi, E. et al. Massive-radius-dependent flow slippage in carbon nanotubes. Nature 557, 210–213 (2016).
5. Xie, Q. et al. Fast water transport in graphene nanofluidic channels. Nat. Nanotechnol. 13, 238–245 (2018).
6. Faucher, S. et al. Critical knowledge gaps in mass transport through single-digit nanotubes: a review and perspective. J. Phys. Chem. C 123, 21309–21326 (2019).
7. Bocquet, L. & Barrat, J. L. Flow boundary conditions from nano- to micro-scales. Soft Matter 3, 685–693 (2007).
8. Thomas, J. A. & McGaughey, A. J. Reassessing fast water transport through carbon nanotubes. Nano Lett. 8, 2788–2793 (2008).
9. Falk, K., Sedlmeyer, F., Joly, I., Netz, R. R. & Bocquet, L. Molecular origin of fast water transport in carbon nanotube membranes: superfluibricity versus curvature dependent friction. Nano Lett. 10, 4061–4073 (2010).
10. Tocci, G., Joly, I. & Michaelides, A. Friction of water on graphene and hexagonal boron nitride from ab initio methods: very different slippage despite very similar interface structures. Nano Lett. 14, 6672–6677 (2014).
11. Kavokin, N., Netz, R. R. & Bocquet, L. Fluids at the nanoscale: from continuum to subcontinuum transport. Annu. Rev. Fluid Mech. 53, 377–410 (2021).
12. Sam, A. et al. Fast transport of water in carbon nanotubes: a review of current accomplishments and challenges. Mol. Surf. 47, 905–924 (2021).
13. Maali, A., Cohen-Bouhacina, T. & Kelley, H. Measurement of the slip length of water flow on graphene surface. Appl. Phys. Lett. 92, 2007–2009 (2008).
14. Misra, R. P. & Blankschtein, D. Insights on the role of many-body polarization effects in the wetting of graphitic surfaces by water. J. Phys. Chem. C 121, 28166–28179 (2017).
15. Weddle, A. M., Tully, J. C. & Auerbach, D. J. Electronically non-adiabatic interactions of molecules at metal surfaces: can we trust the Born-Oppenheimer approximation for surface chemistry? Int. Rev. Phys. Chem. 23, 513–539 (2004).
16. Dou, W. & Subotnik, J. E. Perspective: how to understand electronic friction. J. Chem. Phys. 148 (2018).
17. Sikoloff, J. B. Enhancement of the water flow velocity through carbon nanotubes resulting from the radius dependence of the friction due to electron excitations. Phys. Rev. E 97, 031018 (2018).
18. Volokitin, A. I. & Persson, B. N. Near-field radiative heat transfer and noncontact friction. Rev. Mod. Phys. 79, 1291–1329 (2007).
19. Song, X., Chandler, D. & Marcus, R. A. Gaussian field model of dielectric solvation dynamics. J. Phys. Chem. 100, 1954–1959 (1996).
20. Rammer, J. & Smith, H. Quantum-field-theoretical methods in transport theory of metals. Rev. Mod. Phys. 58, 323–359 (1986).
21. Bocquet, L. & Charlaix, E. Nanofluidics, from bulk to interfaces. Chem. Soc. Rev. 39, 1073–1095 (2010).
22. Pendry, J. B. The shear quantum – Quantum friction. J. Phys. Condens. Matter 9, 10301–10320 (1997).
23. Carlson, S., Brujinig, F. N., Loche, P., Bonhuis, D. J. D. & Netz, R. R. Exploring the absorption spectrum of simulated water from MHz to infrared. J. Phys. Chem. A 124, 5598–5605 (2020).
24. Sato, T. & Buchner, R. Dielectric relaxation processes in ethanol/water mixtures. J. Phys. Chem. A 108, 5007–5015 (2004).
25. Koeberg, M., Wu, C. C., Kim, D. & Bonn, M. Thz dielectric relaxation of ionic liquid water mixtures. Chem. Phys. Lett. 439, 60–64 (2007).
26. Lang, N. D. & Kohn, W. Theory of metal surfaces: charge density and surface energy. Phys. Rev. B 17, 4555–4568 (1978).
27. Parragh-Guerra, L. E., Gonzalez-Valle, C. U. & Ramos-Alvarado, B. Effects of the interfacial modeling approach on equilibrium calculations of slip length for nanoconfined water in carbon slits. Langmuir 36, 14772–14781 (2020).
28. Radha, B. et al. Molecular transport through capillaries made with atomic-scale precision. Nature 538, 222–225 (2016).
29. PORTAIL, M., Carrere, M. & Layet, J. M. Dynamical properties of graphite and peculiar behaviour of the low-energy plasmon. Surf. Sci. 343, 863–867 (1996).
35. Franklin, R. E. The structure of graphitic carbons. Acta Crystallogr. 4, 253–261 (1951).
36. Speck, J. S., Endo, M. & Dresselhaus, M. S. Structure and intercalation of thin benzene derived carbon fibers. J. Cryst. Growth 94, 834–848 (1989).
37. Charlier, J. C., Blase, X. & Roche, S. Electronic and transport properties of nanotubes. Rev. Mod. Phys. 79, 677–732 (2007).
38. Xie, Y., Fu, L., Niehaus, T. & Joly, L. Liquid-solid slip on charged walls: the dramatic impact of charge distribution. Phys. Rev. Lett. 125, 014501 (2020).
39. Pham, T. A., Ping, Y. & Galli, G. Modelling heterogeneous interfaces for solar water splitting. Nat. Mater. 16, 401–408 (2017).

Publisher’s note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.

© The Author(s), under exclusive licence to Springer Nature Limited 2022
**Data availability**

The MD simulation data (Fig. 2 and Supplementary Figs. 1 and 2) are available on Zenodo (https://doi.org/10.5281/zenodo.5242930). The rest of the data are included with the paper.

**Acknowledgements**

We thank A. Robert for help with MD simulations and acknowledge fruitful discussions with A. Robert, B. Douçot, R. Netz, B. Coasne, N. Lorente and B. Rotenberg. L.B. acknowledges funding from the EU H2020 Framework Programme/ERC Advanced Grant agreement number 785911-Shadoks and ANR project Neptune. This work has received the support of ‘Institut Pierre-Gilles de Gennes’, programmes ANR-10-IDEX-0001-02 PSL and ANR-10-LABX-31. We acknowledge the French HPC resources of GENCI for grant number A9-A0070807364. The Flatiron Institute is a division of the Simons Foundation. We acknowledge the inspiration and contributions to science of late Jorge Iribas Cerdà.

**Author contributions**

L.B., M.-L.B. and N.K. conceived the project. N.K. developed the theoretical framework. N.K. and L.B. co-wrote the paper, with input from M.-L.B. All authors discussed the results and commented on the manuscript.

**Competing interests**

The authors declare no competing interests.

**Additional information**

**Supplementary information**

The online version contains supplementary material available at https://doi.org/10.1038/s41586-021-04284-7.

**Correspondence and requests for materials**

Correspondence and requests for materials should be addressed to Nikita Kavokine or Lydéric Bocquet.

**Peer review information**

Nature thanks Mischa Bonn and the other, anonymous, reviewer(s) for their contribution to the peer review of this work. Peer reviewer reports are available.

**Reprints and permissions information**

is available at http://www.nature.com/reprints.