

# Impact of molecular ordering on lubrication

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The dynamical and lubricating properties of solid-liquid nanointerfaces control many natural and industrial processes, from the functioning of our joints, to water purification and engine efficiency. Still, our understanding is largely based on semi-empirical macroscopic models, with only a few direct links between molecular-level effects and the technologically relevant macroscopic forces<sup>1-3</sup>. Furthermore, experimental and computational methods tend to assume an ideal solid-liquid interface, whereas in real life scenarios singularities and environmental factors significantly modify the system behaviour.

Here, I address the problem by Atomic Force Microscopy (AFM), complemented by molecular dynamics simulations, to build a functional picture of two model lubricated systems down from single molecule details and up to molecular group effects (~100 nm). The investigations focus on exploring the role of molecular ordering of lubricant molecules on the friction forces [1-5].

First, I explore the effect of point defects in the lubricant liquid: single metal ions in aqueous solutions [1-2]. Ions disrupt the hydrogen bond network of the water molecules nanoconfined between two solids; locally destroying order reduces friction [1-2].

I then examined point defects in the surface, using carbon-based solids and squalane (a commercially used organic lubricant). Topographical defects limit the configurations lubricant molecules can explore inducing their organisation into well-ordered structures which strongly oppose any applied shear. My study provided the molecular mechanisms whereby roughness is able to affect lubricated friction indirectly and not only through the well-known tribological contacts [4].

Finally, using AFM and contact angle measurements, I considered more realistic systems, with undesired water particles due to humidity mixing with the main oil lubricant and creating microphase separation. The study provided a nanoscale explanation of macroscale observations: the detrimental effect of even nanoscopic quantities of water molecules on lubrication is due to effectively forcing two phases to remix as the confining solids slide one against the other with an energy penalty related to mixing/demixing. This can be mitigated by adding a surfactant reducing the interfacial energy [5]

Overall, the results contribute to bridging the current gap between atomistic models and observed macroscale phenomena with the ultimate goal of developing efficient tribological solutions for real-life systems.

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[3] Cafolla, C., et al. (2018). A non-destructive method to calibrate the torsional spring constant of atomic force microscope cantilevers in viscous environments. *Journal of Applied Physics*, 124, 154502. <https://doi.org/10.1063/1.5046648>. DOI.

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