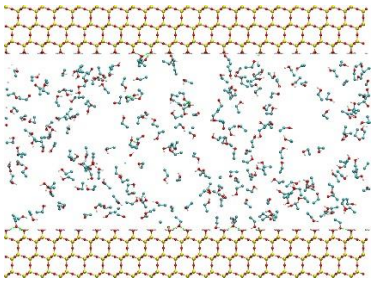
Master 1 internship; MMCI group; publication date: 04/01/2018

Osmotic flows of water-ethanol solutions on silica – toward high or low concentration?



Osmotic effects refer to the flow of liquid mixtures (often water-based) between two regions with different concentration, driven by the presence of interfaces. Usually, these interfaces correspond to the walls of a porous medium – a membrane – connecting two liquid reservoirs. Osmotic effects play a key role in living systems, in sustainable energies (with for instance the "blue energy" systems), or in water treatment and desalination processes.

Combining nanofluidic experiments and simulations at the atomic scale, we have recently shown that the standard description based on liquid-wall interactions can fail to describe the mere direction of osmotic flows for aqueous solutions of ethanol on silica surfaces [1]. We have then related the observed flow reversal to the slowdown of ethanol dynamics at the interface [1]. However, another numerical study did not observe this flow reversal on a similar system [2].

The aim of this internship is to solve this apparent discrepancy. In particular, the student will compare different approaches to measure the osmotic response used in Refs. [1] and [2] on identical systems. Moreover, the silica surfaces considered up to now in the numerical works are idealized (uncharged, crystalline) and not representative of experimental charged amorphous silica surfaces. The student will develop realistic models of water-ethanol/silica interfaces, measure their response to concentration gradients, and compare the results to experimental values.

Informal enquiries and/or applications may be addressed to Laurent Joly: laurent.joly@univ-lyon1.fr.

[1] C. Lee, C. Cottin-Bizonne, R. Fulcrand, L. Joly, C. Ybert: "Nanoscale Dynamics versus Surface Interactions: What Dictates Osmotic Transport?", J. Phys. Chem. Lett. 8, 478 (2017)

[2] H. Yoshida, S. Marbach, L. Bocquet: "Osmotic and diffusio-osmotic flow generation at high solute concentration. II. Molecular dynamics simulations", J. Chem. Phys. 146, 194702 (2017)