# Supporting information for:

# Effect of an external electric field on capillary filling of water in amorphous silica nanochannels

Nabin Kumar Karna,[†] Andres Rojano Crisson,[†] Enrique Wagemann,[†] Jens Honore Walther,[‡,¶] and Harvey A. Zambrano[*,§]

*Department of Chemical Engineering, Universidad de Concepcion, Concepcion, Chile, Department of Mechanical Engineering, Technical University of Denmark, DK-2800 Kgs. Lyngby, Denmark, Computational Science and Engineering Laboratory, Department of Mechanical and Process Engineering, ETH Zurich, CH-8092 Zurich, Switzerland, and Department of Mechanical Engineering, Universidad Tecnica Federico Santa Maria, Valparaiso, Chile*

E-mail: harveyzambrano@usm.cl

---

[*] To whom correspondence should be addressed

[†] Universidad de Concepcion

[‡] Technical University of Denmark

[¶] ETH Zurich

[§] Universidad Tecnica Federico Santa Maria

## S1. Average velocity during the viscous regime during nanocapillary imbibition in amorphous silica channels

The maximum velocity during the viscous regime of the nanocapillary imbibition is calculated from the slope of the length vs time plot, and is shown in fig S1. The maximum velocities are calculated as an average velocites observed between 4-8 nm from the channel distance, which guarantees that the inertial effects are negligible. We observe a monotonic decrease in the maximum velocity of the meniscus with increase in the field strength of the applied electric field.

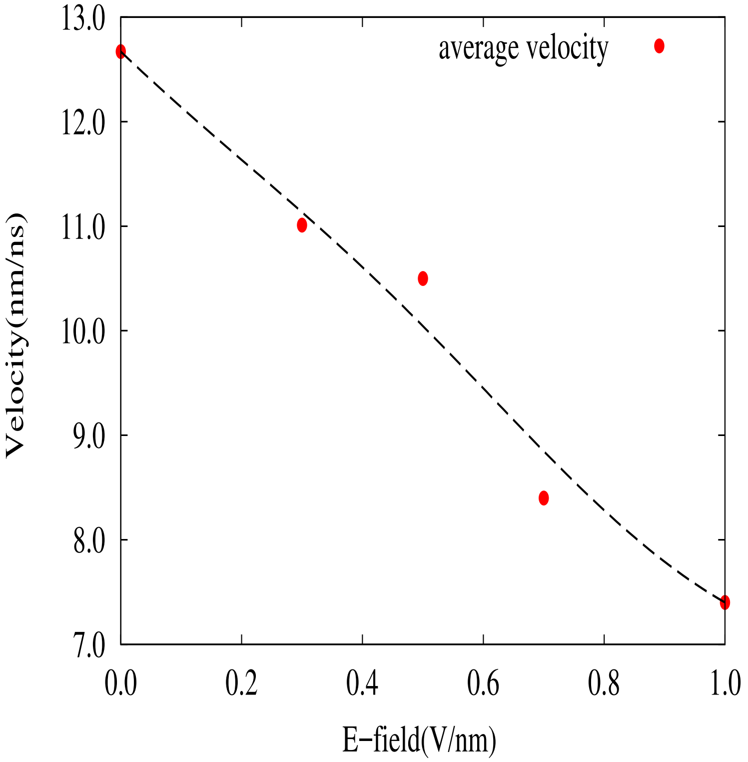

Figure S1: Average velocity during the viscous regime during the nanocapillary imbibition at different electric field strength applied parallel to the flow direction. The dotted lines represents the tendency of monotonic decrease of the maximum velocity observed during the process.

## S2. Orientation distribution of angle between the water dipole vector and the vector normal to the silica surface at different distance from the silica-wall for case without applied electric field

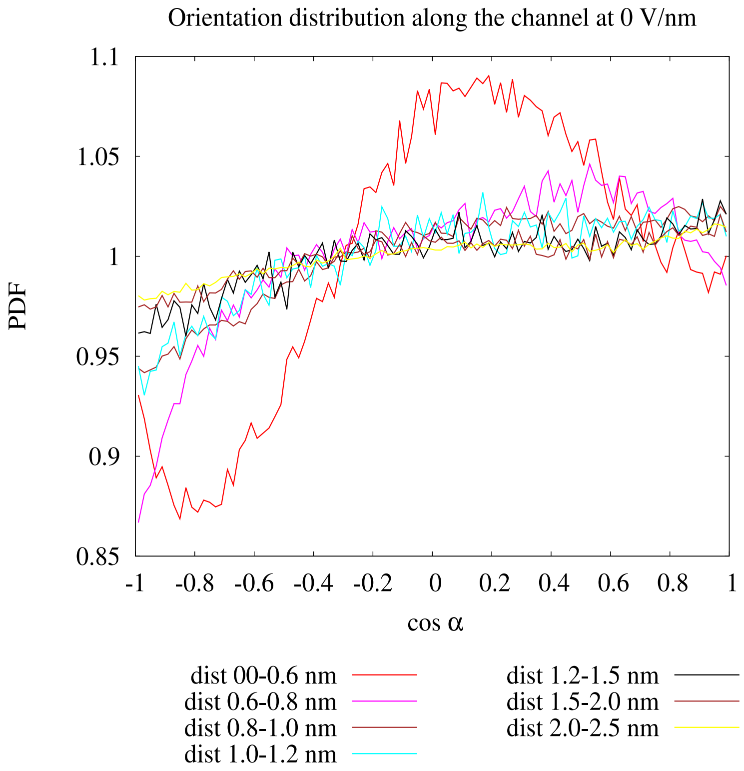

Figure S2: Distribution function of angle between the water dipole and the normal to the silica wall for case without applied electric field.

It can be observed figure S2 that the dipole orientation quickly converge to the bulk value at the distance away from 0.6 nm. This indicates that the surface walls of the capillary nanochannel significantly alter the water dipole orientation at the wall-water interface even in the absence of external electric field. This could probably be caused by the interaction of water molecules with the local electric field produced by the atoms of the wall.

## S3.Orientation distribution of the angle between the vector normal to the silica wall and the vector joining the two hydrogen bonds for different applied field strength.

A complete picture of orientation of water molecules near a surface requieres the distribution function of two important angles made by the atoms of water molecules: 1) The angle between the water dipole and the vector normal to the silica walls. 2) The angle made by the vector connecting two hydrogen atoms with the vector normal to the silica walls. We plot the latter in figure S3.

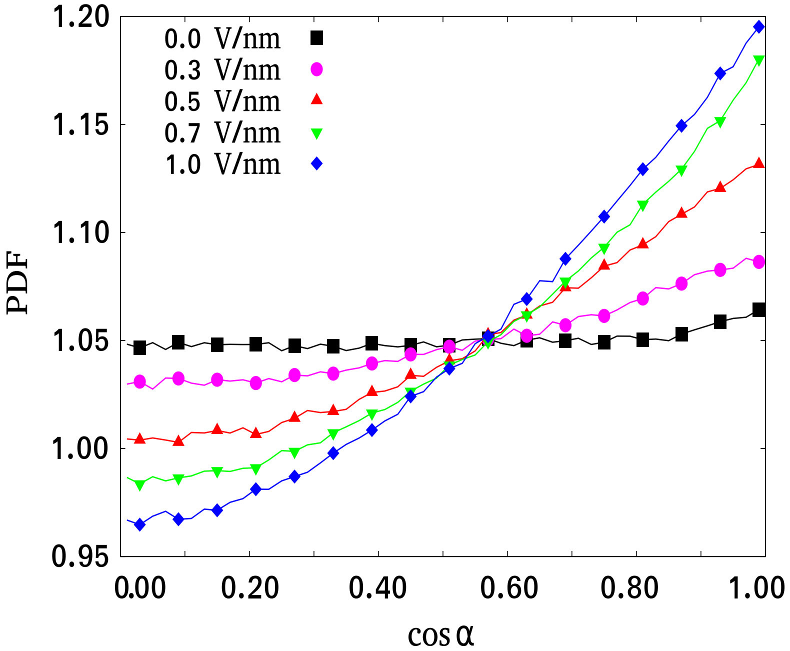

Figure S3: Orientation distribution function of the angle between the vector normal to the silica wall and the vector joining the two hydrogen bonds for different applied field strength. This function is calculated at a distance between 1.5–2.0 nm from the lower wall surface.

## S4. Orientation distribution of angle between the water dipole vector and the vector normal to the silica surface distance between 0-0.5 nm from the silica-wall for different applied electric field

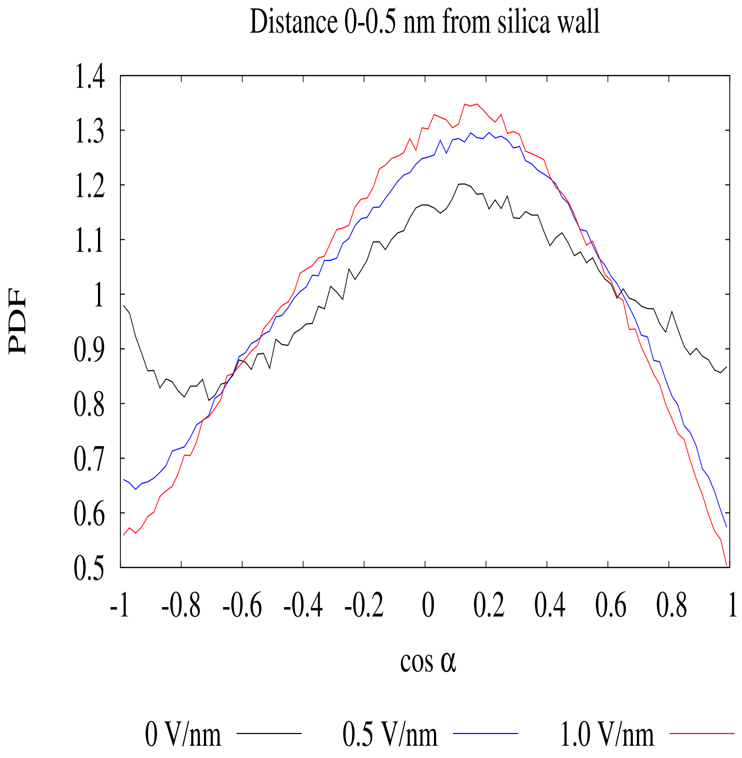

Figure S4: Distribution function of angle between the water dipole and the normal to the silica wall for different applied electric field at a distance between 0-0.5 nm from the silica surface.

It can be inferred from figure S4 that the preferred orientation of water molecules near the wall surface does not change significantly upon the application of electric field which indicates that the application of electric field orients the water molecules more strongly towards the bulk with that compared to the interfacial regions.