Abstract Submitted
for the DFD20 Meeting of
The American Physical Society

Effect of Charge Inversion on Electroosmotic Transport in Nanochannels[1] ANDRES ROJANO, DIEGO BECERRA, Universidad de Concepcion, JENS HONORE WALTHER , Technical University of Denmark, HARVEY A. ZAMBRANO, Universidad Tecnica Federico Santa Maria — The employment of electroosmosis in nanofluidic pores holds great potential for biotechnological applications. Hence, a complete understanding of the transport properties of nanoconfined multivalent electrolytes is key to enable electrokinetics as driving mechanism in nanodevices. Here, Non-equilibrium Molecular Dynamics (NEMD) simulations are conduced to study phenomena related to the presence of charge inversion in electrolytes confined in nanopores. In particular, we perform NEMD simulations of electroosmotic transport of multivalent electrolyte solutions in silica nanochannels. The solutions consist of water, chlorine as co-ion and different amounts of counter-ions i.e. sodium, magnesium and aluminum. The electroosmotic velocities are computed for different applied electric fields and magnitudes of inverted charge. Furthermore, we compute friction coefficient, zeta potential, water ordering and interfacial and bulk diffusivities and viscosities. We find that overscreening related to interfacial charge inversion modifies the electrokinetic driving force and shear stress near the walls. Our results suggest that due to charge inversion, zeta potential and water ordering are altered which induces flow reversal.

[1]We thank funding from CONICYT scholarship 21181167 and computational support from DTU

Andres Rojano
Universidad de Concepcion

Date submitted: 06 Aug 2020 Electronic form version 1.4