Abstract Submitted
for the DFD11 Meeting of
The American Physical Society

Electroosmosis in a nanofilm of chloride-aqueous solution with counter-charged surface patches[1] HARVEY ZAMBRANO, MARIE PINTI, A.T. CONLISK, SHAURYA PRAKASH, The Ohio State University — We study Electroosmotic flow (EOF) by conducting Non-Equilibrium MD Simulations (NEMDS) of water and chloride on a silica substrate. The system response is studied as axial electric fields (AEF) are imposed and as the surface charge (SC) is modified by implementing counter-charged patches (CP). The density profiles reveal that the CP result in an ionic depletion in bulk solvent and in a higher hydrophilicity than on regular silica. We compute lower velocities for the cases with higher SC on the CP. Our velocities are in agreement to results from previous MD studies. Density and velocity profiles reveal a stationary chloride layer and a stagnant water region on the CP. This stationary layer grows as CP with higher charges are settled and as weaker AEF are imposed. We infer that ionic accumulation on the CP and hydrophilicity are responsible for the EOF velocity changes for systems with different CP and the same AEF imposed. We perform continuum calculations and the EOF velocities agree with the results obtained from NEMDS. We show that by modifying SC on a substrate, systematic changes can be induced in EOF at the nanoscale.

[1]Partially supported by the Army Research Office.

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Date submitted: 11 Aug 2011 Electronic form version 1.4