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Multiscale study of nanoparticle-wall interactions in electroosmotic flow[1] A.T. CONLISK, HARVEY ZAMBRANO, ZHIZI PENG, The Ohio State University — In electroosmotic transport (EOT), particle mobility results not only from the dragging exerted by the electrolyte, but also from the force exerted by the External Electric Field (EEF), and from the interactions with the walls and with the solvent. The objective of this work is to develop a unified theory of the motion of colloidal particles near walls and compare with the experiments of Kazoe and Yoda for EOT. In the present study a novel continuum approach is developed to study the particle interactions with polystyrene beads. Moreover, we conduct Non-equilibrium Molecular Dynamics Simulations (NEMDS) of a nanoparticle as it moves near a solid-liquid interface subjected to an EEF. We investigate the response of the particle to changes in the surface electrostatics and the electrolyte concentration. Therefore, we perform NEMDS of a silica particle immersed in an electrolyte. The electrolyte solution is mounted on a silica substrate and the particle is constrained to move parallel to the surface so that we can extract the forces acting between the particle and the wall. We vary the electrolyte concentration, the particle size and the surface electrostatics.

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