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Atomistic simulations of nanoscale electrokinetic transport[1] JIN LIU, University of Pennsylvania, MORAN WANG, Tsinghua University, Beijing, China, SHIYI CHEN, Peking University, Beijing, China, MARK ROBBINS, Johns Hopkins University — An efficient and accurate algorithm for atomistic simulations of nanoscale electrokinetic transport will be described. The long-range interactions between charged molecules are treated using the Particle-Particle Particle-Mesh method and the Poisson equation for the electric potential is solved using an efficient multi-grid method in physical space. Using this method, we investigate two important applications in electrokinetic transport: electroosmotic flow in rough channels and electowetting on dielectric (EWOD). Simulations of electroosmotic and pressure driven flow in exactly the same geometries show that surface roughness has a much more pronounced effect on electroosmotic flow. Analysis of local quantities shows that this is because the driving force in electroosmotic flow is localized near the wall where the charge density is high. In atomistic simulations of EWOD, we find the contact angle follows the continuum theory at low voltages and always saturates at high voltages. Based on our results, a new mechanism for saturation is identified and possible techniques for controlling saturation are proposed.

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