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Molecular simulations of electro-osmotic flows in nano-channels: from molecules to continuum MORAN WANG, JIN LIU, SHIYI CHEN, Johns Hopkins University (Mechanical Engineering) — Most previous molecular dynamics simulations of electro-osmotic flows claimed that the continuum-based Poisson-Boltzmann theory is failed at nanoscale. Here we present our MD results of electroosmotic flows in nanochannels, and compare our results with predictions from continuum theory. Our results show that: 1) the MD results are strongly dependent on the bin size, in which the macroscopic characteristics are sampled. When the bin size is larger than one molecular diameter size, the MD results are comparable with the continuum theoretical solutions. 2) the MD results agree well with the Poisson-Boltzmann theory in the diffusion layer as long as the ion-density is not too high. Furthremore, our MD results are not dependent on the channel size as reported previously by others.

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