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On break-down of continuum theories for electroosmotic flow in nanoscale channels MORAN WANG, SHIYI CHEN, Johns Hopkins University — Most previous researches on electro-osmotic flows in nanochannels found that the continuum theories, such as PB theory for electric potential distribution and NS equation for fluid flow, broke down at the nanoscale. There has not been a perfect explanation for it yet though several factors were ever suspected, such as the transport properties of water near the charged surface and the immobilization of couterions absorbed on the channel wall. In this work, we present our NEMD simulations of electroosmotic flows in nanochannels by changing the molecular parameters freely, and compare with corresponding continuum theory. Our results show that the break-down of continuum theories for nanoscale electroosmosis is mainly caused by the differences of the non-Coulombic interaction between the solvent molecules and the ions. The effect of Coulombic force on the break-down is negligible. When the difference of interactive potential between solvent molecules and ions is artificially eliminated, the MD results agree well with the continuum predictions.

Shiyi Chen
Johns Hopkins University

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