Abstract Submitted
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Accounting for Finite Size of Ions in Nanofluidic Channels Using Density Functional Theory[1] CHRISTOPHER MCCALLUM, Univ of California - Santa Barbara , DIRK GILLESPIE, Rush Medical College, Rush University Medical Center , SUMITA PENNATHUR, University of California - Santa Barbara — The physics of nanofluidic devices are dominated by ion-wall interactions within the electric double layer (EDL). A full understanding of the EDL allows for better exploitation of micro and nanofluidic devices for applications such as biologic separations, desalination, and energy conversion, Although continuum theory is generally used to study the fluidics within these channels, in very confined geometries, high surface charge channels, or significant solute concentration systems, continuum theories such as Poisson-Boltzmann cease to be valid because the finite size of ions is not considered. Density functional theory (DFT) provides an accurate and efficient method for predicting the concentration of ions and the electrostatic potential near a charged wall because it accounts for more complex electrostatic and hard-sphere correlations. This subsequently allows for a better model for ion flux, fluid flow, and current in electrokinetic systems at high surface charge, confined geometries, and concentrated systems. In this work, we present a theoretical approach utilizing DFT to predict unique flow phenomena in nanofluidic, electrokinetic systems.

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