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Electrokinetic transport in realistic nanochannels¹ MORAN WANG, EES16 and CNLS, Los Alamos National Laboratory, JIN LIU, Department of Bioengineering, University of Pennsylvania, QINJUN KANG, EES-16, Los Alamos National Laboratory — When an electrolyte solution contacts with a solid surface, the surface will likely be charged through an electrochemical adsorption process. The surface charge in general varies with the local bulk ionic concentration, the pH value and the temperature of the solution, and even with the double layer interactions in the narrow channel. Most of the previous studies are based on a constant zeta potential or surface charge density assumption, which does not reflect the realistic charge status at interfaces and may lead to inaccurate predictions. In this work, we first develop a generalized model for electrochemical boundary conditions on solid-liquid interfaces, which can closely approximate the known experimental properties. We further present nonequilibrium molecular dynamic (NEMD) simulations of electrokinetic transport in nanochannels. We take silica and carbon as examples of channel materials. Both monovalent and multivalent ionic solutions are considered. The electrokinetic transport properties for realistic nanochannels are therefore studied and a multiscale analysis for a new energy conversion device is performed.

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