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Effect of charge inversion on Poiseuille flow of multivalent electrolyte solutions in nanochannels: an atomistic study

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Body:

Miniaturized devices integrated by nanoconduits have a great potential for clinical and biotechnological analysis due to amplified sensibility, faster response and increased portability. In nanoconduits, wherein the electrical double layer can occupy a considerable part of the cross section, Electro-Kinetic Phenomena (EKP) play a key role in determining transport properties of electrolytes. Hence, a comprehensive understanding of EKP and related phenomenology such as charge inversion (CI), is essential to develop more efficient nanodevices. Here, atomistic simulations of Poiseuille flow of aqueous multivalent electrolyte solutions in silica nanochannels are conducted to study the influence of CI on fluid properties. The solutions consist of water as solvent, chloride as co-ion and different amounts of counter-ions i.e. sodium, magnesium, aluminum and calcium. From atomistic trajectories, the relation between the concentration of different cations and, local and effective viscosities is analyzed considering the particular hydration shell around each ionic species. Moreover, the effect of CI on flow velocity, stick boundary condition, shear stress and friction coefficient is examined.

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