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Ion conduction in nanoscale Janus membranes: Molecular dynamics vs Continuum. JOHNSON DHANASEKARAN, JOAN M. MONTES DE OCA, JUAN J. DE PABLO, Pritzker School of Molecular Engineering, University of Chicago. — An accurate, comprehensive continuum theory of the physical processes that underlie ionic conduction in nanometric size pores is essential for the design and development of new technologies, such as Janus membranes used for power generation. In this work, we compare extensive molecular dynamics (MD) simulations of a complex Janus membrane embedded in an explicit solvent, with classical continuum given by coupling of Poison electrostatics, steady ion transport via Nernst-Planck, and convection described by Navier-Stokes. We find the continuum approach provides good qualitative and quantitative agreement of features such as Ionic distribution and potential with respect to MD simulations. We show the critical role convection plays in achieving this. However, we observe significant discrepancies in the dynamics (Current, ionic velocities, convection flux, etc). After inspection of the molecular mechanisms of ionic conduction, we argue that the significant slip velocity observed in MD simulations, enhanced by the predominantly electroosmotic nature of the flux, plays an important role in the discrepancies observed with the continuum.

Joan Montes de Oca
University of Chicago

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