Middleweight ions win the race in confined carbon pores

Matthew C. F. Wander and Kevin L. Shuford

Department of Chemistry, Drexel University, Philadelphia, PA

Achievement

Classical molecular dynamics (MD) was used to determine the diffusivity of aqueous alkali halides in contact with microscopic pores of carbon electrodes to provide insights into electrical energy storage systems that will deliver both high power and large storage capabilities. Medium atomic weight ions such as potassium, chloride, and bromide show the greatest enhancement of diffusivity in confined pores relative to bulk. Larger ions have difficulty moving through the pores, and the motion of smaller ions is inhibited by strong water-water hydrogen bonding interactions. We find that the brines undergo a charge separation behavior in the direction perpendicular to an interface due to rotations of the water molecules. These studies explain how electrical energy may be stored in aqueous electrolyte supercapacitor systems.

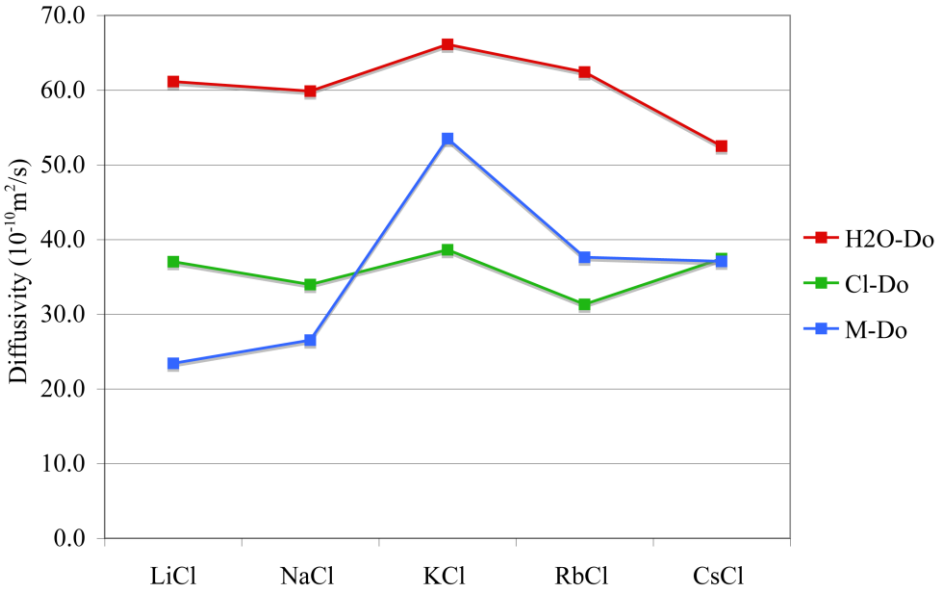

Figure: Alkali ion diffusivities for a 1M solution (paired with a Cl^- anion) confined within a 4 nanometer graphene slit pore.

Significance

Molecular level understanding of ion diffusivity trends that explain the anomalous enhancement of capacitance for potassium found experimentally in supercapacitors and desalination systems that employ nanoporous carbon electrodes.

Credit

This material is based upon work supported as part of the FIRST Center, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number <ERKCC61>.

Citation

Matthew C. F. Wander and Kevin L. Shuford "Electrolyte Effects in a Model System for Mesoporous Carbon Electrodes" J. Phys. Chem. C, 2011, 115 (11), pp 4904–4908.