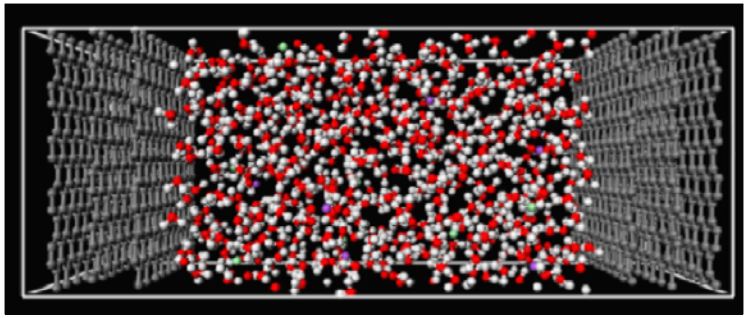
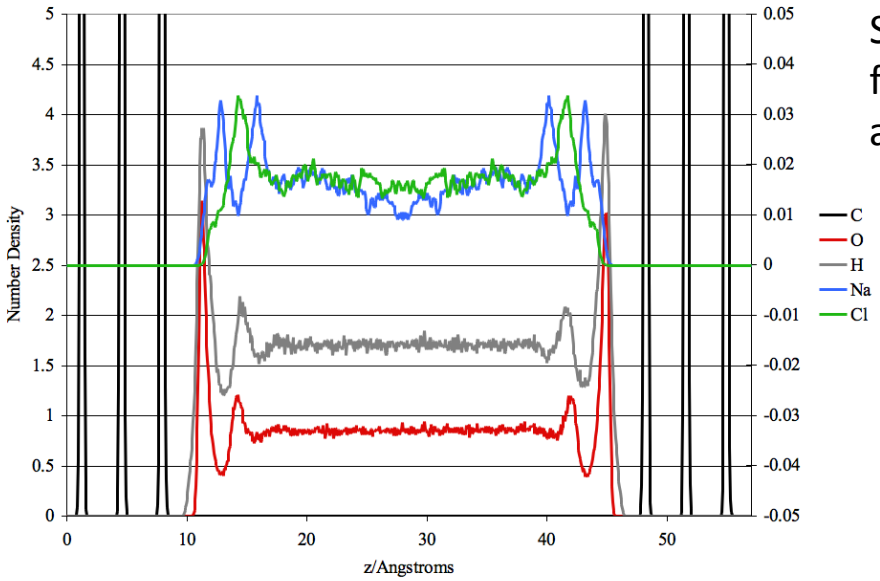
Aqueous Electrolytes in Carbon Slit Pores



NaCl brines in contact with graphite sheets have been simulated using classical molecular dynamics to model dynamics of aqueous electrolyte supercapacitors.

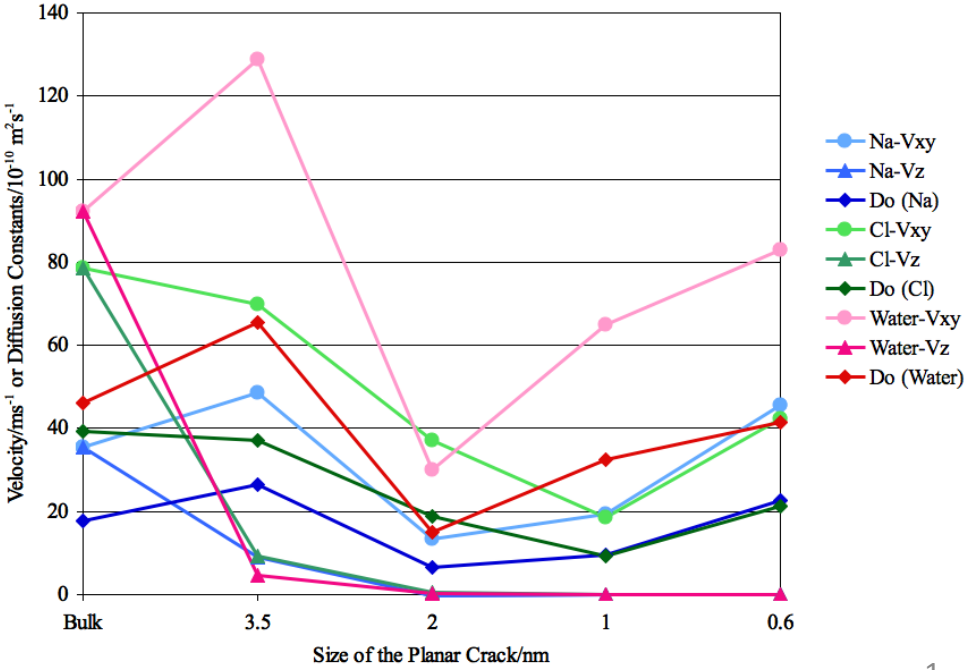
Ordered layers form parallel to the carbon surface as shown to the left for a 3.5 nm nanocrack.

Slight confinement enhances the diffusivity constants (D_0) for sodium and water relative to bulk while chloride is approximately constant.



Velocities perpendicular to the surface (Vz) quickly decay upon confinement as shown to the right.

Ion pairing and correlated motion is significant for cracks less than 2 nm.



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