NaCl Ions Feeling the Pinch in Tight Carbon Spaces

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Achievement:

Pore geometries and solution properties that enhance power of aqueous electrolyte supercapacitors have been determined. Scientists from Drexel University have used modeling to understand the structure and transport behavior of NaCl solutions confined within microscopic pores in carbon electrodes. There is an ever-increasing need for inexpensive and efficient electrical energy storage devices to complement alternative energy sources and applications. Aqueous electrolyte supercapacitors show great promise as systems that combine sizeable energy storage capabilities with rapid charging/discharging properties. Here, the origin of these effects has been investigated on a molecular level using classical molecular dynamics simulations. Two different model pore geometries were examined: planar slits and cylindrical pores. The brines undergo a charge separation behavior perpendicular to an interface due to rotations of the water molecules, which focuses ion motion parallel to the surface. Moderately confined planar systems (~4 nm interstices) display an enhancement of ion motion relative to bulk. Further confining the solution within smaller pores (~1 nm) severely hinders the ion diffusion. In all cases, ion diffusivity and surface structure indicate that water, particularly water-water hydrogen bonding, dictates the overall system behavior. Understanding and ultimately controlling molecular interactions at interfaces could have a transformative impact on future electrical energy storage devices, designs, and materials.

Significance: Molecular interactions and solvation behavior that lead to unique transport phenomena have been identified and examined.

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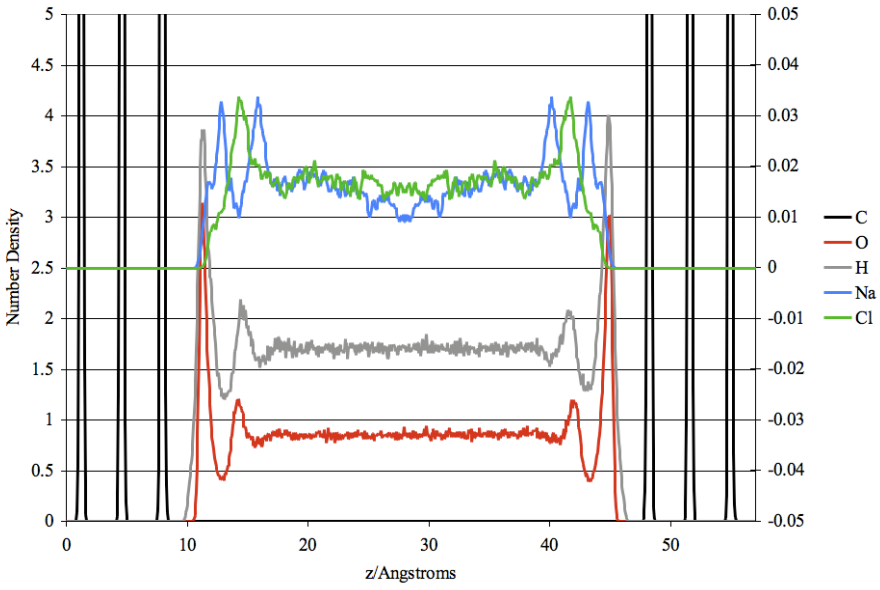

Figure: Vertical profile for a 1 M NaCl solution in a 4nm slit pore.

Citation:

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