

Supporting Information:

Selectivity of Nitrate and Chloride Ions in Microporous Carbons: The Role of Anisotropic Hydration and Applied Potentials

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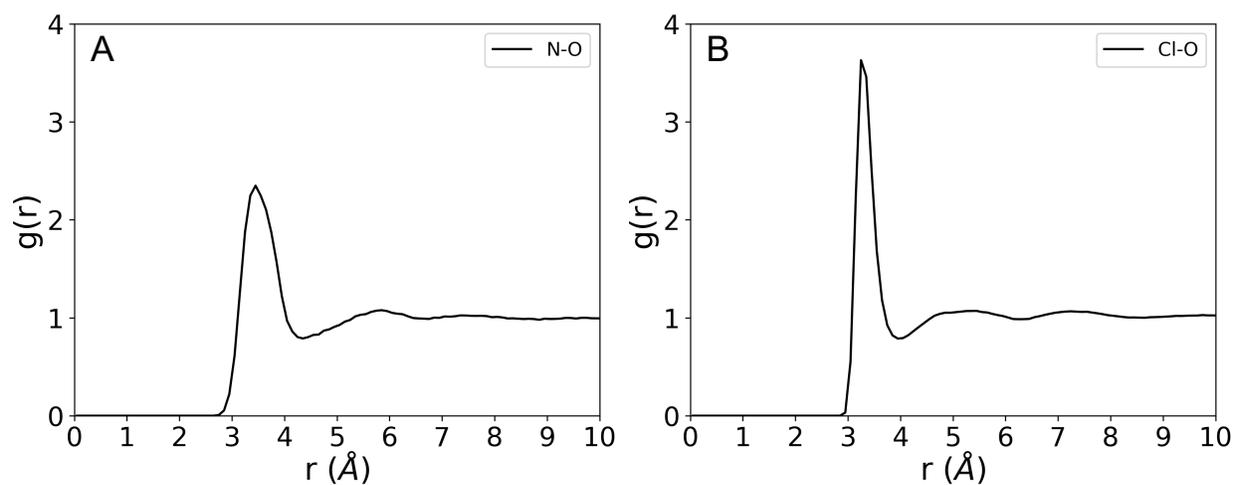


Figure S1. Ion-oxygen radial distribution functions for nitrate (N-O) and chloride (Cl-O) obtained from WT-MetaD simulations.

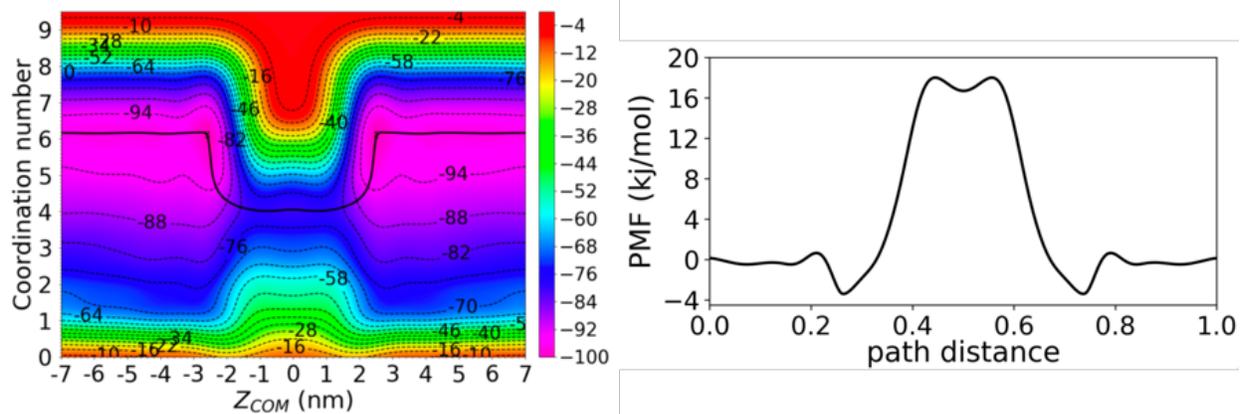


Figure S2. (Left panel) Two-dimensional free energy profiles of Na⁺ transport through a slit pore with a pore size of 0.8 nm. (Right panel) One-dimensional free energy profiles of Na⁺ transport through a slit pore with a size of 0.8 nm as a function of path distance.

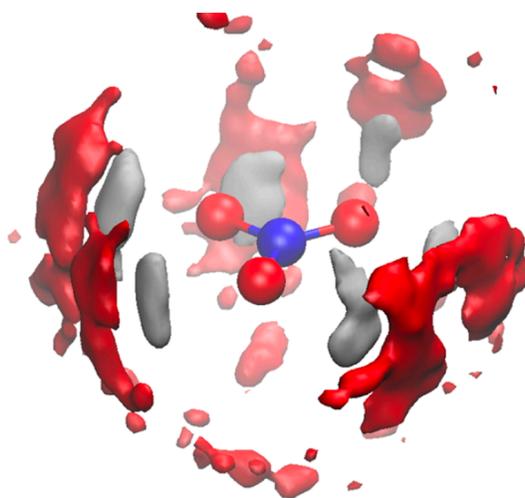


Figure S3. The spatial distribution function of the hydration shell of nitrate. The image is obtained from Ref. 14.

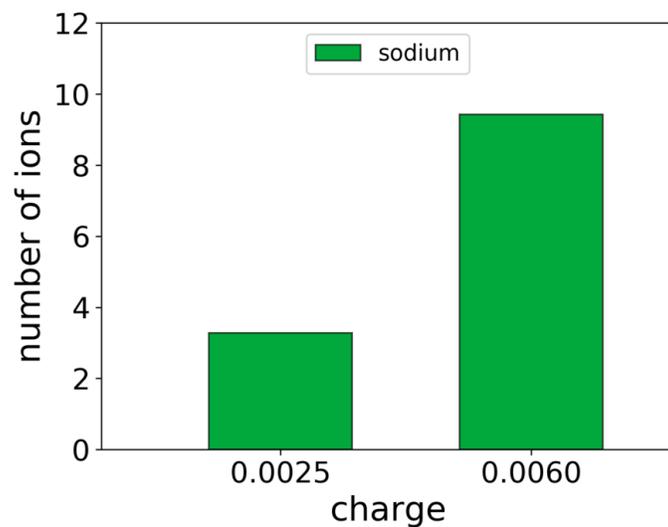


Figure S4. Number of Na⁺ ions inside the negatively charged pore at two different charges, 0.0025 and 0.006 e/carbon.

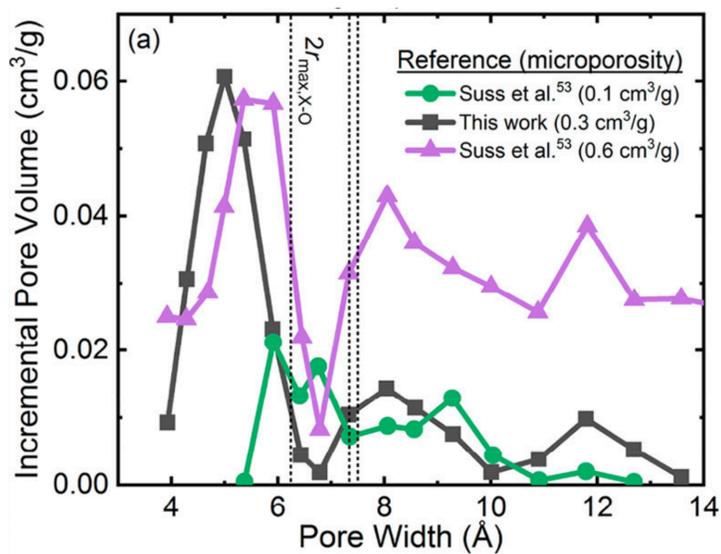


Figure S5. Micropore-size distribution as a function of pore width from N₂ adsorption measurements. The image is obtained from Ref. 14.

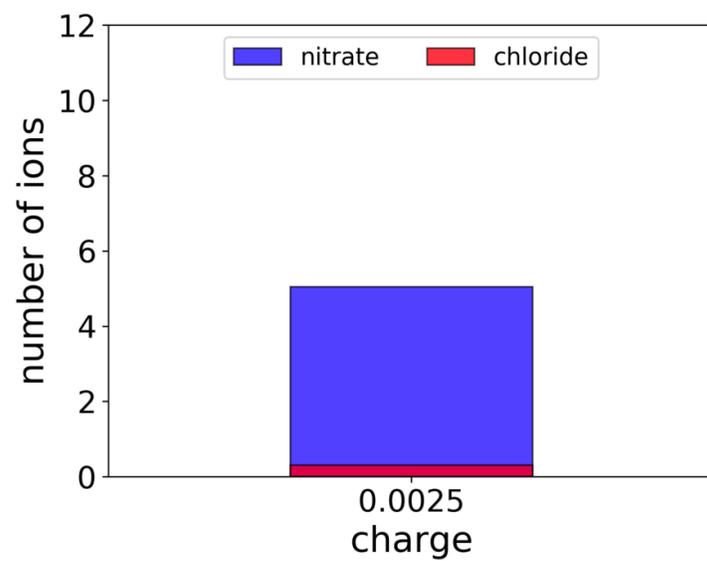


Figure S6. Number of NO_3^- and Cl^- ions inside the larger pore (1.1 nm) at charge of 0.0025 $-e/\text{carbon}$.