Excited state methods for electronic structure in the Green's function formalism

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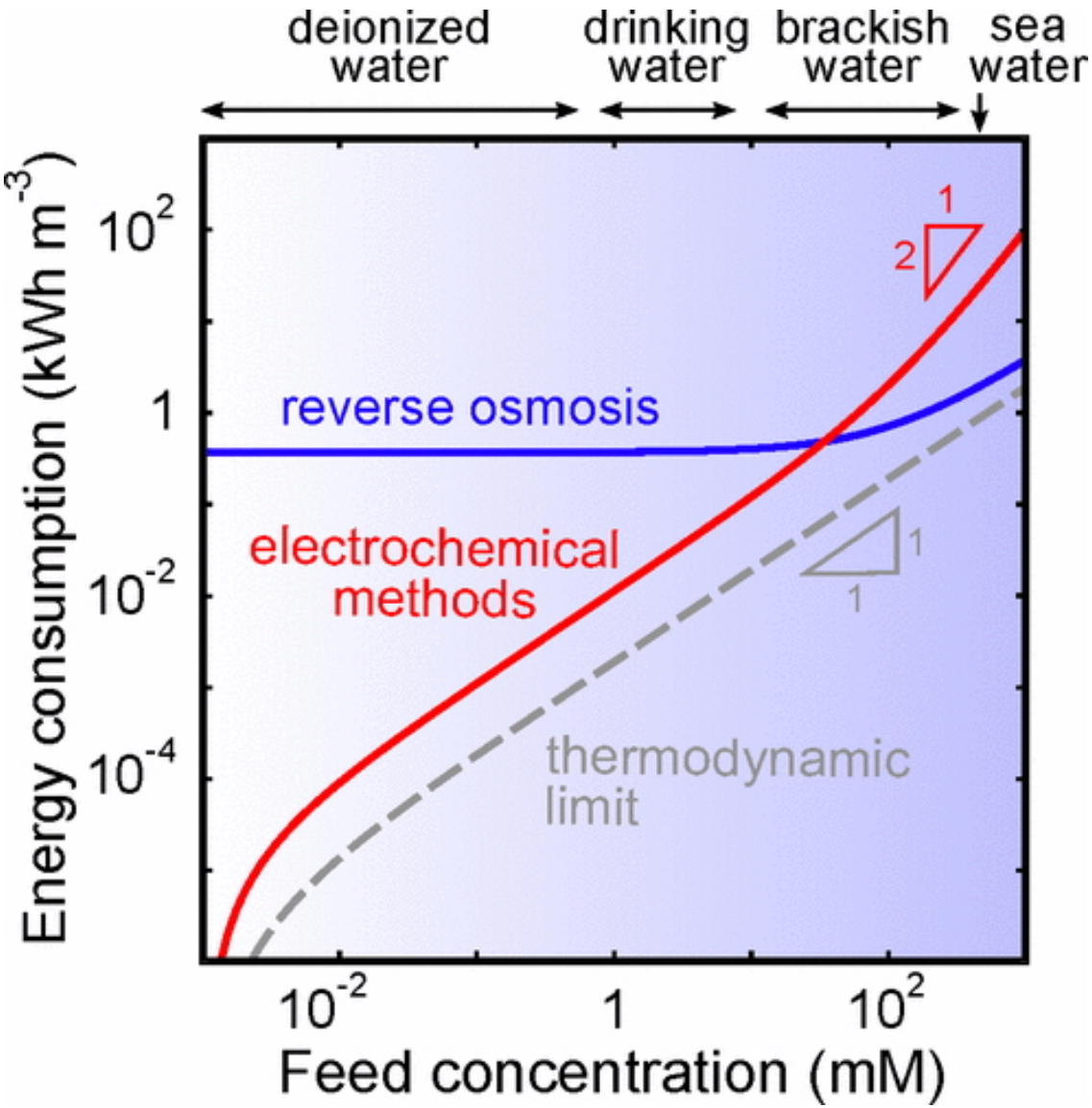
Outline

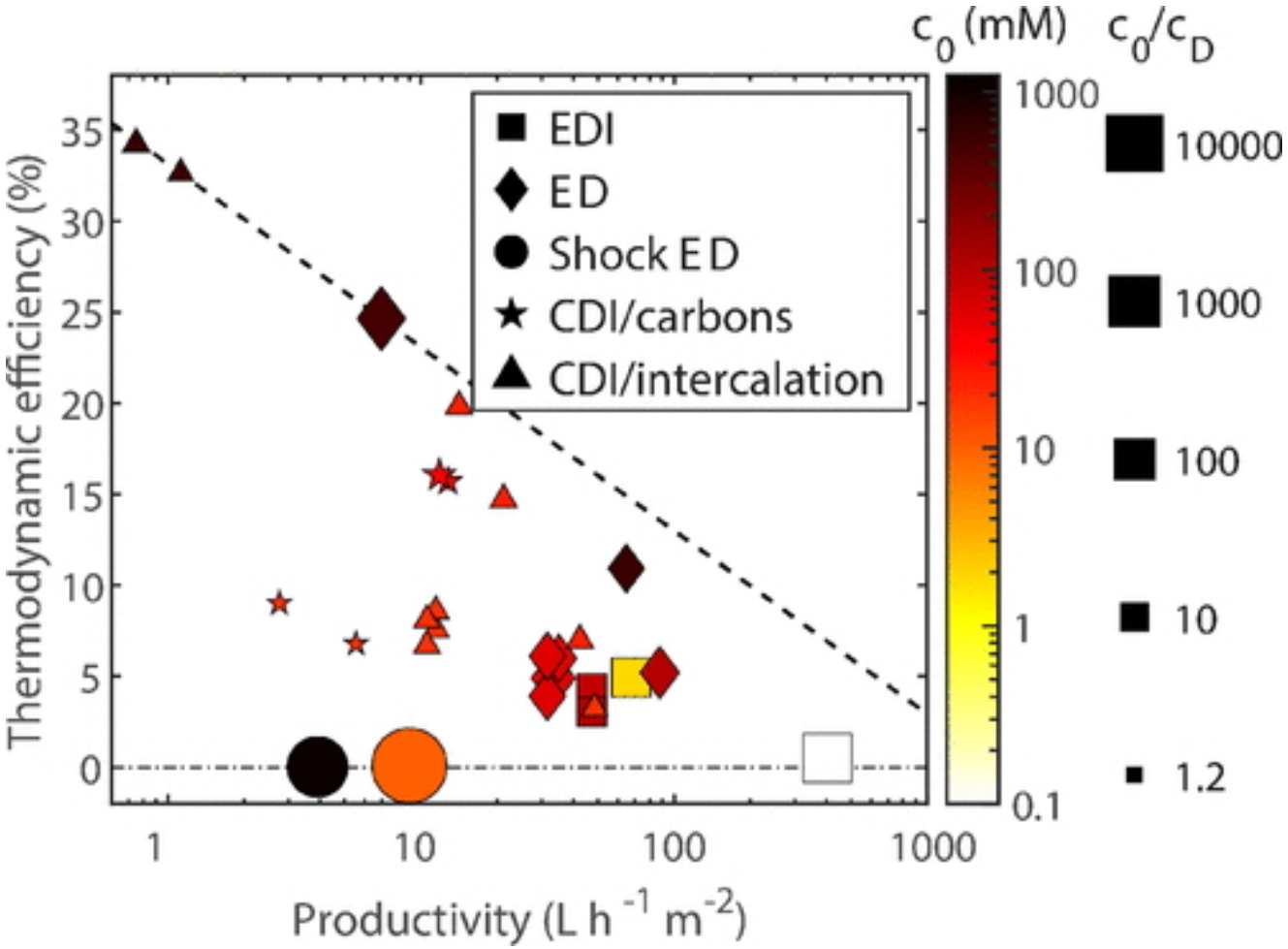
1. Motivation
2. Thermodynamic efficiency of different methods
3. Kinetics of capacitive deionization
4. Transport: Identifying mechanisms of electrosorption

Why the status quo is not enough

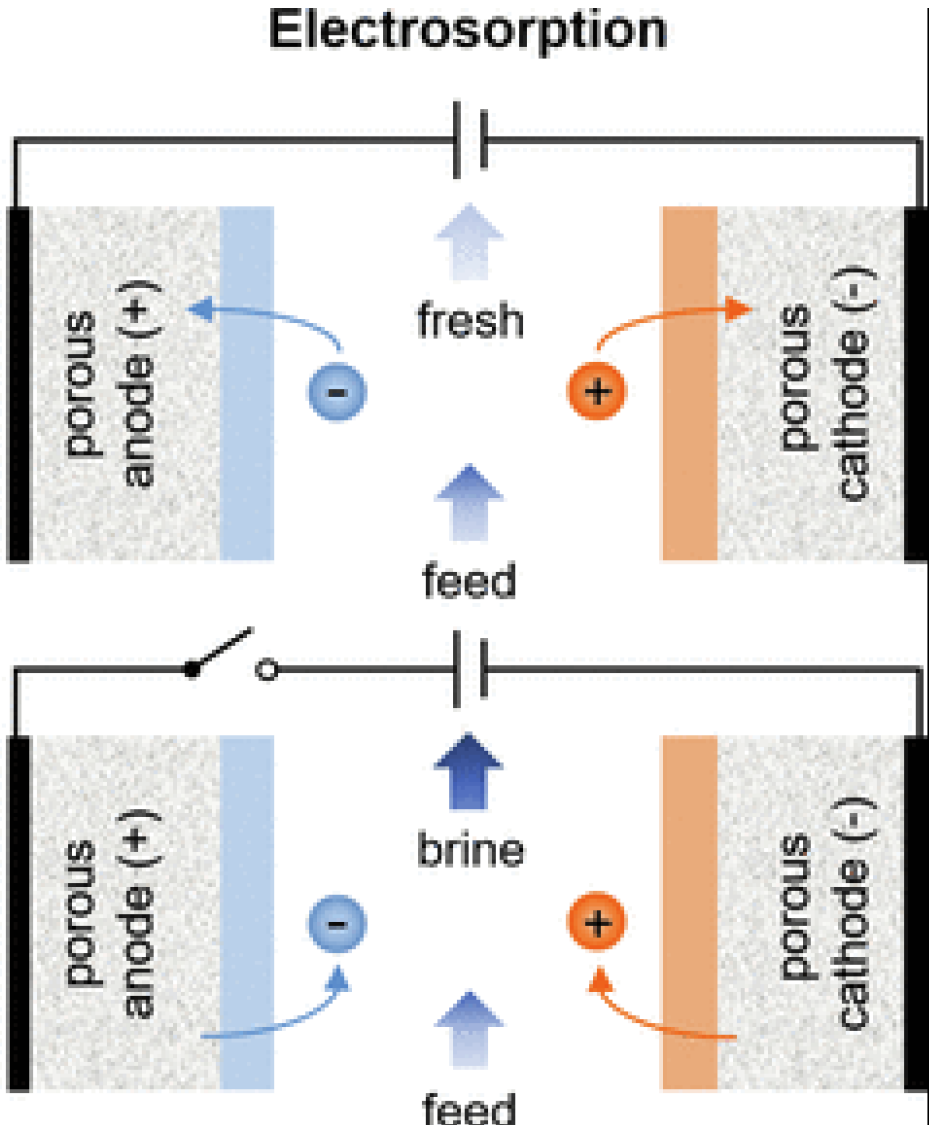


Thermodynamic efficiency of different methods

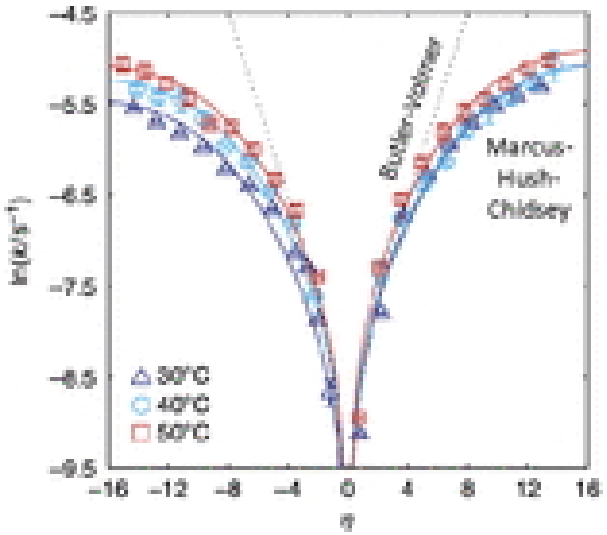
We can plot $\mathcal{P} = \frac{V_D}{nA}$ vs. $\eta = \Delta \hat{G}/\hat{E}$

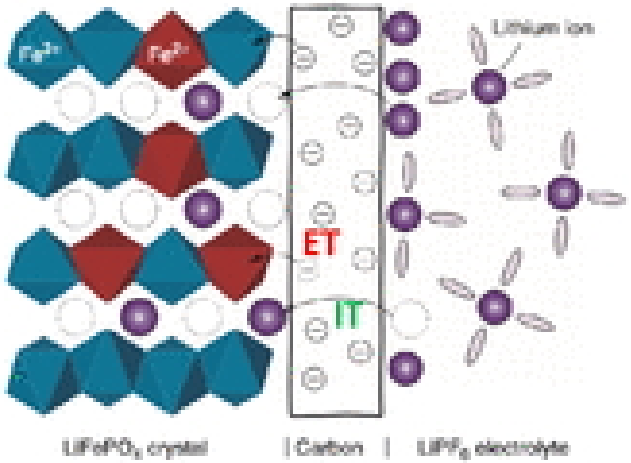


What electrosorption looks like



A coupled ion-electron transfer mechanism for CDI





$$\lambda_{\mathrm{o}} = \frac{e^2}{8\pi\varepsilon_0 k_{\mathrm{B}} T}\left(\frac{1}{a_0} - \frac{1}{2d}\right)\left(\frac{1}{\varepsilon_{\mathrm{op}}} - \frac{1}{\varepsilon_{\mathrm{s}}}\right)$$

Identifying Faradaic vs. electrostatic electrosorption