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Charge relaxation dynamics of an electrolytic nanocapacitor¹

VAIBHAV THAKORE, JAMES HICKMAN, Department of Physics and NanoScience Technology Center, University of Central Florida, Orlando FL — Understanding charge relaxation dynamics in confined nanospaces with overlapping electric double layers (EDLs) is critical for the development of efficient electrochemical energy storage, energy conversion and bioelectrochemical sensing devices. Using Lattice Boltzmann (LB) method, results from simulations of an electrolytic nanocapacitor subjected to a step potential at $t = 0$ are presented here for various degrees of EDL overlap, solvent viscosities, ratios of cation to anion diffusivity and electrode separations. A continuously varying molecular speed dependent relaxation time is proposed for use with the LB equation that, unlike the single relaxation time Bhatnagar-Gross-Krook approximation, recovers the correct microscopic description of molecular collision phenomena and holds promise for enhancing the stability of the LB algorithm. Simulations for large EDL overlap showed oscillatory behavior for ionic current densities as opposed to monotonic relaxation to equilibrium for low EDL overlap. Further, at low solvent viscosities and large EDL overlap, an anomalous plasma-like collective behavior of oscillating ions at a frequency much lower than the plasma frequency of the electrolyte was observed and as such it appeared to be purely an effect of nanoscale confinement.

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