

Making Sense of Electrical Noise by Simulating Electrolyte Solutions

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Seemingly unrelated experiments such as electrolyte transport through nanotubes, nano-scale electrochemistry, NMR relaxometry and Surface Force Balance measurements, all probe electrical fluctuations: of the electric current, the charge and polarization, the field gradient (for quadrupolar nuclei) and the coupled mass/charge densities^{1,2}. Using molecular and mesoscopic simulations, it is possible to predict the fluctuations of these observables from the dynamics of ions and solvent molecules, thereby enabling experimentalists to decipher the microscopic properties encoded in the measured electrical noise. This presentation will illustrate this idea, focusing on quadrupolar NMR relaxation as a probe of subpicosecond collective dynamics in aqueous electrolyte solutions^{3,4} and on the link between the electrode charge fluctuations in nanocapacitors and the dynamics of the interfacial electrolyte.

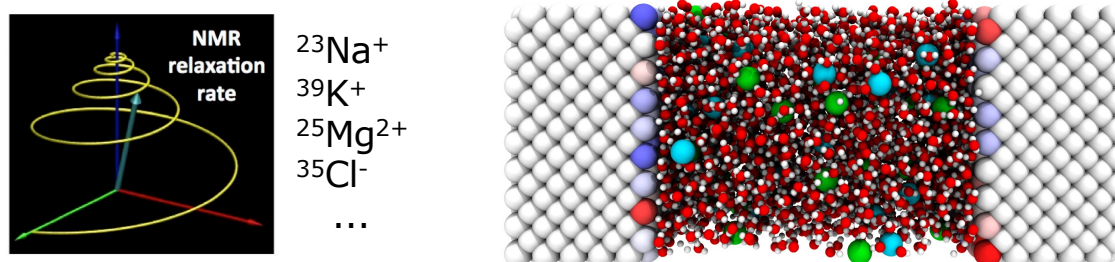


Figure 1. Left: the NMR relaxation rate of quadrupolar ions (with spin $I > 1/2$) reflects the collective dynamics of their environment via the fluctuations of the electric field gradient. Right: the electrode charge fluctuations in a nanocapacitor, related to the frequency-dependent impedance, reflect the dynamics of the confined liquid.

Keywords: Electrical fluctuations, NMR relaxation, nanocapacitors, dynamics, electrolytes.

¹ ERC project SENSES <https://benrotenberg.github.io/erc-senses/>

² Electrical noise in electrolytes: a theoretical perspective. T. Hoang Ngoc Minh, J. Kim, G. Pireddy, I. Chubak, S. Nair, B. Rotenberg, *Faraday Discuss.*, **246**, 198 (2023). <https://doi.org/10.1039/D3FD00026E>

³ NMR Relaxation Rates of Quadrupolar Aqueous Ions from Classical Molecular Dynamics Using Force-Field Specific Sternheimer Factors. I. Chubak, L. Scalfi, A. Carof, and B. Rotenberg, *J. Chem. Theory Comput.*, **17**, 6006 (2021). <https://doi.org/10.1021/acs.jctc.1c00690>

⁴ Quadrupolar $^{23}\text{Na}^+$ NMR Relaxation as a Probe of Subpicosecond Collective Dynamics in Aqueous Electrolyte Solutions. I. Chubak, L. Alon, E. Silletta, G. Madelin, A. Jerschow, and B. Rotenberg, *Nature Commun.*, **14**, 84 (2023). <https://doi.org/10.1038/s41467-022-35695-3>

⁵ Frequency-dependent impedance of nanocapacitors from electrode charge fluctuations as a probe of electrolyte dynamics. G. Pireddu and B. Rotenberg, *Phys. Rev. Lett.*, **130**, 098001, (2023). <https://doi.org/10.1103/PhysRevLett.130.098001>