3D Pulse Field Gradient NMR measurements of transport in anisotropic materials for energy storage applications

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Recent advances in material fabrication and assembly processes has fostered the development of micro and nanostructures with anisotropic diffusion or transport properties. These materials are important for advancing energy storage, catalysis, and bioengineering applications. For instance, in battery electrodes, engineering the tortuosity to enhance diffusion through the thickness of the electrode is currently pursued to improve rate performance.

Direct measurement of 3D diffusion in these non-transparent nanoscale pores is extremely challenging with classic optical techniques. To address this challenge, we demonstrate that pulse field gradient (PFG) NMR allows us to measure anisotropic diffusion in a model porous silicon substrate. We show that the solvents, in our case H_2O, DMSO and battery electrolyte $LIPF_6$:DC:EMC in and outside the pores exhibit distinct NMR signals with derived root mean square displacements that correlate well with the expected values i.e. length and width of the pores.

The results demonstrate that PFG-NMR can serve as a non-destructive characterisation method for both in- and ex-situ analysis of future complex battery and supercapacitor electrodes.

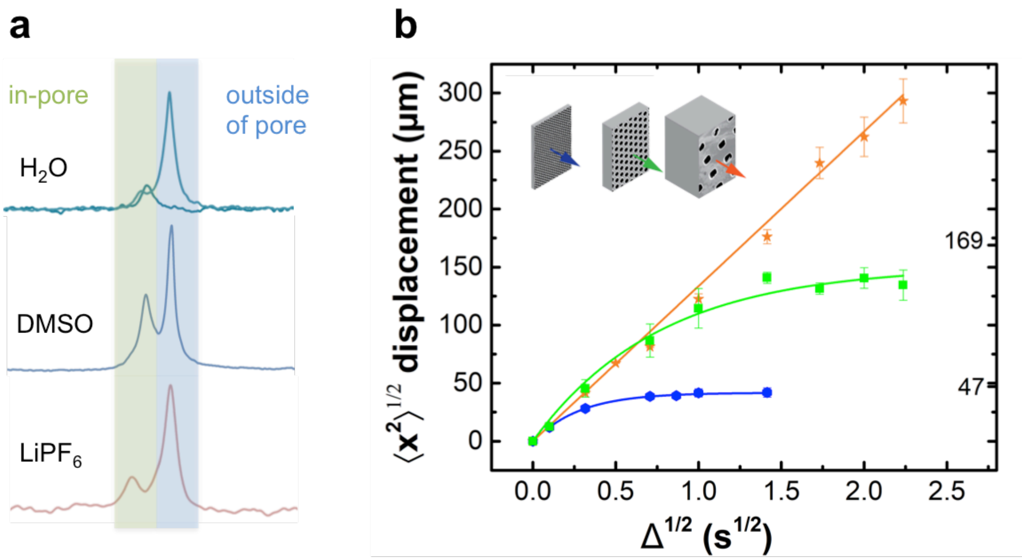

Figure 1. a) 1D slices of ^{1}H and ^{7}Li diffusion measurements for Si samples with H_2O, DMSO and $LiPF_6$, b) root mean square displacements for diffusion measurements along the pores for 500, 169 and 47 μm lengths. Error bars are 2σ. 3D pore width measurements will be shown on the poster.