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Electrophoretic NMR of Concentrated Electrolytes for Li-Ion Batteries: Understanding the Role of Solvent Motion

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A predictive understanding of phenomena at atomic and molecular levels to enable "bottom up" battery design

P1 - THE ROLE OF CATION-DRIVEN SOLVENT MOTION IN LITHIUM BATTERY ELECTROLYTES

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The rational design of new battery systems rests on a fundamental understanding of the factors that underpin the transport of the working ion (frequently a cation). While conductivity reflects the motion of both the cation and the anion, the transference number t_{+}^{0} reflects the fraction of current carried by the cation relative to a reference velocity that is usually taken to be that of the solvent. At any instant, the cations can be present in different solvation environments, *e.g.*, some cations may be entirely solvated by solvent molecules while others may have an anion in the first solvation shell. In this study, we combine electrophoretic NMR (eNMR) measurements of ion and solvent velocities under applied electric fields with computer simulations to interrogate the different solvation environments in a model liquid electrolyte: a mixture of bis(trifluoromethanesulfonyl)imide (LiTFSI) and tetraglyme. Measured values of t_{+}^{0} agree quantitatively with simulation-based predictions. The simulations further reveal two dominant solvation motifs: (1) where the cation is solvated by two solvent molecules, and (2) where it is solvated by one solvent molecule and an anion. While the eNMR data reflect the average velocity of all solvent molecules, combining these results with insights from simulation enables estimation of the field-induced velocity of *only* those solvent molecules within the two solvation motifs. At a particular electrolyte concentration, 1.8 *m*, $t_{+}^{0} = 0$ because the average field-induced velocities of the cation and solvent are identical; most of the solvent molecules are in solvation motif (1) at this concentration.