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Molecular Dynamics of Electrolytes Based on Ionic Liquids by means of Fast Field Cycling NMR Relaxometry, Infrared Spectroscopy and Molecular Dynamics Simulations

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Triglyme-lithium salt complexes show low volatility, high thermal stability, high ionic conductivity, and a wide potential window. It has been shown by Yoshida et al. that the mixtures of lithium bis(trifluoromethylsulfonyl)amide [Li][NTf_2] and triglyme (G3) behave like conventional room temperature ionic liquids [1,2]. In particular the equimolar triglyme-lithium complexes are presumed to be resistive against oxidation and thus thought to be promising electrolytes for lithium batteries. With a combination of experiments and molecular dynamics (MD) simulations we studied the transport properties and molecular motion of G3-lithium salt mixtures as a function of salt concentration and temperature. Self-diffusion coefficients, viscosities and ionic conductivities were measured by conventional methods. We also used fast-field-cycling NMR relaxometry to understand the molecular motion of the different components in the electrolyte system. Relaxation times T_1 have been measured on three different nuclei: ^{1}H of the triglyme, ^{7}Li of the cation and ^{19}F of the anion. The dispersion profiles were recorded in the range from 10 kHz to 30 MHz by using a Spinmaster FFC2000 instrument. From the intra- and intermolecular relaxation rates reorientational correlation times and self-diffusion coefficients could be achieved. Both dynamical properties are sensitive for ion pair formation with increasing salt concentration. Additional molecular dynamics (MD) simulations provide insight at molecular level about the change from glyme solutions to quasi-ionic liquids for the binary mixtures [3]. The results can be used for developing promising electrolytes for battery systems.

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