Cluster Formation in Mixtures of [Li][NTf_2] and Triglyme

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The recent search for more environmentally-friendly energy conversion technologies is also accompanied by developments in energy storage devices. Lithium ion batteries offer great prospects regarding their high energy density and are therefore often a preferred choice. However, currently used electrolytes also often possess a high inflammability and other undesirable properties [1]. In order to study possible alternative electrolytes for lithium-ion batteries with hopefully less problematic properties, we have studied mixtures of [Li][NTf_2] and the glycol ether triglyme by means of molecular dynamics simulations. The added triglyme molecules coordinate to the lithium cations, thus separating cations and anions and improving the transport properties of the mixture significantly. However, the structure and thereby the physical properties of the mixtures are primarily dependent on the composition of the mixture. In particular, we observe an equilibrium of lithium being coordinated by either one or two triglyme molecules. By adding more triglyme to the lithium salt, this equilibrium is shifted towards a two-fold coordinated state leading to higher mobility (gauged through computed diffusion coefficients) and therefore lower viscosities, which is preferred for the application as an alternative electrolyte. As a consequence, a quasi-ionic liquid can be obtained, which could be used in battery research [2]. Simulated and observed transport properties are in good qualitative agreement for this system, and the simulations can give insights into the microscopic origin of the macroscopic properties.

REFERENCES

[1] K. Xu, Chem. Rev., 114 (2014) 11503-11618
[2] K. Yoshida, M. Tsuchiya, N. Tachikawa, K. Dokko, M. Watanabe, J. Phys. Chem. C, 115 (2011) 18384-18394

FIGURES

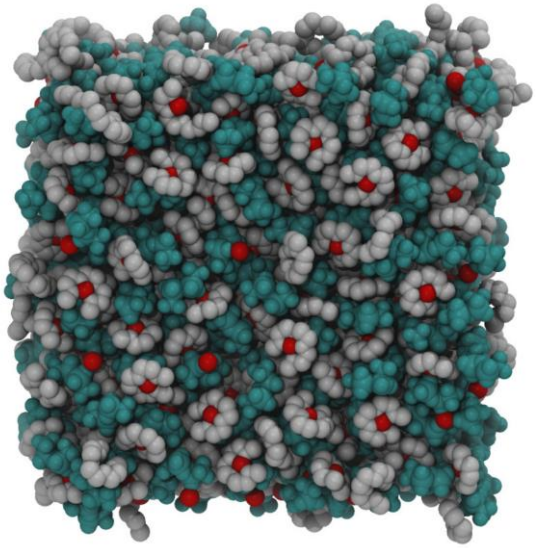

Figure 1: Snapshot taken from MD simulations of [Li-G3][NTf_2] system at T = 300 K. Lithium cations have a red colour, NTf_2 anions are coloured in cyan and triglyme molecules are shown in grey.