Influence of self-organization induced local clustering on self-diffusion of [C_nMIm^+] [NTf_2^-] in bulk and nanoconfined systems

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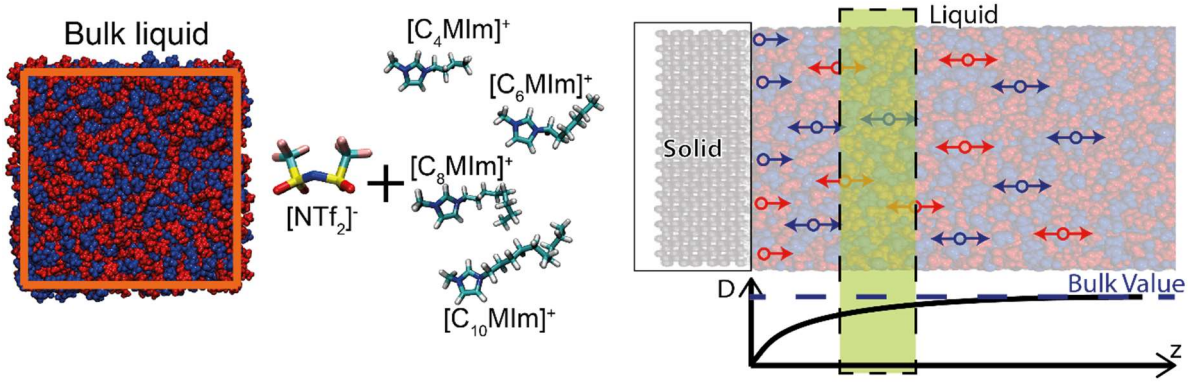

The various applications of ionic liquids require comprehensive knowledge of both their static and dynamic properties. Molecular dynamics simulations can be employed in order to obtain an understanding of how these properties emerge by analyzing the behavior of individual particles within different unconfined as well as confined systems.

We extend the previous study on the properties of [C_2MIm^+] [NTf_2^-] carried out by our group [1] to additional members of the [C_nMIm^+] [NTf_2^-] - family of ionic liquids with larger cations, namely n=4, 6, 8, 10. The static and dynamic properties of these ionic liquids are analyzed in a bulk system as well as in a nano confined solid-liquid-vacuum system with a supporting sapphire crystal.

We will provide evidence that the dynamic properties of the liquids with longer cation chains are governed by the formation of local ion clusters acting as meta-particles by employing the known measure of ion pair lifetimes as well as devising the mean number of encountered closest neighbors of ions within a certain simulation timeframe as a measure for how strongly a particle is confined to a stable local environment [2].

Furthermore, we will devise a theoretical model for obtaining the absolute diffusion coefficient of particles perpendicular to an interface by determining their mean lifetime within a confined subspace without relying on mean square displacement fitting in confined subspaces [2,3].

The influence of relevant parameters of the observed ionic liquids not considered in the theoretical derivation of the estimator are studied and possible corrections to the estimator depending on rotational speed and deformation of particles examined.

[1] Vucemilovic-Alagic, N.; Banhatti, R. D.; Stepic, R.; Wick, C. R.; Berger, D.; Gaimann, M. U.; Baer, A.; Harting, J.; Smith, D. M.; Smith, A.-S. *arXiv*, **2019**, *1903.09450*
[2] Höllring, K.; Smith, A.-S. *Master thesis*, **2019**
[3] Höllring, K.; Vucemilovic-Alagic, N.; Smith, D. M.; Smith, A.-S. *in preparation*