Diffusion coefficients of ionic liquids

in water and methanol:

A combined experimental and molecular dynamics

study

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Supporting Information

In Fig. S 1 and Fig. S 2 the pair correlation function between the hydrogen atom bound at the C(2)-atom of cation and the oxygen atoms of the anion are shown. In Fig. S 1 the results of the simulations in water are compared with the pair correlation function of the pure $[C_2MIM][NTf_2]$. For $[C_4MIM][NTf_2]$ it is not shown because it is similar to the one of $[C_2MIM][NTf_2]$. The first maximum and the first minimum are found at 0.2 nm respectively 0.3 nm. An ion pair is defined by the first minimum. The second oxygen atom bound at the same sulfur atom gives the second maximum at 0.45 nm. The broad maximum at about 0.6 nm shows the two oxygens bounded at the second sulfur atom. The pair correlation functions of the simulations with $[C_2MIM][NTf_2]$ and $[C_4MIM][NTf_2]$ in water are almost similar. The characteristics described above can also be found in Fig. S 2 where the results of the simulations in methanol are shown.
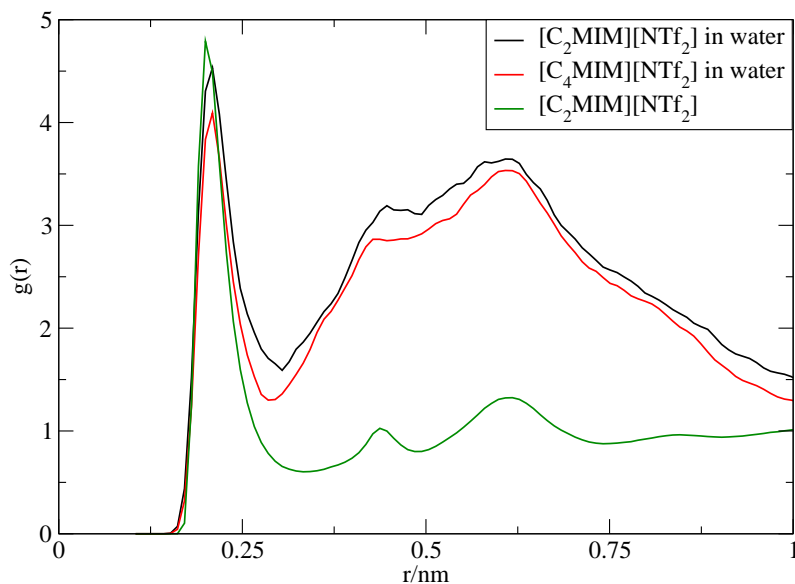
Fig. S 1: Pair correlation function between the hydrogen atom at C(2) of the cation and the oxygen atoms of the anion calculated of the simulation with $[C_nMIM][NTf_2]$ in water.
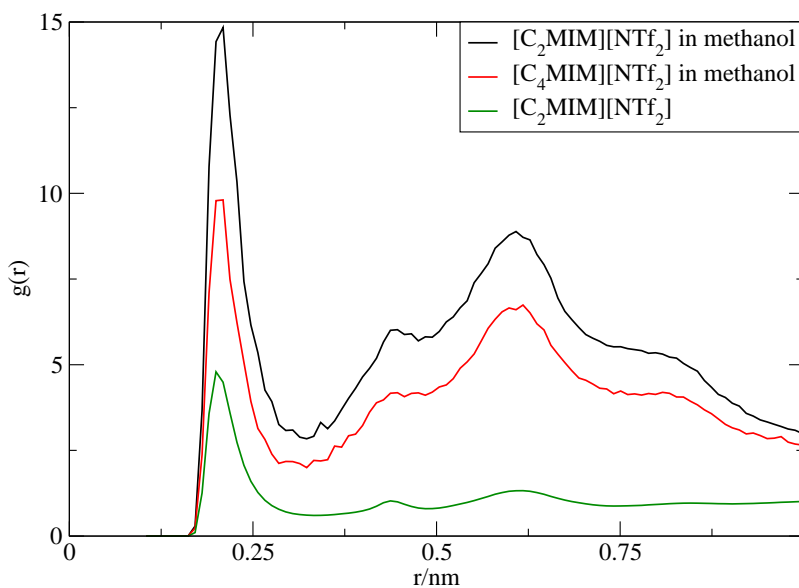

Fig. S 2: Pair correlation function between the hydrogen atom at C(2) of the cation and the oxygen atoms of the anion calculated of the simulation with $[C_nMIM][NTf_2]$ in methanol.