K. Gholizadeh Atania, J Phys Chem Biophys 2021, Volume 11

Using molecular dynamics simulation to study hydrogen bond in 1-n-Alkyl-3-methylimidazolium tris(pentafluoroethyl)trifluorophosphate ionic liquids

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Introduction: During the last decade, ionic liquids have been subject of enormous studies. Some of these properties are concerned to the imidazolium structure. For example, the evidence of the importance of hydrogen bonding in 1-alkyl-3-methylimidazolium ionic liquids was already highlighted by Seddon and coworkers in 1986. In this article, we investigate the hydrogen bond between particular atoms in anion and cations in the [Cnmim][eFAP] (n=2, 4, 6 and 8) ionic liquids with MD simulations. Considering distance and angle criteria between involved atoms in hydrogen bonding between cation and anion, the effect of hydrogen bonding on the structural properties of [Cnmim][eFAP] (n=2, 4, 6 and 8) ionic liquids.

Methods: Molecular dynamics (MD) simulation is used to study structural properties in the homologue series of [Cnmim][eFAP] ionic liquids. We have employed Lopes et al. based on the OPLS-AA force field to determine the intra- and inter-molecular interactions in the four interested ionic liquids. LAMMPS package was used to perform MD simulations.

Results and Discussion:

1. Ionic liquids density

Densities of [Cnmim][eFAP] ionic liquids at 298.15 K and 1 atm were calculated in NPT ensemble simulations and shown in Table 1. The densities of these ILs are in good agreement with experimental and simulated densities reported in literatures.

Table1. The calculated densities of four [Cnmim][eFAP] ionic liquids at 25 0C and compare with other studies

error %	Density /gr.cm-3 (in this work)	Density /gr.cm-3 [4]	Ionic liquid
0.58	1.72	1.71	n=2
-3.68	1.57	1.63	n=4
-3.20	1.51	1.56	n=6
-	1.60	NA	n=8

2. Combined distribution functions (CDFs)

To discuss on the difference between center of mass RDFs in details, we draw Combined Distribution Function (CDF) for different center of mass. As shown in Figure 1 (left Figure), surface area at high occurrence illustrates the interaction type and side chain effects on the different species distribution. Also, in the studied ILs, there is a condition to form hydrogen bonding between cation and anion. In this work, we analyze the hydrogen bonding between special atoms in imidazolium cation and eFAP anion by CDFs counter maps (right Figure).

Fig. 1. The Combined Distribution Functions for cation-anion center of mass and of F…HR bond and F… HR-CR angle in studied ILs

Conclusion

Our results obtained from CDFs maps showed that hydrogen bonding between F and HR atoms occur at ~300 pm and more than ~135 degree. These criteria correspond to strong hydrogen bonding between atoms F and HR.