

Local environment structure and dynamics of CO₂ in the 1-ethyl-3-methylimidazolium bis(trifluoromethanesulfonyl)imide and related ionic liquids

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Abstract: Ionic liquids (ILs) have been considered as advanced materials for different applications, due to the ability to be tuned and, as consequence new physical and chemical properties can be reached, such as low steam pressure, low flammability, chemical and thermal stability as well as good solubility of greenhouse gases. The combination of these specific properties makes of the ionic liquids good candidates for CO₂ capture technologies.[1] In this present work molecular dynamics (MD) were carried out in order to correlate the effect of the gas absorption in the local liquid structure and its correlations with the dynamical properties of the system.[2] It were simulated three different ionic liquids, 1-ethyl-3-methylimidazolium bis(trifluoromethanesulfonyl)imide [C₂mim][Tf₂N], 1-ethyl-3-methylimidazolium acetate [C₂mim][Ac] and 1-Butyl-1-methylpyrrolidinium bis(trifluoromethanesulfonyl)imide [BMpyr][Tf₂N] with six different concentrations of CO₂ at 1 atm and 313 K. In Figure 1 can be seen the a combined distribution function (CDF) of the g(r) of H9-S and the angle of H9-O-S for the neat [C₂mim][Tf₂N] and the mixture [C₂mim][Tf₂N]/CO₂ with 50 gas molecule. It is possible to see a slightly change in the orientation of the cation and anion, which was correlated to the detachment of the ions in order to create an empty space to receive the carbon dioxide. However no change was observed in the g(r) on the top of the figure, evidencing that these changes occur just in the local structure of cation and anion.

Figure 2 shows that the addition of CO₂ in the ionic liquid has shown an increase for the diffusivity of ions, which was related to the decrease of cation-anion interaction strength caused by the presence of the gas between the ions. The transport properties results showed that the addition of CO₂ in the IL generates a fluidization[3] of the system, decreasing the viscosity as a consequence of the local environment structure changing. Likewise, the effect of the type of anion and cation on the systems properties was studied considering [Ac]⁻ and [BMpyr]⁺ ions, showing large effects by the change of anion to [Ac]⁻ which rise from the strong [C₂mim]⁺-[Ac]⁻ interaction, which conditions the solvation of ions by CO₂ molecules.

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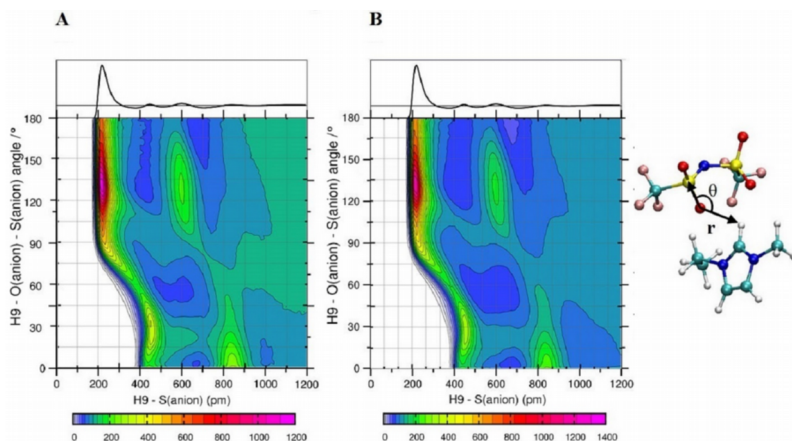


Figure 1 - Combined Distribution Function (CDF) joining the angle and distance distribution for the H9-O(anion)-S(anion) and H9-S(anion), respectively, for the cation-anion interaction in (a) neat $[C_2mim][Tf_2N]$, and (b) fraction 0.24 $[C_2mim][Tf_2N]/CO_2$ at 313 K with a snapshot representing this interaction from MD simulations.

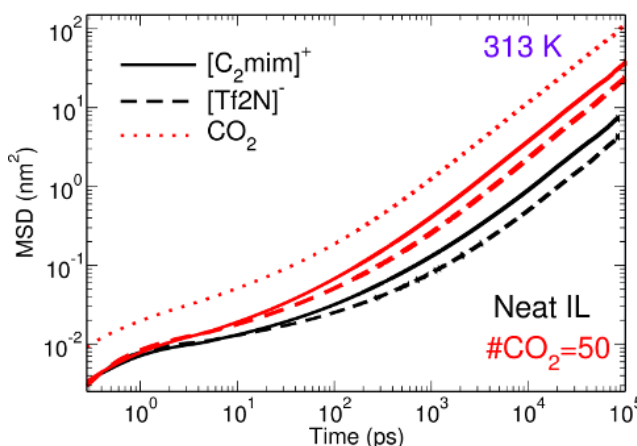


Figure 2 - Mean square displacement of $[C_2mim]^+$ and $[Tf_2N]^-$ in neat ionic liquid and mixture containing 50 molecules of CO_2 at 313 K.

Key-words: Molecular Dynamics, CO_2 , Ionic Liquids

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