When Like-charged Ions Attract: The Influence of Hydroxyl Defects on the Size and Distribution of Cation Clusters in Ionic Liquids

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Attraction between opposite-charged and repulsion between like-charged particles is a commonly accepted concept in science. In contrast, like-charged attraction seems to be counterintuitive at first glance. However, in specifically designed ionic liquids (ILs) with hydroxyl functionalized cations, we found evidence for clustering of cations [1]. Structural and dynamical features, such as the formation of cation clusters, strongly affect the properties of ILs, and a deeper understanding of the relationship between both is worthwhile.

By utilising molecular dynamics simulation as well as neutron diffraction experiments, we are able to investigate the liquid nanostructure of mixtures of $[HOC_4Py][NTf_2]$ and $[C_5Py][NTf_2]$. Data from these studies provide us insight into the formation of cation clusters, and the effects of hydroxyl defects on the clusters' structure and distribution. These clusters are formed via hydrogen bonding between the hydroxyl groups terminating the alkyl chains of the cation. The cations of both ILs are very similar except that the alkyl chain of the former is terminated by a hydroxyl and the latter by a methyl group. The study is aimed towards better understanding the relationship between cluster structures and larger scale nanostructures, which has a strong impact on the properties of ILs.

References:

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