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Weak intermolecular Interactions and Molecular Cluster in Ionic Liquids

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Presently, we are working on weak intermolecular interaction (aliphatic H-bondingand π-π stacking interaction) in imidazolium and piperidinium based ionic liquids. The weak interactions play crucial role on physical properties of ILs. Further, significance of weak interactions on cluster formation and extended intermolecular interaction in these ILs have been investigated in our laboratory. The vibrational spectroscopic techniques (Raman and FTIR) have been employed to understand effect of H-bonding interaction on physical property and molecular cluster formation of ILs. Further, DFT calculations help for better understanding the intermolecular interactions at molecular level.

Ionic liquids (ILs) are a designer ionic materials and influence on scientific interests due to their several applications in different research fields.[1,2] Tunable chemical and physical properties of ILs can be achieved considering different intermolecular interactions among cations and anions. In structure of imidazolium ILs, strong interionic coulombic interaction is observed with different anions.[3,4] Significant contribution from three-dimensional H-bonding network between the counter-ions, dispersion interaction and self-assembly of ILs is observed at microscopic level for explaining mesoscopic heterogeneity.[5,6] several reports aiming on H-bonding and intermolecular interaction as decisivesubject, but it is not clearly understood at molecular level. Relative interaction energy from H-bonding interaction, hydrophobic interaction and molecular orientation, plays a decisive role to generate micro/mesoscopic local domains in ILs.[7,8] Studying ILs with functionalized side chains is alternative exceedingly active area of research that targets at understanding structure-property relationships and number of interesting applications.[9,11] Most research efforts are focused on primarily on intermolecular interactions between cation and anion.

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The aliphatic H-bonding is considered as non-covalent interactions & plays significant role on physical behavior of imidazolium based ILs.[12]

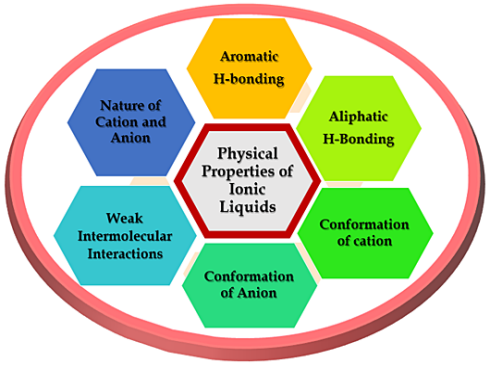

Fig. 1: Different molecular Parameters Effected on Physical properties of ILs

Although aliphatic H-bonding is weaker than aromatic H-bonding, but it has severe impact on physical properties.[13] Aliphatic H-bonding interaction is considered by intra and inter cation-anion interaction in ILs. Impact of weak intermolecular interactions on physical properties of ILs has been investigated on basis of strength cation-anion.[14,15] Due to non existence of suitable structural-properties relationship, & inadequate experimental information, there is open changes and wide scope to explore the ILs research fields.

Conclusion

In our lab, we pragmaticexistence of several aromatic, aliphatic H-bonding & π-π stacking interactions in imidazolium and piperidinium based ILs. Detail analysis of all these interactions show that inconsequential variation of relatively weaker interaction (π-π stacking interaction) can lead to robust packing of constituent ions. In addition, numerousdiverse types of π-π stacking interactions have been recognized in these ILs. These out comes recommend that physical properties of ILs can be alteredradically by amendment these weak interactions alone. It is consequently quite likely that multiple interactions (weak &strong interionic interaction) along with exceedingly estimated mesoscopic structured provides this stability to ILs.

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