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Hydrogen-Bonded Anion Clusters in Choline Phenylalaninate, an Unexpected Origin of Nanostructure in Biocompatible Ionic Liquid

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Recently, a number of choline amino-acid salts have been reported to form ionic liquids (ChILs), creating the possibility of biocompatible ILs with a sustainable production cycle.[1,2] Since their discovery, these designer solvents have proven useful across many applications, including drug synthesis and delivery, electrochemistry, biomass processing and CO2 capture, often in mixtures with water.[3] However, little is still known about how the structure of their constituent ions determines properties and performance of both the pure IL and its solutions, limiting the capacity to design task-specific ILs and optimise for large scale applications. In this study, we investigate choline DL-phenylalaninate (ChPhe) using time-of-flight neutron diffractionand modelled its structure with simulations. Our aim is to understand how its amphiphilic liquid nanostructure arises from atomic correlations. Surprisingly, we discovered the aromatic moieties of the phenylalaninate anion form distinct, small clusters or non-polar domains, but with no evidence for pi-pi stacking. Detailed analysis of the atomic correlations reveals that inter-anion hydrogen bonds are the main stabilisation factor of these non-polar clusters. This is the first example of self-assembled ionic liquid nanostructure not of solvophobic origin. The unusual suite of interactions also explains its water miscibility but inability to retain nanostructure upon water dilution,[4] as well as its poor performance for biomass pretreatment (relative to other nanostructured ChILs),[5] and provides a new strategy by which to engineer and tune ionic liquid nanostructure for the design of application-specific, renewable solvent systems.

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Speakers Gender

Male

Level of Expertise

Student

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Primary author(s) : MIAO, Shurui

Co-author(s) : JIANG, Haihui Joy; Mr WOOD, Jared; Dr IMBERTI, Silvia; Prof. ATKIN, Rob; Prof. WARR, Gregory

Presenter(s) : MIAO, Shurui

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