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Atomistic studies of solvation in deep eutectic solvents

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05 November 2021 | 14:30
online

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Deep eutectic solvents (DES) are a broad category of liquid mixtures, arising from strongly non-ideal interactions formed between ionic and molecular components on mixing.[1] DES therefore make the liquid window more accessible for a wider variety of ordinarily high-melting components to be used as solvating media.[2] As well as a lower melting point, DES therefore lower the access barrier to 'designer' task-specific solvents, by offering a widened chemical space of potential eutectic mixtures.
Concomitantly with the broad chemical space of DES, their multicomponent mixed nature convolutes their bulk structure and interactions, and hence solvation processes are more complicated than in ILs and molecular solvents.[3] To unlock the potential of DES as task-specific solvents, it is therefore critical to begin by understanding the solvation of pertinent species within DES, which is presently poorly understood. Here, we present the results of non-polarisable, scaled-charge MD simulations of DES as a function of water content. First, we have explored the solvation of chloride in popular cholinium chloride DES, in combination with ^{35}Cl NMR spectroscopy, in order to understand the critical role of the anion int he formation of the eutectic, and how this solvation varies as a function of water content. Secondly, we will present results of how DES component choice and water content can be used to modify the solubility of the hydrophobic clothing dye, indigo. We will demonstrate the molecular origin of counterintuitive changes in solvation asymmetry and solubility on addition of water.

[1] Abranches, D. O.; Schaeffer, N.; Silva, L. P.; Martins, M. A. R.; Pinho, S. P.; Coutinho, J. A. P. The Role of Charge Transfer inthe Formation of Type I Deep Eutectic Solvent-Analogous Ionic Liquid Mixtures. Molecules 2019, 24 (20),3687. https://doi.org/10.3390/molecules24203687.
[2] Kollau, L. J. B. M.; Vis, M.; van den Bruinhorst, A.; Esteves, A. C. C.; Tuinier, R. Quantification of the Liquid Window ofDeep Eutectic Solvents. Chem. Commun.2018, 54 (95), 13351–13354. https://doi.org/10.1039/C8CC05815F.
[3] Hammond, O. S.; Edler, K. J. Structure and Implications. In Deep Eutectic Solvents: Synthesis, Properties, and Applications;Wiley-VCH: Weinheim, 2019; pp 25–42.

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