A molecular dynamics investigation of the ionic liquid choline acetate and its application in cellulose solvation

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Choline – (2-hydroxyethyl) trimethylammonium – is an abundantly available, green alternative to commonly studied ionic liquid (IL) cations. Its lack of aromaticity or long aliphatic chains and its protic hydroxyl group make choline an unorthodox IL cation, inviting the question of how these features could influence systemic dynamic and structural behavior. Molecular dynamics (MD) simulations indicate that, when paired with the acetate anion, i.e. [Cho][Ac], choline displays long-lasting heterogeneous dynamics which may be linked to prominent hydrogen-bonding behavior that is distributed unevenly among anions. Moving forward to the exploration of choline's efficacy for carbohydrate solvation, MD simulations were performed on a 12 monomer long single strand of cellulose in [Cho][Ac]. Preliminary studies show minimal direct choline-cellulose interactions, but a notable increase in acetate-cellulose interactions when compared to those found in 1-ethyl-3-methylimidazolium acetate [EMI][Ac]. The distributions of dihedral angles defined along β-D-glucose linkages are broader in [Cho][Ac] than in [EMI][Ac], suggesting less uniform torsion of cellulose chains in [Cho][Ac]. These findings could be representative of greater disruption of cellulose crystallinity, which would bode well for the alluring potential application of [Cho][Ac] as a biomass pretreatment solvent.