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A Computational Study of the Solvation of Chitin in Ionic Liquids and Organic Electrolytes

Exploitation of sustainable and renewable sources of carbon, e.g. cellulose, derived from plant matter such as wood chips, cotton or sugarcane bagasse1 and chitin, which can be isolated from sources such as molluscs, crustaceans, insects and fungi,2 is an important aspect of developing a successful bio–economy. These polymers, however, share a remarkable stability against dissolution by readily available solvents; a result of strong hydrogen bonding within and between polymer chains. Since dissolution is a necessary first step in separation and subsequent degradation through hydrolysis into fermentable sugars, understanding and further developing improved solvents and multicomponent solvent systems is a key step in creating economically feasible routes towards utilization of biomass.

Whereas chitin is insoluble in water and most organic solvents, the derivative chitosan (the deacetylated counterpart of chitin) is soluble in water, albeit at pH below 6.0.3 Ionic liquids (ILs), on the other hand, can dissolve both forms quite readily at moderate temperature and benign conditions.4 We have used classical molecular dynamics simulations to gain molecular insight into the mechanism of dissolution afforded by ionic liquids consisting of the 1–tris(2-hydroxyethyl)methylammonium (THEMA) cation and anions such as acetate and methane sulfonate. This was achieved by simulating large microcrystals/fibrils in solution, at various temperatures and monitoring the changes in the polymeric structure, hydrogen bond formation and ionic liquid solvation structure. In addition, we also used simulation to explore the effect of adding the co-solvent, ethylene diamine (EDA), on the interactions in solution and subsequent dissolution process.

Classical molecular dynamics simulations, extending over a total simulation time in excess of 100 ns each, were run using the PMEMD CPU code, available as part of the AMBER package. PMEMD is one of the fastest MD codes available with a highly efficient MPI implementation and an even more efficient implementation on modern GPU architectures. Benchmarks showed the greatest efficiency when running on a total of 64 cores, distributed across four physical nodes.

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