Computational modelling of cellulose and its modifications

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Cellulose is the most common organic polymer on planet earth. It is produced by a wide range of organism including algae, bacteria and plants, the latter being the most known one as plant-based cellulose is used to produce paper products. Our focus is on bacterial cellulose and its modifications for applications in wound dressings and in biomineralization for artificial joints and bone.

To study these issues, we have performed computer simulations of membrane-cellulose systems using phosphatidylcholine and phosphatidylethanolamine lipids [1] and phophorylate cellulose [2]. In the case of membrane-cellulose systems, hydrogen bonds turned out to be the key player. This is, however, not a simple matter as there is a subtle balance between lipid-cellulose and cellulose-water hydrogen bonds. One of the aims to modify cellulose using common polymers such as polylactic acid [3,4] and I will address some of those issues in this talk.

I will also discuss some difficulties in modelling cellulose in the presence of ions. Significant overbinding of sodium ions was observed independent of the force field. To investigate this further, we set up simpler model systems consisting of poly-α,L-glutamic and poly-α,L-aspartic amino acid and studied the interactions between sodium and potassium ions and the amino acids using several force fields and the so-called NBFIX (non-bonded fix) and ECC (electric continuum) corrections.

References

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