

Modelling the dissolution of cellulose in ionic liquids

Jussi Polvi [1], Tommi T. Järvi [1], Emppu Salonen [2], Kai Nordlund [1]

1 Division of Material Physics, Department of Physics, P.O.Box 64 (Gustaf Hällströminkatu 2a) FI-00014 University of Helsinki, Finland

2 Department of Applied Physics, Helsinki University of Technology, P.O.Box 1100, FIN-02015 TKK, Finland

It has been shown that ionic liquids, such as 1-butyl-3-methylimidazolium chloride (BMIMCl) and 1-allyl-3-methylimidazolium chloride (AMIMCl), can be used to dissolve cellulose without derivation. After the process, cellulose can be separated from its ionic liquid solution by addition of water, ethanol or acetone, and after its regeneration, the ionic liquid can be recovered and reused.

Despite the importance of the subject, relatively few studies have addressed the cellulose-ionic liquid interactions on the atomistic level. Understanding the mechanisms of dissolution and how the ionic liquid affects cellulose-reagent interactions is crucial for allowing the design of better ionic liquids for specific applications.

We present molecular dynamics simulation results of cellulose in ionic liquids, obtained using Gromacs and the Gromos96 and OPLS-AA force fields. We have studied the properties of different ionic liquids and their interactions with crystalline and molecular cellulose.