

Abstract Submitted
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Interaction of Cellulose Chains with Ionic Liquids and Water via MD simulations¹ AHMED ISMAIL, BROOKS RABIDEAU, RWTH Aachen University — One promising route for combustible fuel sources which are both renewable and have a low environmental impact is the conversion of waste biomass into tailor-made fuels. An important aspect of this process is the low-energy separation of cellulose from the biomass. Ionic liquids (ILs) have proven to be very good in dissolving cellulose with the added benefit of being essentially non-volatile making them ideal for “green” processing. IL research, however, remains relatively new, with many parts of this dissolution process remaining uncertain. We examine the behavior of cellulose with the ionic liquids [BMIM]Cl, [EMIM]Ac and [DMIM]DMP as well as water via MD simulation. All three ionic liquids have been observed to dissolve cellulose quite well yet have differently sized anions. We explore these differences and the impacts they have on their interactions with cellulose. First we examine the dynamics of a single cellulose strand in these ionic liquids. We determine the radius of gyration and the hydrogen bonds that are formed between the anions and cellulose. Next, we probe the dissolution mechanism of multiple, bound cellulose strands examining of multiple, bound cellulose strands examining interactions at the IL/cellulose interface and the breakup of inter-cellulose hydrogen bonds.

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