BIOMASS PRETREATMENT USING DESIGNER IONIC LIQUIDS

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Design and development of Ionic Liquid (ILs) is a growing research area that offers the possibility of molecular level control of chemical reactivity and tailored solvation properties. In our work, quantum chemical calculations and molecular dynamics simulations have been used in conjunction with biomass pretreatment experiments to determine the efficiency of ILs. From systematic analyses of the resulting structure-property correlations, our results provides mechanistic understanding of ILs specificity and pretreatment effects on lignin removal and the targeted design of IL:water mixtures with effective dissolution capacity of cellulose. In order to develop novel ILs and to improve IL process selectivity and economics, we have investigated pre-screening ILs for efficient biomass solubility and desired sugar yield using chemoinformatic approaches. A strong correlation between experimental Kamlet and Taft (K-T) parameter values and each of these basicity, acidity, and net basicity quantities for ILs categories have been discovered. The models developed in these studies will guide the targeted design of ILs on superior solubilization of lignocellulosic biomass and will advance the development of IL pretreatment technologies for overcoming biomass recalcitrance to produce fuels, chemicals, and materials.