ABSTRACT

Rapid depletion of the non-renewable fossil fuel resources with fast growing energy demand of the teaming population of the world creates an urgent need to develop alternate and renewable energy sources. In this context, the conversion of 2nd generation biomass to liquefied fuel and fuel additives seems to be a promising solution. In this work, the catalytic conversion of this biomass derived microcrystalline cellulose (MCC) into 5-hydroxymethyl furfural (5-HMF) and its subsequent valorization to fuel additives like HMF cyclic acetal has been attempted using functionalized ionic liquid (IL) catalysts alongwith metal salt cocatalysts. Ionic liquids (ILs) having different functional groups (–SO_3H, –COOH, and –OH) and anions were synthesized in the laboratory and characterized by various spectroscopic techniques like ^{1}H, ^{13}C NMR, FT-IR, TGA, and UV-Vis spectroscopy. Among the synthesized IL catalysts, the IL with –SO_3H functionality and CF_3SO_3 anion showed the highest catalytic activity for MCC conversion into 5-HMF. The structure-activity of the catalyst is theoretically Density Functional Theory (DFT) calculations and experimentally were investigated. In addition, conversion of glucose to levulinic acid (LA) was studied using lab synthesized multifunctional IL catalyst and transition metal salts co-catalyst. The kinetics were investigated in batch reactor, rate constant and activation energies were calculated from the best fitting rate model. Further, valorization of biomass derived 5-HMF and LA into HMF-levulinate was also taken-up under solvent free conditions using dual acidic IL catalysts synthesized and characterized in the laboratory. These laboratory synthesized strong dual acidic IL catalyst showed highest catalytic activity with 97.0% 5-HMF conversion and 78.1% yield of HMF-levulinate. The thermodynamic data for the acetal and esters of 5-HMF were also determined using group contribution methods since these are products which lack this data in reported literature. The valorization of 5-HMF into oxygenated fuel additive acetal compound were studied using IL catalyst. Further, the heterogenization of the IL catalysts thus developed, was attempted in the synthesis of HMF-levulinate and HMF-acetal. This heterogeneous catalyst will have the advantage of easy recoverability and recyclability that can be used on industrial scale.