Indian Institute of Chemical Engineers

Bhubaneswar Regional Centre

Invited Talk Series 2021

Date: 22nd Jan 2021, 4.30 PM

Guest of Honour: Prof. S. Basu, Director, CSIR-IMMT, Bhuaneswar

Atomistic Molecular Dynamic Insights on the Dissolution of Lignocellulosic Biomass with Ionic Liquids and Eutectic Mixtures

Mood Mohan[1] and Vaibhav V. Goud[2] and **Tamal Banerjee**[2,*]

[1]Deconstruction Division, Joint Bioenergy Institute, Emeryville, CA – 94608 & Sandia National Laboratories, 7011 East Ave, Livermore, CA – 94550, email id: mmohan@lbl.gov

[2]Department of Chemical Engineering, Indian Institute of Technology Guwahati, Assam, India

*corresponding author, email id: tamalb@iitg.ac.in

One of the most important drawbacks is that the direct conversion of biomass into value-added chemicals is not possible. Thus, it requires a suitable solvent for the dissolution of biomass without necessitating the pretreatment step. The dissolution of biomass and its derivatives is a demanding task since water and other organic solvents are not able to dissolve these polymers in relatively milder conditions. An extensive research is currently underway to break these complex structures by using different pretreatment methods with green solvents such as Ionic Liquids (IL's) and Deep Eutectic Solvents(DES). These help in reducing the biomass recalcitrance through the following ways namely (a) amorphization of cellulose, (b) delignification, and (c) deacetylation of hemicellulose. Early reports have observed that the solubility of sugars compounds such as glucose and fructose are higher in ILs when compared to other conventional organic solvents It has also been demonstrated that the nature of the cation and anion are dominant factors to be considered for the selection of IL for biomass dissolution. The current talk shall discuss ways to iinitiate screening of these green solvents for the solubility of monosaccharides and disaccharides and also deduce the associated mechanism.

SPEAKER

Prof. Tamal Banerjee
IIT Guwahati

Tamal Banerjee earned his Doctorate degree from Indian Institute of Technology Kanpur in the year 2006. Subsequently, he joined the Indian Institute of Technology Guwahati and is currently a Full Professor at the Department of Chemical Engineering since 2017. He has published over 130 papers in reputed peer-reviewed Journals. In 2011, he was awarded the Indo-US Fellowship in Engineering Sciences. He has also authored two books which discuss experiments and molecular modelling aspect of Ionic Liquids as an extractive agent. His research focuses on the use of Ionic Liquids and Deep Eutectic Solvents (DESs) as green solvents concerning both energy generation and environment mitigation. His group uses both ab-initio methods and Molecular Dynamics methods to predict thermodynamic and transport properties. His other interests lie in the Reactive Force Field simulations of both renewable (alcohols) and non-renewable (coal and chemical hydrides) energy sources. He currently serves in the Editorial Board of *Fluid Phase Equilibria*.

Link: **Join on your computer or mobile MS Teams app**

Click here to join the meeting