Penn Engineering
University of Pennsylvania
Chemical and Biomolecular Engineering

Spring 2023 Seminar Series

LINDA J. BROADBELT

"Developing Strategies for Polymer Redesign and Recycling Using Reaction Pathway Analysis"

Wednesday
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3:30 PM
Wu and Chen Auditorium
Levine Hall

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ABSTRACT

The current lack of sustainability of and the limited portfolio of recycling processes for synthetic polymers have posed serious threats to the environment. Using reaction pathway analysis, we are pursuing a portfolio of strategies for redesign and recycling of polymers for sustainability. Pyrolysis is a promising method for resource recovery from plastic waste that is compatible with current petrochemical infrastructure that thermally converts polymers in the absence of oxygen into valuable chemical feedstocks and monomer. To provide further insight into polymer pyrolysis, a greater understanding of the mechanistic and kinetic details of the underlying reaction network is needed. To handle the complexity of mechanistic modeling of polymer degradation, we have developed both continuum and kinetic Monte Carlo (kMC) models. Alternatively, redesign efforts focusing on polymers that can be reused and recycled to monomers can lead to sustainable solutions for the plastics waste problem. One pathway to success is to identify bioprivileged molecules, biology-derived chemical intermediates that can be efficiently converted to a diversity of chemical products, including both novel molecules and drop-in replacements, and molecules emanating from them that can be used as monomers leading to recyclable polymers. We have developed a framework for molecule discovery and reaction pathway design that is automated and flexible and can be used to screen for bioprivileged candidates and target molecules. The application to discovery of known and novel monomers for poly(hydroxyurethanes) that are derived from biobased molecules and lead to recyclable materials will be discussed, and computational methods to evaluate the recyclability of different polymers will be outlined.

BIO

Linda Broadbelt is Sarah Rebecca Roland Professor in the Department of Chemical and Biological Engineering (ChBE) and Associate Dean for Graduate Research and Education of Engineering at Northwestern University. She was Chair of the Department of ChBE from 2009-2017. Her research and teaching interests are in multiscale modeling, complex kinetics modeling, catalysis, novel biochemical pathways, and polymerization/depolymerization kinetics. She served as the Past Chair, Chair, First Vice Chair and Second Vice Chair of the Catalysis and Reaction Engineering Division of AIChE, and also served on the Executive Board of the National Program Committee of AIChE and the Board of Directors. She is currently an Associate Editor for *Industrial&Engineering Chemistry Research* and *ACS Engineering Au*. Her honors include selection as the winner of the R.H. Wilhelm Award in Chemical Reaction Engineering from AIChE, the E.V. Murphree Award in Industrial Chemistry and Engineering from the American Chemical Society, the Dorothy Ann and Clarence Ver Steeg Award, a CAREER Award from the National Science Foundation, and an AIChE Women's Initiative Committee Mentorship Excellence Award, and selection as a Fellow of the American Association for the Advancement of Science, a Fellow of AIChE, a Fellow of AIMBE, and a Fulbright Distinguished Scholar. She was elected to the National Academy of Engineering in 2019. In 2021, she was elected to the American Academy of Arts & Sciences.