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BENJAMIN M. STATLER COLLEGE OF ENGINEERING AND MINERAL RESOURCES

MATERIALS SCIENCE AND ENGINEERING (MS&E) SEMINAR SERIES
Friday October 15, 2021 at 3:00 pm via Zoom

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"Elucidating the Molecular Origins of Mechanical Properties of Biomass through Molecular and Coarse-Grained Dynamics Simulations of Lignocellulose Assemblies"

Dr. Peter N. Ciesielski
Principal Scientist and Distinguished Member of Research Staff
National Renewable Energy Lab, Golden CO

Plant cell walls are highly-evolved nanocomposite materials with impressive properties and useful functionality. The macromolecular assembly of cellulose, hemicellulose, and lignin, collectively termed lignocellulose, serves multiple functions to plants including structural support, transport of water and nutrients, and biological defense. This same material has also served humanity since the beginning of civilization in applications spanning construction materials, clothing, and fuel. Solving the macromolecular puzzle of lignocellulose structure/property relationships holds the key to efficiently disentangling and deconstructing biomass for conversion to fuels and chemicals, as well as designing new bio-based materials with tailored properties. In this presentation, I will discuss modeling approaches to understand how molecular characteristics give rise the emergent properties that ultimately govern the bulk behavior of lignocellulosic composites. First, I will present findings concerning the interplay between mechanical processing and molecular defect induction in cellulose nanofibrils which have clear implications for enzymatic saccharification and nanocellulose production. Next, I will discuss the construction of simulations of a 3-component system including multiple cellulose nanofibrils, hemicellulose, and lignin. The starting configuration of the polymers is informed by NMR experiments. Simulations varying the monomeric composition of the lignin polymers show that monomers which contain more methoxy groups on the aromatic rings increase the mechanical integrity of the assembly. Finally, I will present recent progress towards development of a coarse-grained dynamics modeling framework that will enable investigations biopolymer assemblies several orders of magnitude larger than those accessible to molecular dynamics simulations.

Bio: Dr. Peter Ciesielski is a Principal Scientist in the Renewable Resources and Enabling Science Center at the National Renewable Energy Laboratory (NREL). He has an interdisciplinary background and training and holds a B.S. degree in Chemical and Biological Engineering from Colorado State University and Ph.D. in Materials Science from Vanderbilt University. Peter's research encompasses many aspects of bioenergy and biobased materials, including biohybrid systems, catalysis, Nano biomaterials, and production of fuels and chemicals biomass. Peter specializes in integrating experimental methods with multiscale modeling to design, understand, and optimize processes that are central to bioenergy and bio-based material applications. During his ten years at NREL, he has published over 80 peer-reviewed journal articles and received numerous awards and honors, which most recently include being named a Distinguished Member of Research Staff and an ACS Energy & Fuels Rising Star both in 2021.

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