



Frontiers in Biorefining

*Chemicals and Products
from Renewable Carbon*

2018

International Conference

St. Simons Island, Georgia, USA
November 5 - November 8

Steering Committee Members

Nourredine Abdoulmoumine
Joseph Bozell
Stephen Chmely
Nicole Labbé
Timothy Rials
Center for Renewable Carbon
The University of Tennessee

Advisory Board Members

Gregg Beckham
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Linda Broadbelt
Northwestern University

Kevin Edgar
Virginia Polytechnic Institute and State
University

Dan Cosgrove
Pennsylvania State University

Roberto Rinaldi
Imperial College London

Andy Sutton
Los Alamos National Laboratory

Hosted By:



CONFERENCE SCHEDULE

MONDAY NOVEMBER 5, 2018

5:00pm-8:00pm Registration/Social Hour

TUESDAY NOVEMBER 6, 2018

6:45am-7:40am Registration/Breakfast

Plenary Session:

Biorefinery Concepts

Session Chair: **Timothy Rials** (*The University of Tennessee*)

7:45-8:00 **Timothy Rials** (*The University of Tennessee*) Welcome and Opening Remarks

8:00-8:40 **Wilfred Vermerris** (*University of Florida*) Genetic enhancement of bioenergy crops to support the bio-economy in the southeastern United States

8:40-9:20 **Brigitte Chabbert** (FARE laboratory, INRA, Université de Reims Champagne-Ardennes) Multimodal characterization of lignocelluloses in the frame of biofuel production

9:20-10:00 **Jeremy Luterbacher** (*École Polytechnique Fédérale de Lausanne*) Protect and serve: acetal formation during biomass fractionation as a toolkit for reducing degradation and introducing new reactivity

10:00am-10:30am Coffee Break

10:30-11:10 **Roberto Rinaldi** (*Imperial College London*) Lignin-first biorefining: past, present and future

11:10-11:50 **Thomas Epps** (*University of Delaware*) From trees to plastics: designer polymers from lignin-rich feedstocks

11:50-12:30 **Jesse Hensley** (*National Renewable Energy Laboratory*) Bio-triptane to re-energize biofuel and to solve our octane shortage

12:30pm-2:00pm Lunch **Toni Grönroos** (*METGEN Oy*) Novel enzymes for biorefinery streams valorisation

Session 2A:

Feedstock-Conversion Interface

Session Chair: **Julie Carrier** (*The University of Tennessee*)

2:30-3:00 **Charles Frazier** (*Virginia Polytechnic Institute and State University*) Plasticity in lignin acidolysis pathways

3:00-3:30 **Joseph Jakes** (*USDA-Forest Service*) Measurement of moisture-dependent ion diffusion constants in secondary lignocellulosic cell walls using time-lapse micro x-ray fluorescence microscopy

3:30-3:50 *Flash Talks*

Valerie García-Negrón (*The University of Tennessee*) Control of carbon composite nano- and meso- structure through feedstock and processing conditions

Enshi Liu (*University of Nebraska-Lincoln*) Microbial production of aryl alcohol oxidase using genetically modified *Aspergillus nidulans* and enzymatic depolymerization of lignin

Xiangchen Huo (*National Renewable Energy Laboratory*) Catalytic upgrading of short chain acids to renewable diesel fuel

Jake Lindstrom (*Iowa State University*) Condensed phase thermal depolymerization of cellulose

3:50pm-4:10pm Coffee Break

4:10-4:40 **Nicholas Thornburg** (*National Renewable Energy Laboratory*) Understanding mesoscale reaction-diffusion phenomena governing lignin extraction from hybrid poplar in methanol

4:40-5:10 **Laurene Tetard** (*University of Central Florida*) Nanoscale exploration of decomposition of lignocellulosic biomaterials in liquid environments

Session 2B:

Biomass Fractionation and Separation

Session Chair: **Nicole Labbé** (*The University of Tennessee*)

2:30-3:00 **Sankar Nair** (*Georgia Institute of Technology*) Nanoporous materials for biorefinery separations

3:00-3:30 **Heather Trajano** (*University of British Columbia*) Capturing the complexity of hemicellulose hydrolysis

3:30-3:50 *Flash Talks*

Tom Renders (*Katholieke Universiteit Leuven*) Catalytic lignocellulose biorefining in butanol/water: a one-pot approach toward phenolics, polyols, and cellulose

Kirsten Davis (*Iowa State University*) Utilization of phenolic monomers by microbes for valorization of lignin

Mohammad Shahinur Rahaman (*University of Louisville*) Mechanistic insights of the acid-catalyzed diphenolic acid production from renewable biomass

3:50pm-4:10pm Coffee Break

4:10-4:40 **Agi Brandt-Talbot** (*Imperial College London*) Low cost ionic liquids for biorefining of lignocellulosic biomass

4:40-5:10 **Abby Engelberth** (*Purdue University*) A molecular modeling approach for solvent screening: extracting hydrogen sulfide with soybean oil

TUESDAY NOVEMBER 6, 2018

6:00pm-7:30pm Group Picture/Social Hour

WEDNESDAY NOVEMBER 7, 2018

6:45am-7:50am Breakfast

Session 3A: Polymers and Soft Materials

Session Chair: **Stephen Chmely** (*The University of Tennessee*)

- 8:00-8:30 **Meisha Shofner** (*Georgia Institute of Technology*) Processing strategies for cellulose nanocrystal/polymer composites
- 8:30-9:00 **Nathalie Lavoine** (*North Carolina State University*) Cell wall deconstruction and conversion into high performance ligno-nanocellulosic materials
- 9:00-9:30 **Kalavathy Rajan** (*The University of Tennessee*) Development of photocurable resins based on lignin-mimics
- 9:30-10:00 **Colleen Scott** (*Mississippi State University*) Sustainable bio-based polymers from lignin-derived precursors
- 10:00-10:15 *Flash Talks*
- Ydna Questell-Santiago** (*École Polytechnique Fédérale de Lausanne*) Carbohydrate stabilization extends the kinetic limits of chemical polysaccharide depolymerization
- Ryan Kalinoski** (*University of Kentucky*) Antimicrobial properties of thermochemically processed lignin derived compounds

10:15am-10:30am Coffee Break

- 10:30-11:00 **Andrew Sutton** (*Los Alamos National Laboratory*) Catalytic carbon chain extension and selective defunctionalization of bioderived building blocks
- 11:00-11:30 **Ngoc Nguyen** (*Oak Ridge National Laboratory*) Intra- and inter-molecular interactions of lignocellulosic biomass in 1-ethyl-3-methylimidazolium acetate ionic liquid: solution spinnability and molecular orientation
- 11:30-12:00 **Peter Olsén** (*Wallenberg Wood Science Center*) Controlled synthesis of functional degradable lignin star-copolymers
- 12:00-12:30 **Martin Lawoko** (*KTH Royal Institute of Technology*) Upgrading crude technical lignins to functional polymers and materials

12:30pm-5:00pm Free Time

Session 3B: Catalytic Conversion of Lignin and Carbohydrates

Session Chair: **Nourredine Abdoulmoumine** (*The University of Tennessee*)

- 8:00-8:30 **Eric Hegg** (*Michigan State University*) [Lignin valorization: biomimetic reductive cleavage of \$\beta\$ -O-4 bonds using small organic thiols](#)
- 8:30-9:00 **Derek Vardon** (*National Renewable Energy Laboratory*) Low-cycle atomic layer deposition for enhanced catalyst stability during biobased adipic acid production
- 9:00-9:30 **Tom Baker** (*University of Ottawa*) Surfing the bioeconomy wave: adventures in catalyzed oxidation of lignin extracts and C6 diacid production from homocitric acid lactone
- 9:30-10:00 **Aditya Bhan** (*University of Minnesota Twin Cities*) [Catalytic deoxygenation](#)
- 10:00-10:15 *Flash Talks*
- Yadong Chiang** (*Georgia Institute of Technology*) Separation and purification of bioderived furanic molecules with metal-organic frameworks
- Jher Hau Yeap** (*École Polytechnique Fédérale de Lausanne*) Selectivity control during the single-step conversion of aliphatic carboxylic acids to linear olefins
- Md. Anwar Hossain** (*University of Louisville*) Novel bio-derived solvents for processing lignocellulose

10:15am-10:30am Coffee Break

- 10:30-11:00 **Basudeb Saha** (*University of Delaware*) Biomass valorization: high value products via C-C coupling and hydrodeoxygenation chemistry
- 11:00-11:30 **Arul Mozhy Varman** (*Arizona State University*) Systems and synthetic biology studies for effective lignin valorization
- 11:30-12:00 **Susan Habas** (*National Renewable Energy Laboratory*) Tunable nanoscale metal phosphide catalysts for thermocatalytic and electrocatalytic conversion of renewable feedstocks
- 12:00-12:30 **Noppadon Sathitsuksanoh** (*University of Louisville*) One-pot acid-catalyzed levulinic acid production from industrial hemp: from controversy to commodity

5:00-6:50pm Poster Session

The Steering Committee members would like to thank the following judges for assessing all the student posters:

Agi Brandt-Talbot (*Imperial College London*)

Nathalie Lavoine (*North Carolina State University*)

Martin Lawoko (*KTH Royal Institute of Technology*)

Meisha Shofner (*Georgia Institute of Technology*)

Aparna Annamraju (*The University of Tennessee*) Investigating the physical and chemical interactions between cellulose, xylan and lignin in three different carboxylate ionic liquids

Student poster competition Second Prize winner

Yadong Chiang (*Georgia Institute of Technology*) Separation and purification of bioderived furanic molecules with metal-organic frameworks

Student poster competition First Prize winner

Raphaël Coste (*FARE laboratory, INRA, Université de Reims Champagne-Ardennes*) The impact of resin embedding on the physicochemical properties of plant cell walls: a nanoscale study

Kirsten Davis (*Iowa State University*) Utilization of phenolic monomers by microbes for valorization of lignin

Courtney L. Ford (*Los Alamos National Laboratory*) A Photochemical Approach to Generate Energy Dense Fuels from Biomass

Valerie García-Negrón (*The University of Tennessee*) Control of carbon composite nano- and meso- structure through feedstock and processing conditions

Wenhui Geng (*North Carolina State University*) Carboxymethylation of hemicellulose isolated from poplar and its potential applications

Arun Ghosh (*The University of Tennessee*) Reactive thermal extrusion of organosolv lignin into thermoplastic materials

Gary Grim (*National Renewable Energy Laboratory*) Bench-scale gasification and techno-economic analysis of pine, poplar, switchgrass, miscanthus, and forest residue feedstocks for the synthesis of high-octane gasoline

Md. Anwar Hossain (*University of Louisville*) Breaking softwood recalcitrance by an integrated thermochemical and biological pathway

Md. Anwar Hossain (*University of Louisville*) Novel bio-derived solvents for processing lignocellulose

Xiangchen Huo (*National Renewable Energy Laboratory, Colorado School of Mines*) Catalytic upgrading of short chain acids to renewable diesel fuel

Mochen Liao (*North Carolina State University*) The predictive life cycle assessment of activated carbon production via different pathways: an artificial neural network and kinetic based model

Jake Lindstrom (*Iowa State University*) Condensed phase thermal depolymerization of cellulose

Enshi Liu (*University of Nebraska-Lincoln*) [Microbial production of aryl alcohol oxidase using genetically modified *Aspergillus nidulans* and enzymatic depolymerization of lignin](#)

Wei Liu (*Virginia Polytechnic Institute and State University*) Valorization of hemicellulose hydrolyzates into eco-friendly surfactants

Jianhua Lyu (*The University of Tennessee & Fujian Agriculture and Forestry University*) Effects of residual lignin on energy consumption during a green manufacturing of switchgrass-based lignin-containing cellulose nanofibers

Ydna Questell-Santiago (*École Polytechnique Fédérale de Lausanne*) Carbohydrate stabilization extends the kinetic limits of chemical polysaccharide depolymerization

Student poster competition Third Prize winner

Chad Peterson (*Iowa State University*) Characterization of phenolic oil produced during autothermal pyrolysis

WEDNESDAY NOVEMBER 7, 2018

5:00-6:50pm Poster Session

Tom Renders (*Katholieke Universiteit Leuven*) Catalytic lignocellulose biorefining in butanol/water: a one-pot approach toward phenolics, polyols, and cellulose

Miguel Santoscoy (*Iowa State University*) Membrane engineering in *E. coli* to increase its robustness for the increased production of biofuels and bio-privileged molecules

Mohammad Shahinur Rahaman (*University of Louisville*) Hydrophobic zeolites enabling acetalization of crude glycerol: influence of water and NaCl on catalytic activity and solketal selectivity

Mohammad Shahinur Rahaman (*University of Louisville*) Mechanistic insights of the acid-catalyzed diphenolic acid production from renewable biomass

Anh To (*National Renewable Energy Laboratory*) Catalytic CO₂ hydrogenation using supported metal modified molybdenum carbide nanoparticles

Xiaokun Yang (*Los Alamos National Laboratory*) [Hydrodeoxygenation of bio-derived ketones with heterogeneous catalysts for fuel and chemical production](#)

Jher Hau Yeap (*École Polytechnique Fédérale de Lausanne*) Selectivity control during the single-step conversion of aliphatic carboxylic acids to linear olefins

Seunghyun Yoo (*North Carolina State University*) Graphite formation kinetics of loblolly pine wood and bio-choice lignin investigated by in situ x-ray diffraction technique

Longfei Zhang (*The University of Tennessee & Chinese Academy of Forestry*) Innovative synthesis of fluorescent carbon nanodots with tunable quantum yields by recycling waste from pressurized hot water extraction of switchgrass biomass

7:00pm-9:00pm Conference Dinner

Keynote speaker: **Timothy Theiss** (*Oak Ridge National Laboratory*) Recent developments and trends in 3D printing with bio-derived materials

6:45am-7:50am Breakfast

Session 4A:**Understanding Biomass Recalcitrance**Session Chair: **Roberto Rinaldi** (*Imperial College London*)

- 8:00-8:30 **Tim Tschaplinski** (*Oak Ridge National Laboratory*)
Metabolomics of populus deltoides plants with modified gene activity prior to and within the lignin pathway reveals alterations in carbon flux to secondary metabolism and the underlying basis of biomass recalcitrance
- 8:30-9:00 **Josh Michener** (*Oak Ridge National Laboratory*)
Identification and reconstruction of pathways for lignin catabolism
- 9:00-9:30 **Toni Grönroos** (*METGEN Oy*) Enzymatic lignin modification
- 9:30am-10:00am Coffee Break**
- 10:00-10:30 **Loukas Petridis** (*Oak Ridge National Laboratory*)
Molecular flexibility in bioenergy applications
- 10:30-11:00 **Thomas Elder** (*USDA-Forest Service, Southern Research Station*) The application of density functional theory calculations to the formation and reactions of lignin
- 11:00-11:30 **Kurt Van Allsburg** (*National Renewable Energy Laboratory*) Catcost: an estimation tool to aid commercialization of catalytic materials

Session 4B:**Thermochemical Transformations of Biomass**Session Chair: **Jesse Hensley** (*National Renewable Energy Laboratory*)

- 8:00-8:30 **Nourredine Abdoulmoumine** (*The University of Tennessee*)
[Capturing the intricacies of lignocellulosic biomass gasification in multiphysics and multiscale analysis: present and future](#)
- 8:30-9:00 **Peter Ciesielski** (*National Renewable Energy Laboratory*)
Multiscale modeling of catalytic fast pyrolysis
- 9:00-9:30 **Lauren Dellon** (*Northwestern University*) Microkinetic modeling of vapor phase upgrading of small oxygenates
- 9:30am-10:00am Coffee Break**
- 10:00-10:30 **Frederick Baddour** (*National Renewable Energy Laboratory*)
A molecular approach to the design of nanostructured metal carbide catalysts for the upgrading of renewable feedstocks
- 10:30-11:00 **Daniel Ruddy** (*National Renewable Energy Laboratory*)
Evaluating Cu/BEA catalyst performance with techno-economic analysis to develop a market-responsive biorefinery concept around the conversion of DME to high-octane hydrocarbons
- 11:00-11:30 **Ofei Mante** (*RTI International*) Biocrude as a source of aroma chemicals in an integrated biorefinery

11:30am-12:00pm Box Lunch