

EFRC: CATALYSIS CENTER FOR ENERGY INNOVATION (CCEI)

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AWARDS: \$17.5M (August 2009 – July 2014); \$12.4M (August 2014 – July 2018) WEBSITES: http://science.energy.gov/bes/efrc/centers/ccei/; http://www.efrc.udel.edu/ TEAM: University of Delaware (Lead): Dionisios G. Vlachos (Director), Stavros Caratzoulas, Douglas J. Doren, Raul F. Lobo, Basudeb Saha, Stanley I. Sandler, Klaus H. Theopold, Donald A. Watson, Bingjun Xu; Brookhaven National Laboratory/Yeshiva University: Anatoly Frenkel; California Institute of Technology: Mark E. Davis; Columbia University/Brookhaven National Laboratory: Jingguang G. Chen; Georgia Institute of Technology: Christopher W. Jones; Lehigh University: Mark A. Snyder; Rutgers University: Marianthi G. lerapetritou; University of Massachusetts Amherst: Wei Fan, Friederike C. Jentoft; University of Minnesota: Paul J. Dauenhauer, J. Ilja Siepmann, Michael Tsapatsis; University of Pennsylvania: Raymond J. Gorte, Christopher B. Murray

SCIENTIFIC MISSION AND APPROACH

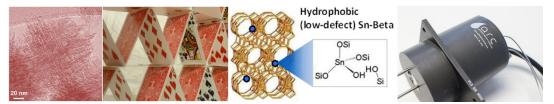
CCEI develops innovative, transformational heterogeneous catalytic technologies for utilization in future biorefineries to economically convert lignocellulosic (non-food-based) biomass into bio-products and fuels. The overarching goals of CCEI are to develop the science that will enable the transformation of lignocellulose to fuels and bio-products, to prepare the workforce for future biorefineries, and to facilitate technology transfer. The center's research consists of three thrusts:

- 1) **Furans**: Efficiently transform sugars (like glucose and xylose) derived from cellulose and hemicellulose biomass to various intermediates, such as furans and fuel-grade compounds.
- 2) <u>Hydrodeoxygenation (HDO)</u>: Selectively upgrade furans and partially-oxygenated compounds to deoxygenated chemicals and transportation fuels.
- 3) <u>Aromatics</u>: Selectively convert and upgrade furans to aromatic compounds (such as BTX benzene/ toluene/xylene), which are important feedstocks in the chemical industry. Existing means of producing BTX are energy-intensive and require petroleum (not shale gas) as a feedstock.

SELECTED SCIENTIFIC ACCOMPLISHMENTS

- Introduced the first-of-its-kind heterogeneous catalyst (Sn- or Ti-Beta zeolite) for the isomerization of glucose to fructose to replace the existing, costly enzymatic process. Used theory and experiment to explain how these hydrophobic molecular sieves work for glucose and related sugar conversions.
- Demonstrated that the Sn-Beta catalyst is active at low pH and in the presence of salt, enabling tandem reactions to convert glucose to fructose to HMF (a furan that is a potential "carbon-neutral" feedstock for fuels and chemicals) in a single pot. Traditional methods require multiple pots, which can be more costly to implement and generate additional waste.
- Synthesized hierarchical multiscale materials that are hydrothermally stable, possess tunable porosity with bio-inspired functionality in the active sites, and minimized resistance to molecular motion while allowing shape selectivity. The new structures improve the effectiveness of traditional catalysts with no increase in cost or unwanted change in functionality.
- Established the first route for the production of renewable aromatics (BTX, benzoic acid, phthalic anhydrite, etc.) from biomass derivatives using acid zeolites on feedstocks from sugars.
- Predicted, and confirmed experimentally, that Mo₂C is an extremely selective deoxygenation catalyst to convert small oxygenates to high demand renewable alkenes, such as propylene.
- Produced the highest yield of dimethylfuran from sugars with an ultra-selective and stable catalyst.





CCEI research, from left: Sheets of zeolite catalysts form an open pore hierarchical structure like a "house-of-cards"; The active site (blue dot) in the Sn-Beta zeolite, surrounded by a hydrophobic sieve, selectively converts sugars derived from biomass; The Polyarc[®] reactor system is an add-on to gas chromatographs that increases accuracy while eliminating the need for calibration.

IMPACT

- Activated Research Company (ARC), a start-up company founded in 2014, is commercializing the Polyarc[®] reactor system, an add-on detector to existing gas chromatographs (GCs) that reduces operating costs and improves the accuracy in quantification without the need for calibration standards. GCs are widely used in the petroleum, chemical and other analytical industries. The core technology is based on CCEI work. In June 2016, Wasson-ECE Instrumentation, a leading provider of GCs, partnered with ARC to distribute the Polyarc[®] reactor system world-wide and incorporate the technology into their own products. <u>http://www.activatedresearch.com/</u>
- Anellotech, co-founded by George Huber (a CCEI member from 2009-2012) in 2008, is developing cost-competitive renewable chemicals from non-food biomass. These biomass-derived chemicals are used to make important plastics that are used in consumer goods such as beverage bottles, clothing, carpeting, automotive and electronic components. Anellotech, a CCEI industrial partner, has licensed patents which include CCEI-supported investigators as inventors. http://www.anellotech.com/
- CCEI's Industrial Consortium accelerates technology transfer by developing long-term relationships with members of industry. Members attend CCEI's annual meetings, recruit EFRC students and postdocs, and have the option to sponsor research projects that are tailored to the sponsoring company's interests and needs. Current and past members include: Activated Research Company (ARC), Air-Liquide, Anellotech, Bridgestone Americas Center for Research & Technology, Dow Chemical Company, DuPont Company, ExxonMobil, Renewable Energy Group, INVISTA, Micromidas, Plant PET Technology Collaborative (PTC), The P&G Company, and Virdia. http://www.efrc.udel.edu/consortium.html
- CCEI research accomplishments have been the basis for over \$1.1M in follow-on funding from several companies including ExxonMobil, Air Liquide, and PTC (CocaCola, P&G, Nike, Ford, Heinz), \$1.3M from other DOE programs, and at least \$900K from other government agencies.

PUBLICATIONS AND INTELLECTUAL PROPERTY

As of May 2016, CCEI had published 257 peer-reviewed publications cited over 7,500 times and filed 20 disclosures, 16 US patent applications, and 39 foreign patent applications. Six patents have been issued and 5 disclosures or patent applications licensed. A selection of highly cited papers are:

- Moliner, M., Roman-Leshkov, Y. & Davis, M. Tin-containing zeolites are highly active catalysts for the isomerization of glucose in water. *PNAS* **107**, 6164-6168, doi:<u>10.1073/pnas.1002358107</u> (2010). [**347 citations**]
- Yu, W., Porosoff, M. & Chen, J. Review of Pt-Based Bimetallic Catalysis: From Model Surfaces to Supported Catalysts. *Chemical Reviews* **112**, 5780-5817, doi:<u>10.1021/cr300096b</u> (2012). [**321 citations**]
- Nikolla, E. *et al.* "One-Pot" Synthesis of 5-(Hydroxymethyl)furfural from Carbohydrates using Tin-Beta Zeolite. *Acs Catalysis* **1**, 408-410, doi:10.1021/cs2000544 | 10.1021/cs2000544 (2011). [**261 citations**]
- Roman-Leshkov, Y. *et al.* Mechanism of Glucose Isomerization Using a Solid Lewis Acid Catalyst in Water. *Angewandte Chemie-International Edition* **49**, 8954-8957, doi: <u>10.1002/anie.201004689</u> (2010). [**240 citations**]
- Carlson, T., Cheng, Y., Jae, J. & Huber, G. Production of green aromatics and olefins by catalytic fast pyrolysis of wood sawdust. *Energy & Environmental Science* **4**, 145-161, doi: <u>10.1039/c0ee00341g</u> (2011). [**194 citations**]