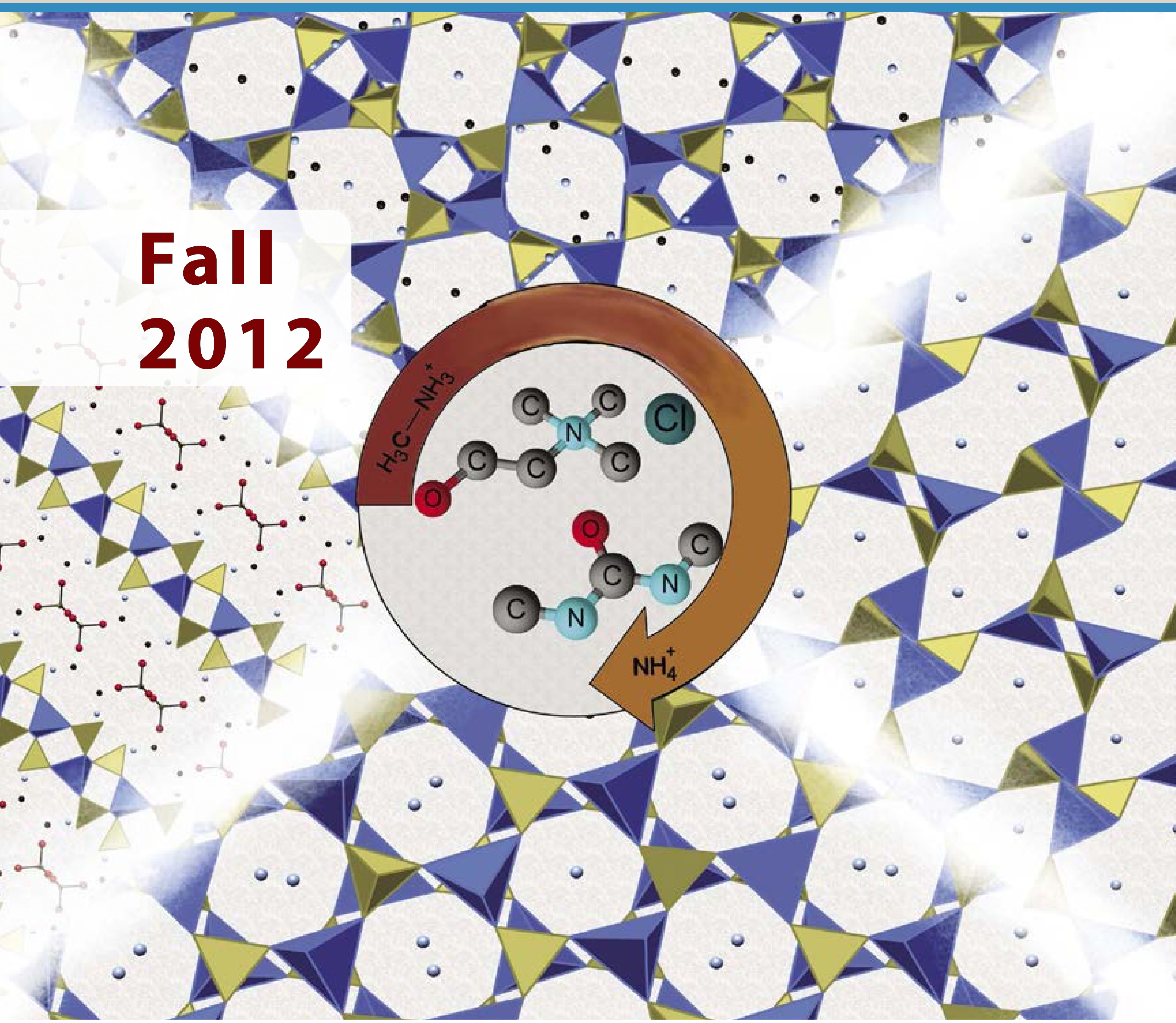
CENTER FOR CATALYTIC SCIENCE & TECHNOLOGY



Cover Image: Chemical Communications | A general synthetic method for MPO4 (M=Co, Fe, Mn) frameworks using deep-eutectic solvents ---**Feng Jiao** *et al*.

Dare to be first.

UNIVERSITY OF DELAWARE

www.che.udel.edu/ccst

FROM THE DIRECTOR

Raul F. Lobo
Chemical & Biomolecular Engineering

RESEARCH INTERESTS
Synthesis, characterization and discovery of novel microporous materials and structure property relationships in catalysts and adsorption.

The Center for Catalytic Science and Technology (CCST) continues to be a leader in catalysis research with substantial efforts in new catalyst discovery, the application of state-of-the-art characterization techniques, and the development of novel computational methods. You have probably noticed the rapid growth in the number of scientific journals devoted to all aspects of catalysis research across the globe. I am glad to report that the CCST's research has a prominent presence in these new publications as well as the more established catalysis journals.

This publication describes some of our most important discoveries reported in 2011-2012, and shows a sample of the intense research activities conducted at the CCST. Our research environment remains dynamic and highly interactive. We continue to attract first-rate students who recognize that CCST is a place that not only fosters innovation, but also nurtures the innate research capacity of the students.

I would like to extend a warm welcome to our newest colleague, Wilfred Chen, the Gore Professor of Chemical Engineering at the University of Delaware (UD). Wilfred joined the Department of Chemical and Biomolecular Engineering at UD in 2011. Prior to joining Delaware, he was professor in the Chemical and Environmental Engineering Department at the University of California, Riverside. Wilfred's research focuses on the development of the next generation of biomolecular tools needed for biofuel production including biocatalysts. We believe the future will see an increased synergy between biocatalysis and classical catalysis in order to meet future technological challenges. We are excited that Wilfred will play a key role in leading CCST in this direction.

I also extend my gratitude to the Eastman Chemical Company for sponsoring our 2012 Spring Seminar Series that featured distinguished seminar speakers who gave enlightening presentations, and also for sponsoring the Eastman Chemical Student Award. This year's award will be presented to Weiting Yu during our Annual Research Review for her important discoveries in the reforming of small oxygenates on bimetallic and carbide surfaces. Last year's award recipient was Mike Salciccioli.

We encourage you to contact us with questions or comments, and we hope you will visit our center either in person or via our web site (www.che.udel.edu/ccst). We look forward to continuing fruitful collaborations with each of you--our institutional partners, industrial sponsors and scientific colleagues.

With best regards,

RAUL LOBO
CCST Director

Industrial Sponsors Program

Our Industrial Sponsors Program embodies the principal mechanisms for industry-university cooperation as they have evolved over the Center's three decades of operation. The tangible benefits of such cooperation are many and include joint research programs, publications, and patents, as well as significant opportunities for support through established industry-university cooperative research funding mechanisms.

Benefits of Sponsorship

CCST sponsors benefit from the full portfolio of the Center's research activities including a number of programs designed to provide early access to nonproprietary research:

Access to CCST Facilities

- Sample analysis
- Discounted rates for experiments
- Use of CCST software

Faculty Expertise

- Consultation by CCST faculty

Recruitment

- Recruitment of outstanding students

Research Programs and Activities

- Invitation to the Center's annual research review at which the results of ongoing research programs are presented by center faculty and students
- Annual report of the Center's research activities and accomplishments

CCST Seminars

- Invitation to Center seminars by catalysis experts from around the world

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CENTER FACULTY

Mark A. Barteau
Chemical & Biomolecular Engineering

RESEARCH INTERESTS

Surface science and catalysis by metal oxides and metals; acid-base catalysis; application of density functional theory to surface reactions; self-assembly of inorganic materials, scanning probe microcopies

Douglas J. Buttrey
Chemical & Biomolecular Engineering

RESEARCH INTERESTS

Synthesis of complex oxides and alloys, composition-structure-property relationships in catalytic and electronic materials; high-resolution electron microscopy

Jingguang Chen
Chemical & Biomolecular Engineering

RESEARCH INTERESTS

Synthesis and characterization of metal carbides and bimetallic alloys as low-cost catalysts and electrocatalysts.

Wilfred Chen
Chemical & Biomolecular Engineering

RESEARCH INTERESTS

Cellular and metabolic engineering, synthetic biology for biofuel production, protein therapeutics, viral detection, drug discovery, protein purification.

Douglas J. Doren
Chemistry and Biochemistry

RESEARCH INTERESTS

Theoretical and computational methods with applications to materials science, surface science, catalysis and solvation

Feng Jiao
Chemical & Biomolecular Engineering

RESEARCH INTERESTS

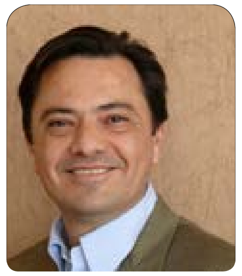
Energy storage and conversion, advanced lithium-ion batteries, solar energy harvesting, and synthesis of nanostructure materials

Michael T. Klein
Chemical & Biomolecular Engineering

www.che.udel.edu/klein

RESEARCH INTERESTS

Chemical Reaction Engineering with special emphasis on the kinetics of complex systems



Raul F. Lobo
Chemical & Biomolecular Engineering

RESEARCH INTERESTS

Synthesis, characterization and discovery of novel microporous materials and structure property relationships in catalysts and adsorption.

S. Ismat Shah
Materials Science & Engineering

RESEARCH INTERESTS

Nanostructured materials synthesis via PVD and CVD processes with applications to environmental catalysis and energy generation

Andrew V. Teplyakov
Chemistry and Biochemistry

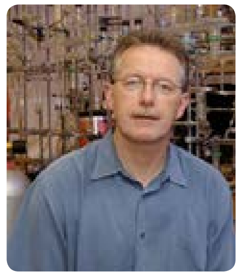
RESEARCH INTERESTS

Experimental and computational surface and thin film chemistry, diffusion barriers, nucleation, growth, self-assembly, surface modification.

Douglass F. Taber
Chemistry and Biochemistry

RESEARCH INTERESTS

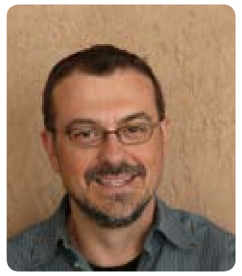
Stereoselective synthesis of natural products, organometallic catalysis, computational organometallic chemistry



Klaus H. Theopold
Chemistry and Biochemistry

RESEARCH INTERESTS

Homogeneous catalysis, coordination polymerization of olefins, activation of dioxygen by novel oxidation catalysis



Dionisios G. Vlachos
Chemical & Biomolecular Engineering

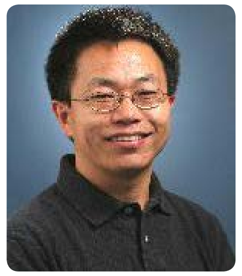
RESEARCH INTERESTS

Multiscale simulation, reacting flows, reaction mechanism development, catalyst design, microreactors, portable power, energy, crystal growth, nanomaterials, zeolites, membranes, separations.

Donald A. Watson
Assistant Professor of Chemistry

RESEARCH INTERESTS

Transition-metal catalysis; organic synthesis; alternative energy chemistry



Yushan Yan
Chemical & Biomolecular Engineering

RESEARCH INTERESTS

His research focuses on new materials for fuel cells, energy storage and solar hydrogen generation and zeolite thin films for semiconductors and aerospace applications.

Welcome new CCST Faculty, WILFRED CHEN

RECENT PUBLICATIONS

BARTEAU GROUP

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M. Salciccioli, W. Yu, M. A. Barteau, J. G. Chen and D. G. Vlachos, **"Differentiation of O-H and C-H Bond Scission Mechanisms of Ethylene Glycol on Pt and Ni/Pt Using Theory and Isotopic Labeling Experiments,"** *Journal of the American Chemical Society,* **133**, 7996 (2011).

A. Kulkarni, M. Bedolla-Pantoja, S. Singh, R. F. Lobo, M. Mavrikakis and M. A. Barteau, **"Reactions of Propylene Oxide on Supported Silver Catalysts: Insights into Pathways Limiting Epoxidation Selectivity,"** *Topics in Catalysis,* **55**, 3 (2012).

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CHEN GROUP

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A.L. Stottlemyer, T.G. Kelly, Q. Meng and J.G. Chen, **"Reactions of Oxygen-Containing Molecules on Transition Metal Carbides: Surface Science Insight into Potential Applications in Catalysis and Electrocatalysis"**, *Surface Science Reports* **(invited review)**, (2012) DOI: 10.1016/j.surfrep.2012.07.001.

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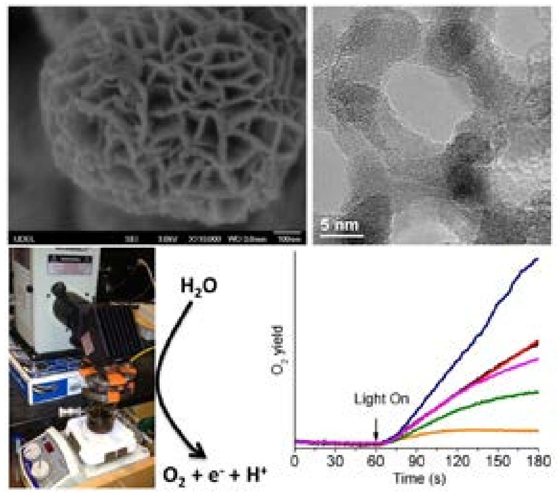
RESEARCH

PHOTOCATALYTIC OXYGEN EVOLUTION

Faculty: Feng Jiao (Chemical & Biomolecular Engineering)
Graduate Students: Seif Yusuf, Gregory Hutchings (Chemical & Biomolecular Engineering)

Oxygen evolution from water is the critical reaction for solar fuel production, because water is the only cheap, clean and abundant source that is capable of completing the redox cycle for producing either hydrogen (from H_2O) or carbonaceous fuels (from CO_2) on a terawatt scale. In our lab, we recently demonstrated that the morphology and crystal structure have negligible effect on the photocatalytic properties of MnO_2 based oxygen evolution catalysts, while the turnover rate is proportional to its surface area (i.e. Mn sites available on the surface). To further enhance the turnover frequencies (TOFs) that limited by surface area, surface active site with a higher TOF rate compared with Mn^{4+} is required. Along this direction, we introduce K^+ doped MnO_2 catalysts into oxygen evolution reaction. By doping MnO_2 with K^+, we create Mn^{3+} sites on the surface of mixed manganese oxides. Our preliminary data show that more than one order higher oxygen evolution rates per surface Mn were observed. In order to explore the origin of the enhancement in oxygen evolution activity, detailed structural characterizations have been performed and the results indicate that Mn^{3+} sites generated by K^+ doping may be responsible for the high TOFs.

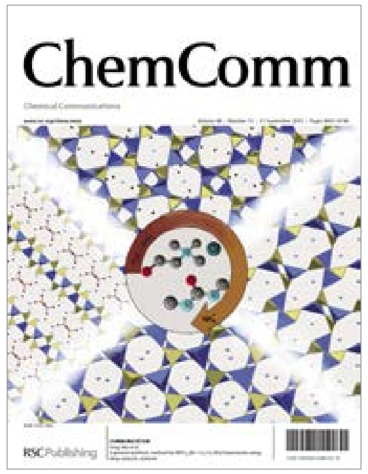


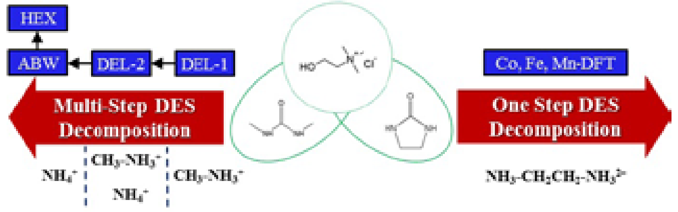
NANOPOROUS METAL PHOSPHATES

Faculty: Feng Jiao (Chemical & Biomolecular Engineering)
Graduate Students: Bryan Yonemoto, (Chemical & Biomolecular Engineering)

Recently, ionothermal synthesis was introduced to the preparation of zeolite and metal-organic frameworks by Morris and his co-workers. The utilization of ILs and DES as solvents to replace traditional aqueous solutions in material synthesis offers new opportunities in synthesis of inorganic solids with unique frameworks, which cannot be obtained through other methods due to highly ionic environment under synthetic conditions.

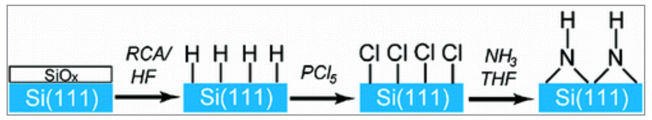
Recently, we have successfully developed a general synthetic approach to synthesize a wide range of transition metal phosphate frameworks via ionothermal synthesis. Using the choline chloride/N,N'-dimethylurea DES yields a layer $CoPO_4$ structure (DEL-1) that phase changes to the 12-member ring DEL-2 structure. It was demonstrated that DEL-2 can further phase change to ABW (8-member ring) and HEX (6-member ring) frameworks with longer reaction times. At low temperature (130⁰C) only DEL-1 is observed, so higher temperatures are necessary to produce 3-D $CoPO_4$ structures. Water usually plays a critical role in organic template decomposition and accelerates phase transition in cobalt phosphate system. The charge disposition and the size of the decomposing organic template have delicate influence on the coordination behaviors of different metal ions. Judicious choice of ionic solvent is important to prepare different transition metal phosphates. Among all the as-synthesized MPO_4 compounds, four new metal phosphate frameworks, $MnPO_4$-DFT, DEL-1, DEL-2 and DEL-3, are reported for the first time. This work provides us a new synthetic approach for design and preparation of transition metal phosphate materials, which opens great opportunities in many important applications.





–NH– TERMINATION OF THE SI(111) SURFACE BY WET CHEMISTRY

Faculty: Douglass F. Taber and Andrew V. Teplyakov (Department of Chemistry and Biochemistry,) Graduate Student: Fangyuan Tian

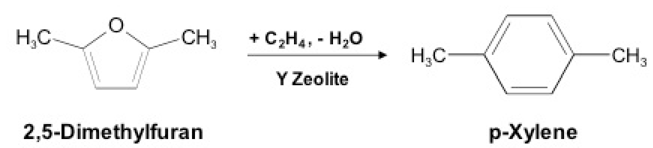


For over a quarter of a century the hydrogen-terminated Si(111) single-crystalline surface has been the gold standard as a starting point for silicon surface modification chemistry. However, creating a well-defined and stable interface based on Si–N bonds has remained elusive. Despite the fact that azides, nitro compounds, and amines do lead to the formation of surface Si–N, each of these modification schemes produces additional carbon- or oxygen-containing functional groups that in turn react with the surface itself, leaving contaminants that affect the interface properties for any further modification protocols. We describe the preparation of a Si(111) surface functionalized predominantly with Si–NH–Si species based on chlorination followed by *the room temperature* ammonia treatment utilizing NH_3-saturated tetrahydrofuran (THF). The obtained surface has been characterized by infrared spectroscopy and X-ray photoelectron spectroscopy. This analysis was supplemented with DFT calculations. This newly characterized surface will join the previously established H–Si(111) and Cl–Si(111) surfaces as a general starting point for the preparation of oxygen- and carbon-free interfaces, with numerous potential applications.

HETEROGENEOUS CATALYST CONVERTS BIOMASS-DERIVED FURANS TO PARA-XYLENE FOR RENEWABLE PLASTICS WITH VERY HIGH YIELD

Caratzoulas, Lobo, and Vlachos Groups (Department of Chemical & Biomolecular Engineering, University of Delaware) and Dauenhauer and Fan Groups (Department of Chemical Engineering, University of Massachusetts)

Biomass naturally produces furan chemical structures (five-member rings), such as 5-hydroxymethylfurfural (HMF) or dimethylfuran (DMF), when undergoing catalytic reactions. However, most of the polymers and products currently used, including packaging, clothing, and computers, require six-member ring structures. Engineers at the University of Massachusetts and University of Delaware have shown that the furan ring can be converted to a six-carbon aromatic chemical, such as p-xylene, at high yield (>75%) [1]. P-xylene is the main component in polyethylene teraphthalate (PET) plastics which make up plastic bottles, adhesives, insulation and substrates in solar cell devices. This discovery bridges the gap between biomass and current petroleum-based products. The same technology can potentially be applied to replace most of the aromatic chemicals currently produced from non-renewable resources.



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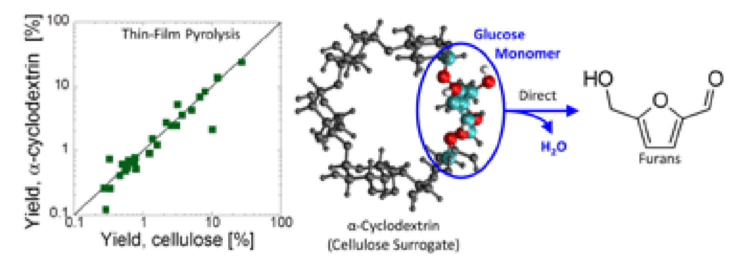
REVEALING PYROLYSIS CHEMISTRY FOR BIOFUELS PRODUCTION

Vlachos Group (Department of Chemical and Biomolecular Engineering - University of Delaware) and Dauenhauer Group (Department of Chemical Engineering - University of Massachusetts)

Next-generation biofuels production utilizes high temperatures (~1000 °F) to convert all parts of a plant to molecules similar in size to those found in fuels. A series of complex processes fracture large biomolecules containing millions of atoms into much smaller molecules with higher energy density and reactivity. While this chemical deconstruction is critical to biofuels production, for decades the fundamental chemical reactions controlling this transformation have been unknown. Researchers at the Catalysis Center for Energy Innovation (CCEI) have unmasked the complex chemistry of high-temperature biomass conversion. A novel thin film technique was developed which utilizes extremely small samples (approximately the thickness of a human hair) for precise control of the deconstruction process. Next a small molecule was identified that gives the same product distribution as cellulose and can be used to mimic the complexity of the biopolymer. These advanced experiments were then coupled with first principles simulations at very high temperatures to understand for the first time the underlying mechanisms of conversion of raw cellulose to fuels and chemicals. These findings can enable development of fundamental chemistry models for optimization of large scale deconstruction of biomass.



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THE MAGIC OF TIN: CONVERTING HEMICELLULOSE BUILDING BLOCKS TO FURFURAL IN AQUEOUS MEDIA

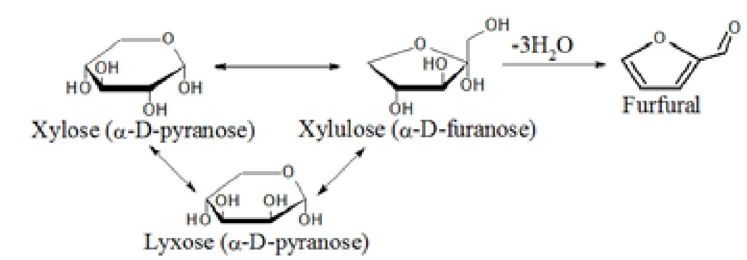
Lobo, Sandler, and Vlachos Groups (Department of Chemical & Biomolecular Engineering - University of Delaware) and Tsapatsis Group (Department of Chemical Engineering and Materials Science - University of Minnesota)

Hemicellulose makes up a large fraction of lignocellulosic biomass. The majority of hemicellulose consists of C5 sugars (pentoses), such as xylose. Biological routes, such as conversion of xylose by yeast or micro-organisms, have not been met with much success. As a result, the key C5 furan, furfural, is currently made from xylose by sulfuric acid heat treatment at high temperatures and is stripped away by steam. This is an energy intensive process, similar to the first industrial furfural production process established by Quaker Oats in 1921.

CCEI researchers at the University of Delaware have recently introduced the Sn-beta zeolite as a Lewis acid to selectively isomerize xylose to xylulose in water at low temperatures[1]. Xylulose is then dehydrated using a Brønsted catalyst to furfural. It was demonstrated that it is possible to combine two heterogeneous catalysts to achieve furfural yields approaching 90% under certain conditions using a reactive separation scheme. CCEI researchers at the University of Minnesota[2] have further demonstrated that the Sn-beta catalyst does its magic for aldo to keto sugar isomerization, further enriching the portfolio of heterogeneous Lewis catalyzed chemistry in water introduced by the CCEI researchers in 2010.

The introduction of selective and active heterogeneous bifunctional catalysts for the transformation of xylose to furfural can be a transformative technology in efficiently utilizing hemicellulose.

Schematic representation of xylose isomerization using the Sn-beta zeolite and the xylulose dehydration using a Brønsted acid catalyst.



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FACULTY & STUDENT NEWS

Wilfred Chen wins Biotechnology Progress Award

Wilfred Chen, Gore Professor of Chemical Engineering in the University of Delaware's Department of Chemical and Biomolecular Engineering, will receive the 2012 Biotechnology Progress Award for Excellence in Biological Engineering Publication at the American Institute of Chemical Engineers (AIChE) annual meeting in Pittsburgh this October. Given annually, the award recognizes outstanding contributions to literature in biomedical engineering, biological engineering, biotechnology, biochemical engineering and related fields.

2011 award recipient, **Mike Salciccioli** with **Zhufang Liu** of Eastman Chemicals, and (left to right) **Jingguang Chen**, **Dion Vlachos**, and CCST Director, **Raul Lobo**.

Yushan Yan Reports Milestone in Fuel Cell Membrane Research

It looks like a plastic candy wrapper that's been charred on both sides, but it may hold the solution to commercially viable fuel cells. About the thickness of a human hair, it is actually a thin polymer membrane sandwiched between two catalysts. The work is that of Yushan Yan, Distinguished Professor of Engineering at the University of Delaware, who is known for developing new catalysts and membranes to reduce the cost and improve the durability of fuel cells.

2012 Eastman Chemical Student Award

Weiting Yu, CCST student advised by Professor Jingguang Chen, is the recipient of the 2012 Eastman Chemical Student Award. This award is in recognition of her valuable scientific discoveries and contributions to CCST, her notable publications and the dedication and ingenuity that she has brought to catalysis research. Weiting will receive the award at the CCST Annual Review this fall. Congratulations Weiting!

CCST Faculty HIGHLIGHTS

Joel Rosenthal

- DuPont Young Professor Award, 2012

Andrew V. Teplyakov

- American Chemical Society Delaware Section Award, 2012.
- Organizer of the Symposium entitled: Molecular Processes at Solid Surfaces" at the 244th National Meeting of the American Chemical Society (Philadelphia, PA 2012), 2012.
- Teplyakov Group work is highlighted in **nanotechweb.org (http://nanotechweb.org/cws/article/tech/46735)** (Polyakova (Stolyarova), E., Rim, K. T., Eom, D., Douglass, K., Opila, R., Heinz, T., Teplyakov, A. V. and Flynn, G. W. Scanning tunneling microscopy and X-ray photoelectron spectroscopy studies of graphene films prepared by sonication-assisted dispersion. ACS Nano **2011**, 5(8), 6102-6108)
- Organizer of the Surface Science Session at the EAS, 2012.

Dion Vlachos

- Executive Editor, Chemical Engineering Science, 2011-2014.
- The para-xylene work was highlighted in Chem. Eng. News and The Catalyst Review, May 2012 pg. 9.
- Pyrolysis paper in *Energy Env. Sci.* **5**, 5414-5424 (2012) was highlighted in *Nature Chemistry* **4**, 68-69 (2012) and in Chemical Engineering Progress (CEP) in March 2012, pages 9 & 10: www.aiche.org/uploadedFiles/CEP/Issues/2012-03/031206.pdf

Yushan Yan

- 27th Outstanding Alumni Lecture, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, 2011.

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