

[www.GCandE.org](http://www.GCandE.org)

Innovating For the Future:  
Progress on the Grand Challenges  
in the Chemical Enterprise

**13th**

# Annual Green Chemistry & Engineering Conference

June 23-25, 2009  
College Park, Maryland



American Chemical Society



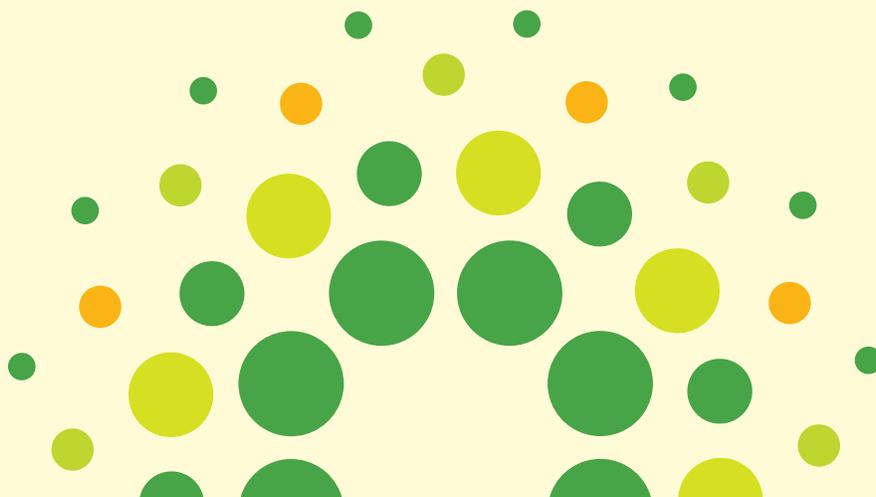
# The ACS Green Chemistry Institute®

The ACS Green Chemistry Institute® is devoted to promoting and advancing green chemistry. First incorporated in 1997, GCI joined with the American Chemical Society in 2001 to pursue joint interests in the area of green chemistry.

The mission of the ACS Green Chemistry Institute® is to enable and catalyze the implementation of green chemistry and green engineering into all aspects of the global chemical enterprise.

Planning for this year's conference included several "green" initiatives.

- A key factor in the selection of the Marriott Inn and Conference Center site was its LEED certification. Every facility in the hotel, from the meeting facilities to the guest rooms, uses recyclable materials and energy-saving systems to ensure a positive role on the environment.
- Carbon emissions of all participants in the conference were calculated and off-set.
- The incorporation of green practices and materials was a consideration in the selection of a designer and printer for the conference program. The printer is FSC-certified and uses recycled paper and soy ink. Even the plastic coils binding the program are made from recycled materials. The program designer has completed special course work in green design and printing and follows sustainable guidelines of the American Institute of Graphic Artists, which includes responsible use of consumable resources and protection of the environment.
- Except for a site visit to the conference site, all planning for the conference was done through "virtual" conferencing.



# Welcome from the Conference Organizing Committee

On behalf of the 2009 conference organizing committee, welcome to College Park, Maryland, and the 13th Annual Green Chemistry & Engineering Conference.

We are pleased to have you join us for what we believe is the premier conference on sustainability. This year's conference theme, "Innovating For the Future: Progress on the Grand Challenges in the Chemical Enterprise," was specifically selected to report on progress made since the National Academies of Science issued its landmark 2006 report, "Sustainability in the Chemical Industry: Grand Challenges and Research Needs." This conference program illustrates the dramatic improvements and opportunities that have been created by uniting chemistry and engineering to the benefit of business and the environment.

Whether your interests are in a specific area of fine chemical synthesis, bulk manufacturing, process optimization, environmental monitoring, education or more generalized around green chemistry and engineering, we are confident you will find cutting edge science you can use among the presentations in the conference's seven special tracks:

- Transforming Green Chemistry and Engineering
- Lifecycle Analysis and Green Metrics
- Toxicology: Environmental Fate and Effects
- Renewable Energy Fuels and Feedstocks
- Process Design and Optimization
- Greenhouse Gas Management and Prevention
- Integrative Education in Green Chemistry and Engineering

Best wishes for a great conference,

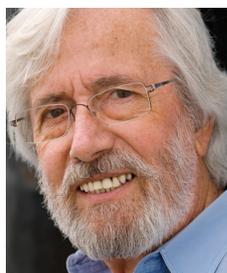
Liz Gron  
*Conference Chair*

## Keynote Speakers



**Len Sauers**  
*Vice President,  
Global Sustainability,  
The Procter & Gamble Company*

**P&G's Environmental  
Sustainability Journey**



**Jean-Michel Cousteau**  
*Founder and President,  
Ocean Futures Society;  
Executive Vice President,  
The Cousteau Society*

**The Call of the Killer Whale**

**Accurate, timely,  
authoritative news on  
research, companies,  
and government  
agencies focusing on  
green  
chemistry**

**C&EN**

**CHEMICAL & ENGINEERING NEWS**

**Email [service@acs.org](mailto:service@acs.org) for pricing and further information.**

# Dream Green!™

February 16<sup>th</sup> - 19<sup>th</sup> 2010 • San Francisco, CA

At this year's Informex – North America's largest chemical ingredient tradeshow – you're invited to 'Dream Green' at our second annual Green Exchange. The Green Exchange will feature both innovators and buyers of green chemistry, along with programming designed to map the opportunities for the green chemistry of the future.

## The Green Pavilion at InformexUSA

Informex 2010 will feature a green chemistry pavilion on the show floor. For exhibitors, the Green Pavilion offers a low-cost opportunity to get in front of sourcing professionals. For attendees, it gathers some of the leading green chemistry in the world in one spot.

2009 participants included:  
SiGNa Chemistry, Newreka, Bioniqs, Archimica, Novomer and more.

### The Green Exchange Breakfast February 18, 2010

The 2009 Green Breakfast Briefing was a huge success, with speakers including:

**John C. Warner** - Director,  
Warner Babcock Institute for Green Chemistry

**Maureen Gorsen** - Director,  
California Department of Toxic Substances

**Ronald Gebhard** - R&D Director,  
DSM Pharmaceutical Products

**Christopher E. Gann** - Chief Executive Officer,  
Genomatica, Inc.

**Thomas Schäfer** - Senior Director, Novozymes A/S

**Moderator:**  
**Clay Boswell** - Senior Editor  
ICIS Chemical Business

If you would like to join the 2010 line-up, co-produced by Informex and the ACS Green Chemistry Institute®, please contact Jennifer Jessup, [jjessup@informex.com](mailto:jjessup@informex.com).

For more information, visit:  
[www.informex.com](http://www.informex.com)  
Or call: 609.759.4746

# 2009 Conference Organizing Committee

**Martin Abraham**

Youngstown State University

**Sharon Austin**

U.S. Environmental Protection Agency

**Berkeley W. "Buzz" Cue, Jr.**

BWC Pharma Consulting, LLC

**Richard Engler**

U.S. Environmental Protection Agency

**Liz Gron**

*Conference Committee Chair*  
Hendrix College

**Julie Haack**

University of Oregon

**Julie Manley**

Guiding Green, LLC

**Robert Peoples**

ACS Green Chemistry Institute®

**Henry Ramsey**

Verrico Associates, LLC

**Matthew Realff**

Georgia Institute of Technology

**Darlene Schuster**

AIChE Institute for Sustainability

**Megan B. Turner - O'Meara**

BASF Corporation

**Anne Wallin**

The Dow Chemical Company

**Denyce Wicht**

Suffolk University

**Conference Administrators**

Marvin Coyner

Jane Day

Joyce Kilgore

Linda Pirrone

Jennifer Young

Special thanks to Jessica Gosling-Goldsmith for promotional assistance

## Please visit our conference exhibitors

ACS Green Chemistry Institute®

ACS Membership & Scientific Advancement

ACS Publications

Beyond Benign

The Dow Chemical Company

Harris LithoGraphics, Inc.

Island Press

Oxford University Press

Royal Society of Chemistry

Taylor & Francis

US EPA Green Chemistry Program

## Local area discounts

Several businesses in the University Town Center, located just one mile from the Marriott Conference Center, are offering a 10% discount to conference attendees during the week of the conference. Just show your registration badge to get your discount.

Gifford's Ice Cream & Candy

Hank's Tavern & Eats

New Town Cleaners

Old Dominion Brewhouse

Qdoba Mexican Grill

Three Brothers Italian Restaurant

Wild Onion Gourmet Café

A special thanks to RITA'S, located on Route 1 in College Park, for providing free scoops of ice cream on Monday to attendees arriving early for the Conference. They also are offering a 10% discount to attendees at their Rte. 1 location.



A CHEMISTRY THAT EMBRACES THE HUMAN

ELEMENT IS A CHEMISTRY THAT IS ALWAYS

ASKING 'WHY NOT?' The Dow Chemical

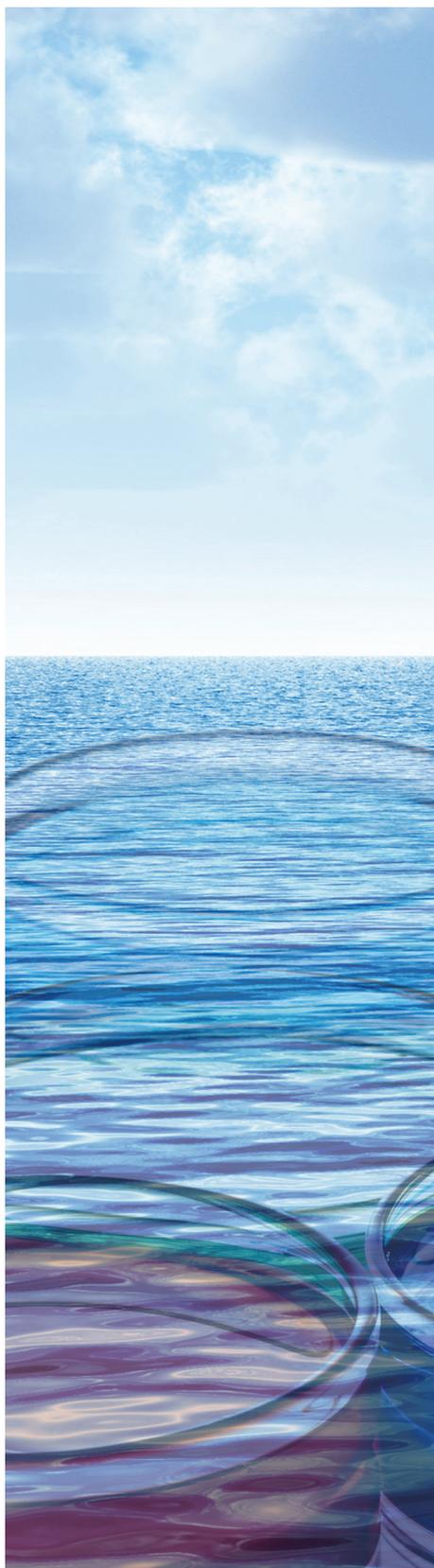


Company proudly supports the Green Chemistry

& Engineering Conference.



# Schedule At A Glance



## Monday morning, June 22

### STUDENT WORKSHOP

8:00 AM – 4:30 PM

This full-day workshop is designed for graduate students attending the GC&E conference; however, undergraduate and postdoctoral fellows are welcome. Leading green chemistry and engineering experts will give presentations and lead discussions. You must be registered for the GC&E conference to attend. Lunch provided.

### ACS GCI PHARMACEUTICAL ROUNDTABLE MEETING

*(by invitation only)\**

8:30 AM – 1:30 PM

### ACS GCI FORMULATOR'S ROUNDTABLE

*(by invitation only)\**

11:30 AM – 5:00 PM

## Monday afternoon, June 22

### STUDENT WORKSHOP

*(continued)*

### ACS GCI PHARMACEUTICAL ROUNDTABLE MEETING

*(continued)*

### ACS GCI FORMULATOR'S ROUNDTABLE

*(continued)*

\* Inquiries about the Roundtables should be addressed to Julie Manley ([j\\_manley@acs.org](mailto:j_manley@acs.org))

### PRESIDENTIAL GREEN CHEMISTRY CHALLENGE AWARDS:

#### **2009 Awards Presentation Ceremony**

*(must be pre-registered to attend).*

The ceremony starts at 5:30 pm at the Carnegie Institution for Science, 1530 P Street, NW, Washington, D.C. Business attire recommended.

## Tuesday morning, June 23

### OPENING SESSION:

#### **Perspectives from Winners of the 2009 Presidential Green Chemistry Challenge Awards**

- Technical presentations by winners of the 2009 Presidential Green Chemistry Challenge Awards
- Incorporation of GC/GE in the Undergraduate Experience
- Technologies for a Hydrogen Economy
- Catalysis

### EXHIBITS

## Tuesday afternoon, June 23

- Catalysis *(cont'd)*
- Environmental Fate and Effects – sponsored by Division of Environmental Chemistry, American Chemical Society

- Taking GC/GE Beyond the Traditional
- Supply Chain
- Green Synthesis I – sponsored by Newreka
- Perspectives On Embedding GC/GE in Different Institutional Contexts
- Surface Preparation, Coatings, and Films – sponsored by Celgard, LLC

#### EXHIBITS

#### OPENING NIGHT RECEPTION

### Wednesday morning, June 24

#### OPENING SESSION:

**Keynote Address – Len Sauers, Vice President, Global Sustainability, The Procter & Gamble Company**

- Green Analytical Chemistry
- Green Corrosion Inhibition and Water Treatment
- Green Synthesis I (*cont'd*)
- New Focuses In Green Chemistry

#### EXHIBITS

### Wednesday afternoon, June 24

- Poster Sessions
- New Focuses In Green Chemistry (*cont'd*)
- Greenhouse Gas Management and Prevention
- Process Safety & Reaction Engineering
- Renewable Feedstocks and Materials
- Design Signals From Environmental Health Sciences: What Every Chemist Should Know – sponsored by Advancing Green Chemistry
- Green Synthesis II
- Suppliers Roundtable meeting (*by invitation only*)

#### EXHIBITS

### Thursday morning, June 25

#### OPENING SESSION:

**Keynote Address – Jean-Michel Cousteau, Founder and President, Ocean Futures Society; Executive Vice President, The Cousteau Society**

- Funding Green Chemistry & Engineering Research
- Lifecycle Analysis and Green Metrics
- Renewable Fuels
- Technologies for the Green Toolbox – sponsored by Warner Babcock Institute for Green Chemistry

#### EXHIBITS

### Thursday afternoon, June 25

- Technologies for the Green Toolbox (*cont'd*)
- Drivers and Strategies for Green Chemistry and Engineering
- Green Synthesis II (*cont'd*)

#### EXHIBITS

### Friday morning, June 26

#### TRAIN-THE-TRAINERS WORKSHOP

8:30 AM – 5:00 PM

Pre-registration required for the workshop. You also must be registered for the conference in order to attend the workshop. This free workshop is for people interested in teaching green chemistry workshops. Continental breakfast and lunch provided for workshop registrants.

#### TOUR OF THE BLUE PLAINS WATER TREATMENT FACILITY

(*pre-registration required*)

9:00 AM – 12:00 PM

#### TOUR OF THE U.S. BUREAU OF ENGRAVING AND PRINTING

(*pre-registration required*)

9:00 AM – 12:00 PM

#### EXHIBITS



**ACS  
Green  
Chemistry  
Institute®**

#### ACS GCI FORMULATOR'S ROUNDTABLE

**Mission: To be a driving force in the formulated products industry to use Green Chemistry in creating innovative products that are environmentally sustainable throughout its product life cycle and safer to make and use.**

**All companies identifying with SIC industry group 284 are welcome.**

**Thank you to our current members:**

Amway Corporation	JohnsonDiversey, Inc.
Bissell Homecare, Inc.	Rug Doctor, Inc.
Church & Dwight Co., Inc.	S.C. Johnson & Son, Inc.
The Clorox Company	Seventh Generation
Johnson & Johnson Consumer Companies	Zep, Inc.

**[www.acs.org/greenchemistry](http://www.acs.org/greenchemistry)**



# Track Descriptions & Leaders

## Transforming Green Chemistry and Engineering

This track describes the fundamental changes in methodology developed by chemists and engineers to create economically viable green processes and technologies.

**Track leader:** Topher Buck, GreenBlue Institute

## Lifecycle Analysis and Green Metrics

Comprehensive assessments of the impact of chemicals and products from raw material extraction through use to recycling and disposal have become key aids to decision-making by companies and governments. There is a growing need for data to support life cycle assessments and ways of combining and streamlining the multiple metrics that can be used to assess performance of products and process systems. We invite contributions in the areas of new life cycle metrics, methods and data, using life cycle assessment methods to inform decision-making, and the development of product standards based on life cycle assessment. Sessions in this track will be aimed at those using, as well as developing, life cycle analysis and green metrics.

**Track Leaders:** Martha Stevenson, GreenBlue Institute; Matthew Realff, Georgia Institute of Technology

## Toxicology: Environmental Fate and Effects

This session will focus on understanding the toxicological fate and effect of chemicals used or generated by the chemical enterprise. It includes measurement methods, results of toxicity or fate studies, and the design of less hazardous chemical substances. Of particular interest are biotechnology and nanotechnology: These two areas have enormous potential to make strides towards sustainability, but there is little understanding of their environmental fate or effects, or how to measure or model them.

**Track Leaders:** John Davis, The Dow Chemical Company; Richard Engler, U.S. Environmental Protection Agency

## Renewable Energy Fuels and Feedstocks

Innovation in chemistry and engineering technologies focused on energy generation from renewable sources such as wind and sunlight will be highlighted. Sessions will also focus on developments in chemistry and engineering technologies for the production of liquid fuels and basic chemical feedstocks from renewable (non-food) sources. Process scale-up and commercial viability will also be discussed.

**Track Leader:** Jim Frederick, National Renewable Energy Laboratory

## Process Design and Optimization

Sessions will cover developments in energy, material, and cost efficient chemical process design and green manufacturing strategies. Contributions are encouraged in the following areas, including but not limited to, biotechnology, novel catalytic reaction chemistry, reaction modeling, reactor engineering, and separation technology. Process optimization and efficiency in the pharmaceutical, fine chemical, and bulk chemical industries are encouraged including the application of process analytical chemistry to monitor and control the reaction.

**Track Leaders:** Berkeley W. "Buzz" Cue, Jr., BWC Pharma Consulting, LLC; Julie Manley, Guiding Green, LLC

## Greenhouse Gas Management and Prevention

The sessions will reflect the broad impact of greenhouse gas emissions on society. Contributions are encouraged in the prevention and management of all greenhouse gas emissions, the storage and sequestration of carbon dioxide, and emerging greenhouse gas policy and legislation.

**Track Leader:** Ron Chance, Georgia Institute of Technology

## Integrative Education in Green Chemistry and Engineering

Chemists and Engineers play a key role in creating and facilitating the transition to green technologies and processes. In order to be most effective, they require new ways of thinking, analyzing, and designing, which have significant implications in the educational programs created for these chemists and engineers. In an effort to showcase ways of approaching this new education enterprise, we invite submissions that describe emerging curricular innovations, established cross-disciplinary programs or learning activities, and transformational teaching and learning tools. In addition, we invite presenters to share their work in the areas of multi-disciplinary programs for science education, public policy, or business training that facilitates the incorporation of green chemistry and engineering into these disciplines. We welcome business leaders from the chemical enterprise to share in-house professional development materials used to educate chemists and chemical engineers regarding strategies that promote sustainable product development. Preference will be given to abstracts that illustrate pioneering concepts.

**Track Leaders:** Julie Haack, University of Oregon; Linda Vanasupa, California Polytechnic State University; Denyce K. Wicht, Suffolk University





# Workshops

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**Monday, June 22, 2009**

## Green Chemistry & Engineering Student Workshop

*(pre-registration required)*

7:30 AM

**BREAKFAST**

8:00 AM

**WELCOME REMARKS AND INTRODUCTION**

8:15 AM

**INTRODUCTION TO GREEN CHEMISTRY**

**John Warner**, Warner Babcock Institute for Green Chemistry & **Paul Anastas**, Yale University

9:45 AM

**DISCUSSION & COFFEE BREAK**

10:15 AM

**INTRODUCTION TO GREEN ENGINEERING**

**Linda Vanasupa**, California Polytechnic State University

11:00 AM

**GREEN CHEMISTRY IN ELECTRONIC APPLICATIONS**

**Michael Korzenski**, ATMI

11:45 AM

**LUNCH**

12:30 PM

**GREEN CHEMISTRY IN PAINTS AND COATINGS**

**Morgan Sibbald**, Sherwin-Williams

1:15 PM

**GREEN CHEMISTRY IN THE CHEMICAL INDUSTRY**

**Anne Wallin**, The Dow Chemical Company

2:00 PM

**DISCUSSION & COFFEE BREAK**

2:30 PM

**GREEN CHEMISTRY IN THE PHARMACEUTICAL INDUSTRY**

**Peter Dunn**, Pfizer

3:15 PM

**PANEL DISCUSSION - CAREERS AND OPPORTUNITIES IN GREEN CHEMISTRY & GREEN ENGINEERING**

**Emily Reichert**, Warner Babcock Institute for Green Chemistry

3:50 PM - 4:00 PM

**CLOSING REMARKS**



**Friday, June 26, 2009**

## Green Chemistry Education Train the Trainer Workshop:

### Sharing Progress on the Grand Challenges of the Chemical Enterprise

*(pre-registration required)*

8:30 AM

**CHECK-IN & BREAKFAST**

9:00 AM

**WELCOME REMARKS AND INTRODUCTION**

9:15 AM

**AN INTRODUCTION TO GREEN CHEMISTRY**

**R. K. Sharma**, University of Delhi

10:15 AM

**ACTIVITY FOR PRESENTATIONS TO K-12/GENERAL PUBLIC — GROUP DISCUSSIONS**

11:00 AM

**BREAK/NETWORKING TIME**

11:15 AM

**WORKING WITH K-12 EDUCATION: GOALS AND RESOURCES**

**Michael Tinneland**, Consultant

12:00 PM

**LUNCH/NETWORKING**

1:00 PM

**REACHING OUT TO INDUSTRY**

**Anne Wallin**, The Dow Chemical Company

1:45 PM

**GREENER APPROACHES TO UNDERGRADUATE EDUCATION: GOALS AND RESOURCES**

**Jim Hutchison**, University of Oregon

2:30 PM

**BREAK/NETWORKING TIME**

2:45 PM

**ACTIVITY FOR INCORPORATING GREENER APPROACHES IN UNDERGRADUATE PROGRAMS — GROUP DISCUSSIONS**

3:30 PM

**STORYBOARD PROJECT**

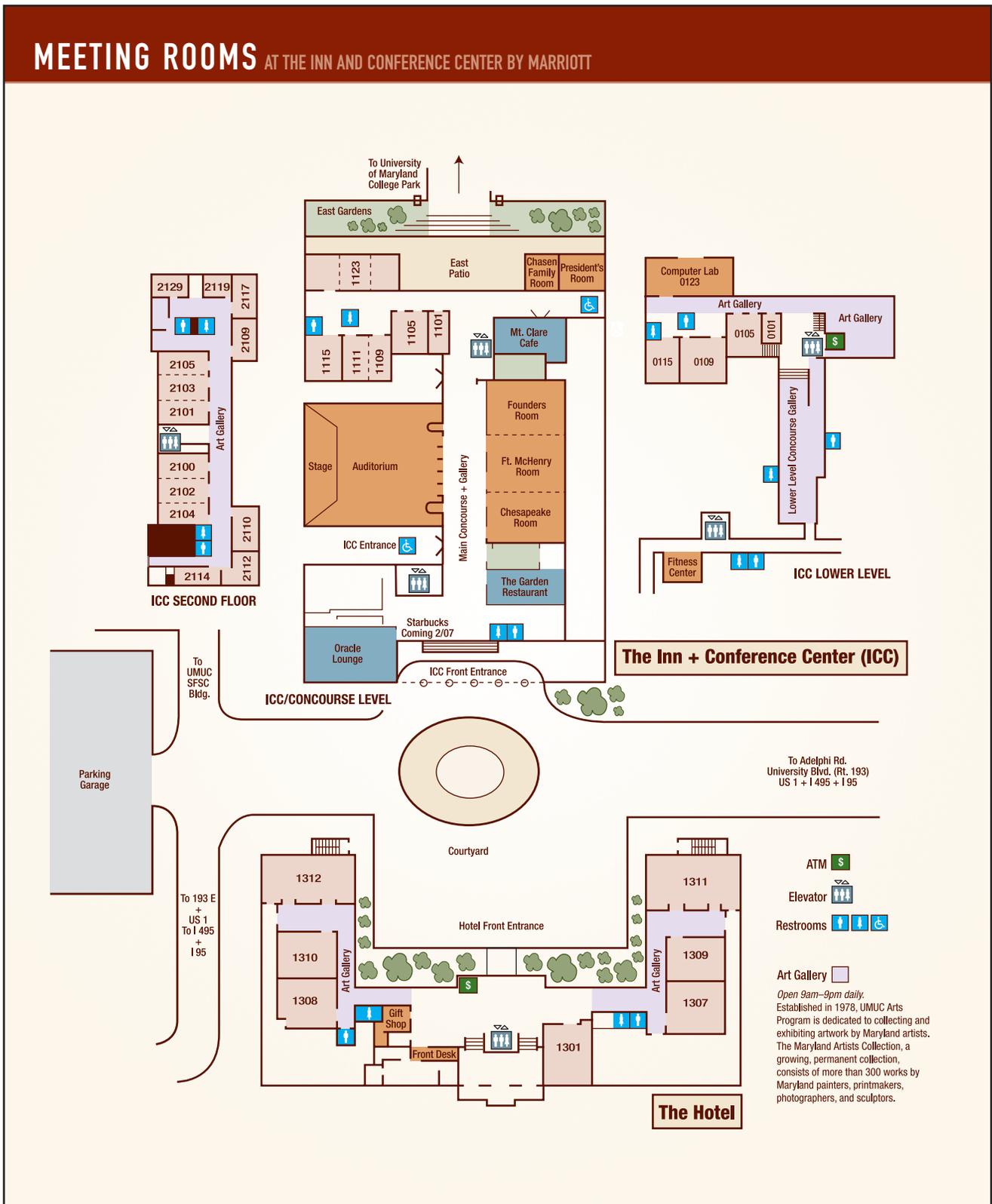
4:30 PM – 4:45 PM

**EVALUATION AND REFLECTIONS**



# Marriott Meeting Rooms

## MEETING ROOMS AT THE INN AND CONFERENCE CENTER BY MARRIOTT





## 2010 ACS GCI PHARMACEUTICAL ROUNDTABLE RESEARCH GRANT

REQUEST FOR PROPOSALS  
Coming this Summer!

For information: [www.acs.org/gcipharmaroundtable](http://www.acs.org/gcipharmaroundtable)  
or E-Mail: [gcipr@acs.org](mailto:gcipr@acs.org)

The Roundtable's mission is to catalyze the implementation of green chemistry and green engineering in the global pharmaceutical industry. Membership is open to all pharmaceutical research, development, and manufacturing companies.

### Strategic Priorities:

- Informing & influencing the research agenda
- Defining & delivering tools for innovation
- Educating leaders
- Collaborating Globally

Thank you to our current members:

*Lilly*

 **gsk**  
GlaxoSmithKline

 **Pfizer**

 **MERCK**

 **Boehringer  
Ingelheim**

  
AstraZeneca  
life inspiring ideas

 **Schering-Plough**

*Johnson & Johnson*

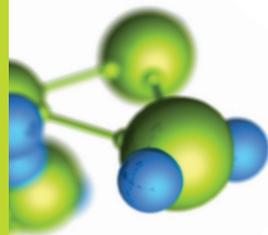
**Wyeth**

 **CODEXIS®**

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 **NOVARTIS**  
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# Technical Program

Tuesday, June 23, 2009

7:00 AM – 5:00 PM

## REGISTRATION

Main Concourse, Marriott Inn and Conference Center

8:00 AM – 5:00 PM

## EXHIBITION

Main Concourse, Marriott Inn and Conference Center

## Tuesday Morning

7:15 AM – 8:15 AM

### CONTINENTAL BREAKFAST

Main Concourse, Marriott Inn and Conference Center

8:15 AM

### WELCOMING REMARKS

Auditorium, Marriott Inn and Conference Center

8:45 AM – 9:45 AM

### OPENING SESSION:

#### PERSPECTIVES FROM WINNERS OF THE 2009

#### PRESIDENTIAL GREEN CHEMISTRY CHALLENGE AWARDS

Auditorium, Marriott Inn and Conference Center

*Session Chair: Rich Engler, US Environmental*

*Protection Agency*

9:45 AM – 10:15 AM

### COFFEE BREAK

Main Concourse

## Process Design and Optimization

10:15 AM – 12:15 PM

### CATALYSIS

1105, Marriott Inn and Conference Center

*Session Chair: Alex Tao, Elevance Renewable Sciences; Romas Kazlauskas, BioTechnology Institute, University of Minnesota*

- 10:15 1** Conversion of Racemic Ibuprofen to (S)-Ibuprofen. **David Chavez** and James Salvador, University of Texas at El Paso
- 10:55 2** Enzymatic Synthesis In Deep Eutectic Solvents. **Johnathan Thomas Gorke**, Friedrich Srienc, and Romas J. Kazlauskas, University of Minnesota
- 11:35 3** Engineering *Candida tropicalis* for conversions of fatty acids to  $\omega$ -hydroxyfatty acids. **Wenhua Lu**<sup>1</sup>, Jon E. Ness<sup>2</sup>, Xiaoyan Zhang<sup>1</sup>, Wenchun Xie<sup>1</sup>, Jeremy Minshull<sup>2</sup>, and Richard A. Gross<sup>1</sup>, (1)NSF I/UCRC for Biocatalysis and Bioprocessing of Macromolecules, Department of Chemical and Biological Sciences, Polytechnic Institute of NYU, Brooklyn, NY, (2)DNA 2.0, Inc., Menlo Park, CA
- 12:15** Lunch

## Integrative Education in Green Chemistry and Engineering

### INCORPORATION OF GC/GE IN THE UNDERGRADUATE EXPERIENCE

Founders, Marriott Inn and Conference Center

*Session Chair: Andrew P. Dicks, University of Toronto*

- 10:15 7** Teaching Green Chemistry and Engineering Concepts in the Undergraduate Organic Laboratory via Biginelli and Hantzsch Reactions. **Andrew P. Dicks**, Evangelos Aktoudianakis, and Sarah Styler, University of Toronto
- 10:55 8** Designing a Green, Inquiry-Based Organic Chemistry Laboratory to Educate the Next Generation of Scientists. **Loyd D. Bastin** and Kaitlyn Gerhart, Widener University
- 11:15 9** Development of an Organic Chemistry for Engineers with a “Sustainable” Spin. **Montserrat Rabago Smith**, and Jennifer Aurandt, Kettering University
- 11:35 10** Empowering Student Education In Chemistry with Novel Green Ideas and Tools. **Chandana Mukherjee**<sup>1</sup>, Malini Rajendran, Poonam Sharma<sup>1</sup>, and S. Bhanumati<sup>3</sup>, (1)Gargi College, University of Delhi, New Delhi, India, (2)NGO Project Roshni, (3)Gargi College, University of Delhi, New Delhi, India
- 11:55 11** Greener Chemistry in the Automotive Industry: A Collaboration Between Academia and Industry. **Kristi A. Kneas**, Elizabethtown College

10:15 AM – 12:15 PM

### PERSPECTIVES FROM WINNERS OF THE 2009 PRESIDENTIAL GREEN CHEMISTRY CHALLENGE AWARDS

Auditorium, Marriott Inn and Conference Center

*Session Chair: Rich Engler, US Environmental Protection Agency*

## Renewable Energy Fuels and Feedstocks

10:15 AM – 12:15 PM

### TECHNOLOGIES FOR A HYDROGEN ECONOMY

2101/2103/2105, Marriott Inn and Conference Center

*Session Chair: Carole Read, US Department of Energy*

- 10:15 12** The DOE Hydrogen Program: Technology Status and R&D Issues. **Carole Read**, US Department of Energy
- 10:35 13** Water Oxidation Using Iridium Catalysts. **Jonathan F. Hull**, Yale University
- 10:55 14** Hydrogen Storage on Carbonized Chicken Feather Fibers. **Erman Senöz** and Richard P. Wool, University of Delaware

**11:15 15** Heterogeneous H<sub>2</sub> Formation Catalyzed by Economical Molecular Coordination Compounds Anchored to High-Surface-Area Metal-Oxide Thin Films. **Shane Ardo**, Siah Hong Tan, and Gerald J. Meyer, Johns Hopkins University

**11:35 16** Copper Oxide Nanoparticles via Flame Spray Pyrolysis for Photoelectrochemical Hydrogen Generation. Ranjan K. Pati<sup>1</sup>, Joshua Emmanuel<sup>1</sup>, Raymond Adomaitis<sup>1</sup>, **Sheryl Ehrman**<sup>1</sup>, Anjana Solanki<sup>1</sup>, Jaya Srivastava<sup>1</sup>, Aadesh Singh<sup>1</sup>, Monika Gupta<sup>1</sup>, Vibha Satsangi<sup>1</sup>, Rohit Shrivastav<sup>1</sup>, and Sahab Dass<sup>2</sup>, (1)University of Maryland - College Park, (2) Dayalbagh Educational Institute

**11:55 17** Heterogeneous Catalysis Reactions of Carbon Dioxide. **Heather D. Willauer**<sup>1</sup>, Dennis R. Hardy<sup>1</sup>, Frederick W. Williams<sup>1</sup>, and Robert W. Dornier<sup>2</sup>, (1)Naval Research Laboratory, (2) National Research Council Postdoctoral Research Associate at Naval Research Laboratory

12:15 PM – 1:15 PM

#### LUNCH

Chesapeake/Ft. McHenry, Marriott Inn and Conference Center

### Tuesday Afternoon

#### Process Design and Optimization

1:15 PM – 3:15 PM

#### CATALYSIS

(continued)

1105, Marriott Inn and Conference Center

*Session Chairs: Alex Tao, Elevance Renewable Sciences; Romas Kazlauskas, BioTechnology Institute, University of Minnesota*

**1:15 4** A Greener, Biocatalytic Manufacturing Route to Sitagliptin. **John Grate**, Emily Mundorff, and Christopher Savile, Codexis, Inc.

**1:55 5** The Development of a Greener, Enzymatic Manufacturing Process to Sitagliptin. **Gregory J. Hughes**, Paul N. Devine, Jeffery C. Moore, and Jacob M. Janey, Merck & Co.

**2:35 6** Sustainable Chemical Production Using Engineered Microorganisms. **Mark J. Burk**, Genomatica, Inc.

#### Toxicology, Environmental Fate and Effects

1:15 PM – 3:15 PM

#### ENVIRONMENTAL FATE AND EFFECTS

2101/2103/2105, Marriott Inn and Conference Center

*Session Chair: Rich Engler, US Environmental Protection Agency*

**1:15 18** Chlorantraniliprole: Design of Green Chemistry for Insect Control. **George P. Lahm**, Thomas M. Stevenson, Thomas P. Selby, John H. Freudenberger, Daniel Cordova, Lindsey Flexner, Robert T. Roche, Mary Ellen McNally, Michael D. Woodward, and Richard A. Carver, DuPont Crop Protection

**1:55 19** Application of the Concept of Green Chemistry to Pathology Clearing Agents. **A. Moghissi**, Institute for Regulatory Science

**2:15 20** Towards the Development of Green Plasticizers. **Azadeh Kermanshahi pour**, David G. Cooper, Milan Maric, and Jim A. Nicell, McGill University

**2:35 21** Dissolvine GL: A New, Biodegradable Chelating Agent with an Excellent Safety Profile. **Edwin Bisinger Jr.**, SHERA Americas

**2:55 22** Plastics Scorecard: Applying Life Cycle Thinking to Environmental Assessments of Plastics. **Mark Rossi**, Clean Production Action, and Tim Greiner, Pure Strategies

#### Process Design and Optimization

1:15 PM – 5:30 PM

#### SUPPLY CHAIN

Auditorium, Marriott Inn and Conference Center

*Session Chairs: Joel A. Tickner, University of Massachusetts Lowell Ken; Geiser, Lowell Center for Sustainable Production, University of Massachusetts Lowell*

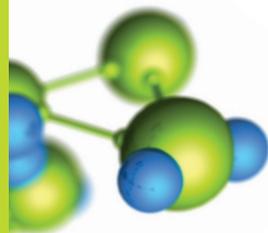
**1:15 23** Collaboration through Green Chemistry Roundtables Can Promote and Commercialize Green Chemistry. Robert J. Israel, Johnson-Diversey, Inc., **David Long**, ACS Green Chemistry Institute®, Schubert Pereira, Rug Doctor, Inc., Rob Predale, Johnson & Johnson Consumer Companies, Inc., Herbert VanderBilt, Bissell Homecare, Inc., Philip G. Sliva, Access Business Group, and **Stanley R. Weller**, Zep, Inc.

**1:55 24** Moving towards Greener Solvents for Pharmaceutical Manufacturing – An Industry Perspective. **Peter J. Dunn**, Pfizer, Inc., Richard K. Henderson, GlaxoSmithKline, Ingrid Mergelsberg, Schering-Plough and Andrew S. Wells, AstraZeneca

**2:35 25** Botanical Drug Products: Sustainable Pharmaceuticals. **Zelleka Getahun**, CDER / FDA

**2:55 26** Working with Suppliers to Manage Total Environmental Footprint of Active Pharmaceutical Ingredient Manufacture. **Caireen R. Hargreaves**, AstraZeneca

**3:15** Break



# Technical Program continued

- 4:10 27** The Green Chemistry and Commerce Council. **Ken Geiser**, Lowell Center for Sustainable Production, University of Massachusetts Lowell
- 4:50 28** Feasibility Study for Establishing a Center for Green Innovation & Technology Transfer for the Automotive Industry in Michigan. **Carol Henry**<sup>1</sup>, Cindy Reese<sup>2</sup>, and Jack Pokryzwa<sup>2</sup>, (1)Chemical Society of Washington, (2)SAE Automotive
- 5:10 180** California's Green Chemistry Initiative – Application of Lca in Public Policy. **Bob Boughton**, California EPA

## Integrative Education in Green Chemistry and Engineering

1:15 PM – 3:15 PM

### TAKING GC/GE BEYOND THE TRADITIONAL

Founders, Marriott Inn and Conference Center  
*Session Chair: Linda Vanasupa, California Polytechnic State University*

- 1:15 29** Incorporating Green Chemistry and Engineering Into a Non-Majors Course. **Lloyd D. Bastin**, Widener University
- 1:35 30** Green Chemistry Education for Chemical Workers. **Paul Renner**, Labor Institute
- 1:55 31** Business Education and GC/GE. **Andrea Larson**, Darden Graduate School of Business
- 2:15 32** Science Education and Civic Engagement. **Richard D. Sheardy**, Cynthia Maguire, and Jennifer DaRosa, Texas Woman's University
- 2:35 33** Green Chemistry at Wilkes University. **R. Gregory Peters** and Terri Wignot, Wilkes University
- 2:55 34** Green Chemistry Education: Facilitating Transition to Green Technologies and Processes in India. **R.K. Sharma**, University of Delhi

## Process Design and Optimization

3:30 PM – 5:30 PM

### GREEN SYNTHESIS I

1105, Marriott Inn and Conference Center  
*Session Chair: Chao-Jun Li, McGill University*

- 3:30 35** Achieving Synthetic Efficiency through New Method Development. **Jeff Song**, Boehringer Ingelheim Pharmaceuticals, Inc.
- 4:10 36** Ammonia-Free Birch Reductions Using Stabilized Sodium In Silica Gel for Safer, More Sustainable Synthesis. Michael J. Costanzo,

**Michael Lefenfeld**, Mitul N. Patel, Kathryn A. Petersen, and Paul F. Vogt, SiGNa Chemistry, Inc.

- 4:50 37** Recycle Solutions Reduce E-Factor for Pharma Intermediate by 90%. **Nitesh Mehta**, Bhadresh Padia, Anand Hunoor, and Hari Ramsubramani, Newreka GreenSynth Technologies

## Integrative Education in Green Chemistry and Engineering

3:30 PM – 5:30 PM

### PERSPECTIVES ON EMBEDDING GC/GE IN DIFFERENT INSTITUTIONAL CONTEXTS

Founders, Marriott Inn and Conference Center  
*Session Chair: Loyd D. Bastin, Widener University*

- 3:30 38** The New Center for Green Chemistry at the University of California, Berkeley: Integrating Approaches. **Michael P. Wilson**, University of California, Berkeley
- 3:50 39** Green Chemistry in Chinese Higher Education. **Kira JM Matus**, Harvard University
- 4:10 40** Worcester State College: Towards a Green Chemistry Center. **Meghna Dilip**, Margaret E. Kerr, and Eihab Jaber, Worcester State College
- 4:30 41** Connecting Green Chemistry to the 'TEM' In the K-12 STEM Curriculum. **Rachel Pokrandt**, Beyond Benign
- 4:50 42** Promoting Green Chemistry Education through Short-Term Courses. **Anju Srivastava** and Reena Jain, University of Delhi
- 5:10 43** Recent Educational Activities by the ACS Green Chemistry Institute®. **Jennifer L. Young**, ACS Green Chemistry Institute®

## Transforming Green Chemistry and Engineering

3:30 PM – 5:30 PM

### SURFACE PREPARATION, COATINGS, AND FILMS

2101/2103/2105, Marriott Inn and Conference Center  
*Session Chair: Topher Buck, GreenBlue*

- 3:30 44** Non-Acidic Electrochemical Polishing of Some Metals. **Tarek M. Abdel-Fattah**, Christopher Newport University
- 3:50 45** RegenSi™: Low Carbon Footprint Alternative Wafer Reclaim Solution for Extending Life Cycle of Silicon Test Wafers. **Michael B. Korzenski** and Ping Jiang, Advanced Technology Materials, Inc.
- 4:10 46** Nonisocyanate Polyurethanes: Alternative Nontoxic Process of Polyurethane

Coatings Manufacturing. **Oleg L. Figovsky**, Leonid D. Shapovalov, Olga V. Birukov, and Dmitry A. Beilin, Polymate, Ltd., International Nanotechnology Research Center

- 4:30 47** Water-Based Refractory Coatings with Wet/Dry Color Change Indication. **Jörg Kroker**, Flavia Duncan, and Lee Horvath, Ashland Performance Materials
- 4:50 48** Novel Biobased Technologies for Coatings Applications. **Madhukar (Duke) Rao**, The Sherwin Williams Company
- 5:10 49** Celgard Solvent-Free Microporous Film Technology. **Lie Shi** and Jill Watson, Celgard LLC

6:00 PM - 7:30 PM

#### RECEPTION

Main Concourse, Marriott Inn and Conference Center

## Wednesday, June 24, 2009

7:15 AM – 8:15 AM

#### CONTINENTAL BREAKFAST

Main Concourse, Marriott Inn and Conference Center

7:30 AM – 5:00 PM

#### REGISTRATION

Main Concourse, Marriott Inn and Conference Center

8:00 AM - 5:00 PM

#### EXHIBITION

Main Concourse, Marriott Inn and Conference Center

### Wednesday Morning

8:15 AM – 9:30 AM

Opening Remarks

#### KEYNOTE ADDRESS

Auditorium, Marriott Inn and Conference Center



- 50 Len Sauers**  
Vice President,  
Global Sustainability  
The Procter & Gamble Company  
**P&G's Environmental  
Sustainability Journey**

9:30 AM – 10:00 AM

#### COFFEE BREAK

### Transforming Green Chemistry and Engineering

10:00 AM – 12:00 PM

#### GREEN ANALYTICAL CHEMISTRY

1105, Marriott Inn and Conference Center  
*Session Chair: Douglas Raynie, South Dakota State University*

- 10:00 51** Green Assessment of Chemical Methods. **Douglas Raynie** and Julee Driver, South Dakota State University
- 10:20 52** The Way of Greening Analytical Chemistry. **Mihkel Koel** and Mihkel Kaljurand, Tallinn University of Technology
- 10:40 53** Green Analytical Chemistry. **Ellen R. Campbell** and Wilbur H Campbell, NECi: The Nitrate Elimination Company, Inc
- 11:00 54** Extraction Methods That Focus On Green Chemistry. **Fulgentius N. Lagemwa** and Eric J. Lawrence, Pennsylvania State University – York Campus
- 11:20 55** Thermodynamic Evaluation of the Greenness of Supercritical Fluid Chromatography in the Pharmaceutical Industry. **Geert Van der Vorst<sup>1</sup>**, Herman Van Langenhove<sup>1</sup>, Frederik De Paep<sup>1</sup>, Wim Aelterman<sup>2</sup>, Jules Dingenen<sup>2</sup>, and Jo Dewulf<sup>1</sup>, (1)Ghent University, (2)Janssen Pharmaceutica
- 11:40 181** Solvent-Free Method for Membrane Recoverable Oil and Grease by Infrared Determination. **Dean Smith**, Orono Spectral Solutions

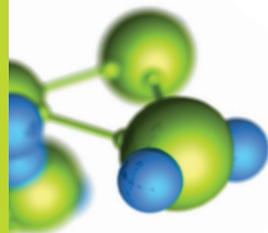
10:00 AM - 12:00 PM

#### GREEN CORROSION INHIBITION AND WATER TREATMENT

Auditorium, Marriott Inn and Conference Center

*Session Chair: Topher Buck, GreenBlue*

- 10:00 56** Sustainable Natural Green Chemistry (NGC) for Cooling Water Treatment. **Dan A. Duke**, Water Conservation Technology International, Inc.
- 10:40 57** The Development of Green Corrosion Inhibitors. **Andrea Hansen**, Margarita Kharshan and Alla Furman, Cortec Corporation
- 11:00 58** A New Cooling Water Treatment Strategy Significantly Reducing Chemical and Water Usage. Henry A. Becker, Jon J. Cohen, and **Thomas F. Hutchison**, H-O-H Water Technology, Inc



# Technical Program continued

**11:20 59** Solar Photo Oxidative Treatment System (SPOTS) Part 4: Treatment of Bacteria in Drinking Water by Induced Oxidation with Transparent Colloidal Systems. **Mohammad Musaddaq**<sup>1</sup>, Shyam Shukla<sup>1</sup>, Kenneth Dorris<sup>1</sup>, Paul Anastas<sup>2</sup>, Julie B. Zimmerman<sup>2</sup>, S. Bhanumati<sup>3</sup>, and Anh Tran<sup>1</sup>, (1)Lamar University, (2)Yale University, (3)Chemistry Department, Cargi College, Dehli University, New Delhi, India

**11:40 60** Novel Biomaterial: Designing, Characterization and Modifications for Decontamination of Metals from Waste Water: A Green Approach. **Man Mohan Srivastava**, Shalini Srivastava, and Pritee Goyal, Department of Chemistry, Agra, India.

## Process Design and Optimization

10:00 AM – 12:00 PM

### GREEN SYNTHESIS I

(continued)

Founders, Marriott Inn and Conference Center

Session Chair: *Chao-Jun Li, McGill University*

**10:00 61** A Green Protocol for the Synthesis of Pharmacologically Active Spiro-Indoles and 2-Aryl Benzimidazoles. **Siva Shankar Panda**, Rohtash Kumar and Subhash C. Jain, University of Delhi

**10:40 62** Membrane Separations for Greener Operations in the Chemical Process Industries. **C. Stewart Slater** and Mariano J. Savelski, Rowan University

**11:20 63** Benzamide as a Solvent for the Leuckart Reaction. **Mikhail M. Bobylev** and Lioudmila I. Bobyleva, Minot State University

10:00 AM – 12:00 PM

### NEW FOCUSES IN GREEN CHEMISTRY

2101/2103/2105, Marriott Inn and Conference Center

Session Chair: *Berkeley W. Cue, BWC Pharma Consulting, LLC*

**10:00 64** Climate Change – How Can Green Chemistry Help? **Peter J. Dunn**, Pfizer, Inc.

**10:40 65** Using Process Mass Intensity (PMI) to Guide Process Development and Design. Aaron S. Cote, Jason G. Dorwart, Paul F. Fernandez, D. Michael Hobbs, Viviane Massonneau, **Marguerite A. Mohan**, Aaron J. Moment, Anthony W. Moses, Rositza I. Petrova, Debra J. Wallace, and Timothy J. Wright, Merck & Co., Inc.

**11:20 66** Surfactants in Green Chemistry Part 1: Their Use as Solvents for Titrations of Water Insoluble Compounds. **Shyam Shukla**<sup>1</sup>, Paul Anastas<sup>2</sup>, Julie B. Zimmerman<sup>2</sup>,

S. Bhanumati<sup>3</sup>, and Mohammad Musaddaq<sup>1</sup>, (1)Lamar University, (2)Yale University, (3)Chemistry Department, Cargi College, Dehli University, New Delhi, India

12:00PM – 1:00PM

### LUNCH/POSTER SESSION

Chesapeake/Ft. McHenry, Marriott Inn and Conference Center

## Wednesday Afternoon

### POSTER SESSION

12:00 PM – 2:00 PM

Lower Level Concourse, Marriott Inn and Conference Center

Session Chair: *Darlene Schuster, AIChE Institute for Sustainability*

## Greenhouse Gas Management and Prevention – Poster

**69** Analysis of the CO<sub>2</sub> and NH<sub>3</sub> Reaction In An Aqueous Solution: Influence of the Operating Temperature. **Bong Gill Choi**<sup>1</sup>, Won Hi Hong<sup>1</sup>, Jong-Nam Kim<sup>2</sup>, Kwang Bok Yi<sup>2</sup>, Jong-Duk Kim<sup>1</sup>, and Sung yuol Park<sup>3</sup>, (1)Korea Advanced Institute of Science and Technology, (2)Separation Process Research Center, Korea Institute of Energy Research, (3)Korea Institute of Energy Research

## Integrative Education in Green Chemistry and Engineering – Poster

**70** Green Chemistry and Analytical Techniques: Undergraduate Laboratory Experiments. **Keith Duso** and Meghna Dilip, Worcester State College

**71** Reclaiming and Recycling Silver (a precious metal) from Lab Waste of Undergraduate Students. **Chandana Mukherjee**<sup>1</sup>, Minakshi Bhardwaj<sup>1</sup>, and S. Bhanumati<sup>2</sup>, (1)Gargi College, University of Delhi, New Delhi, India, (2)Gargi College, Delhi University, New Delhi

**72** Liquid CO<sub>2</sub> as an Apt Solvent in Undergraduate Labs. **Pragya Sidhwani**, Sri Venkateswara College, Delhi University, Sunita Dhingra, Miranda House, University of Delhi and Indu Tucker Sidhwani, Gargi College, University of Delhi

## Process Design and Optimization – Poster

**75** Extension of the Environmentally Benign Catechol Method to the Synthesis of Barium-Based Perovskites. **Heather Sheridan**,

Samantha DeCarlo, and Anne Marteel-Parrish, Washington College

- 76 Scalable Green Chemistry: A Catalytic Asymmetric Hydrogenation Case Study. **Stefan G. Koenig**, Sepracor, Inc
- 78 Implementation of Green Chemistry and Engineering Principles into Nanomaterial Synthesis and Processing. **Juncheng Liu Sr.** and Christopher B. Roberts, Auburn University
- 79 The Study on the Hollow Titanium Silicalite Zeolite (HTS). **Min Lin**, Bin Zhu, Xingtian Shu and Xieqing Wang, Research Institute of Petroleum Processing, SINOPEC
- 80 Epoxidation of Propylene and Hydrogen Peroxide. **Min Lin**<sup>1</sup>, Hua Li<sup>2</sup>, Bin Zhu<sup>1</sup>, Wei Wang<sup>2</sup>, Shunxian Huang<sup>1</sup>, Xingtian Shu<sup>1</sup>, Chijian He<sup>2</sup>, Jizao Gao<sup>2</sup>, and Xiaoju Wu<sup>2</sup>, (1)Research Institute of Petroleum Processing, SINOPEC, (2)China Petroleum & Chemical Corporation Changling Company
- 81 A Study on Noble Metal Modified Titanium Silicalite. **Min Lin**, Chunfeng Shi, Bin Zhu, and Jun Long, Research Institute of Petroleum Processing, SINOPEC
- 82 Development of Safe and Environmentally Friendly Halogenation Reagents. **Rodrigo Cristiano**, Kefeng Ma, George Pottanat, and Richard G. Weiss, Georgetown University

### Renewable Energy Fuels and Feedstocks – Poster

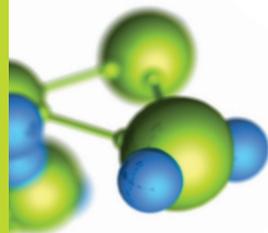
- 84 Homogeneous Modification of Cellulose in Ionic Liquid Using Iodine as a Catalyst. **Run-Cang Sun**, Beijing Forestry University
- 85 Plants as Factories; Enzymes, Electricity, and Light as Transformative Reagents. **Ian D. Brindle**, Brock University
- 88 Properties and Characterization of a Renewable Water Soluble Polymer: Polyitaconic Acid. **Mathieu Chirat**, University of New Hampshire; Yvon Durant, Itaconix
- 89 Evaluation of Different Combinations of *E. Coli* Strains and Cellulase Genes for Cellulosic Substrate Degradation. **Angelica Cavalett**, André L. Rodrigues, Larissa G. Paludo, Filipe A. T. Paulo, and Andre O. S. Lima, Universidade do Vale do Itajaí
- 90 2009 HANCOCK AWARD RECIPIENT: Chemical Transformation of Lignocellulosic Biomass into Fuels and Chemicals. **Joseph B. Binder**, Energy Biosciences Institute; Ronald T. Raines, University of Wisconsin-Madison

### Toxicology, Environmental Fate and Effects – Poster

- 91 Fate of *Jatropha curcas* Phorbol Esters in Soil. **Rakshit K. Devappa**, Harinder PS Makkar, and Klaus Becker, University of Hohenheim
- 92 Web-Based Toxic Information Clearinghouse. **George R. Thompson**, Chemical Compliance Systems, Inc.
- 93 Oligonucleotide-Based Fluorescence Probe for Sensitive and Selective Detection of Mercury(II) in Aqueous Solution. **Huan-Tsung Chang** and Cheng-Kang Chiang, National Taiwan University

### Transforming Green Chemistry and Engineering – Poster

- 94 Catalytic Activity of Ce MgO Catalyst in the Oxidation of Cumene to the Cumenehydroperoxide. **Biaohua Chen**, Shuai Xu, Chongpin Huang, and Jie Zhang, Beijing University of Chemical Technology
- 95 The Concept of a Green Drug, Curcumin, and its Derivatives as a Prototype. **Krishnaswami Raja**, College of Staten Island, CUNY
- 96 Synthesis of Ionic Liquids under Ultra-High Pressure. **Dora Lucia Sousa**<sup>1</sup>, Laurence Harwood<sup>1</sup>, and Janet L. Scott<sup>2</sup>, (1)University of Reading, (2)Monash University
- 97 A Green Pathway: Investigation of Corrosion Inhibitors and Inhibitive Effect of Some Novel Organic Dyes on the Corrosion of 2S Aluminium in Alkaline Media. **Popatbhai kuberbhai Patel Sr.**, Tushar Gopinath Barot Jr., and Pravinbhai Ranchhodbhai Patel, M.G. Science Institute (Gujarat University)
- 98 Highly Efficient and Practical Selective Monohydrolysis of Symmetric Diesters. **Satomi Niwayama**, Texas Tech University
- 99 An Exploratory Study of Propargylation of Aromatics in Ionic Liquids Employing Metallic Triflates as Catalysts. Viorel D. Sarca<sup>1</sup>, Levente Fabry-Asztalos<sup>1</sup>, **Kelley Brown**<sup>1</sup>, Casey Kellar<sup>1</sup>, and Kenneth K. Laali<sup>2</sup>, (1)Central Washington University, (2)Kent State University



# Technical Program continued

- 100** New Binary Mixture Ionic Liquid Based On  $(C_4H_9)_4NHSO_4$  and Caprolactam. **Dishun Zhao**<sup>1</sup>, Hongyan Cui<sup>1</sup>, and Erhong Duan<sup>2</sup>, (1)Hebei University of Science and Technology, (2)Tianjin University
- 101** Hydrolysis of Nitriles to Amide in Water Under Microwave Irradiation. **Joo Ho Kim**<sup>1</sup>, Ui Yong Kim<sup>1</sup>, and Jong Chan Lee<sup>2</sup>, (1)ChungAng University, (2)Chung-Ang university
- 102** Delineation of More Environmentally Benign Pathways for the Synthesis of Doped Barium Titanate. **Samantha DeCarlo**, Heather Sheridan, and Anne Marteel-Parrish, Washington College
- 103** Surfactants in Green Chemistry Part 2: The Use of Surfactant-Modified Clays for Removal of Traces of Organics from Aqueous Systems. **Shyam Shukla**<sup>1</sup>, Paul Anastas<sup>1</sup>, Julie B. Zimmerman<sup>1</sup>, S. Bhanumati<sup>2</sup>, and Mohammad Musaddaq<sup>3</sup>, (1)Yale University, (2)Chemistry Department, Cargi College, Dehli University, New Delhi, India, (3)Lamar University
- 104** Phase Transfer Catalysis with Microwaves: Green Synthetic Approaches to Metal Carbonyl Complexes. **Kurt Birdwhistell**, Brian E. Schulz, and Kathryn Conroy, Loyola University New Orleans
- 105** Extraction of Toxic Metal Ions Using Aqueous Biphasic System. **Sushmita Chowdhury** and Indu Tucker Sidhwani, Gargi College, University of Delhi
- 106** 1,3,5-Triisopropylbenzene Synthesis by Alkylation of Benzene with Propylene Using Chloroaluminate Ionic Liquids as Catalysts. **Biaohua Chen**, Chongpin Huang, and Jie Zhang, Beijing University of Chemical Technology
- 107** Adsorption and Reduction of Cr(VI) Using Orange Peels. **Bryan Bilyeu**<sup>1</sup>, Carlos Barrera-Diaz<sup>2</sup>, Patricia Balderas-Hernández<sup>2</sup>, and Gabriela Roa-Morales<sup>2</sup>, (1)Xavier University of Louisiana, (2)Universidad Autonoma del Estado de México
- 108** Solar Photo Oxidative Treatment System (SPOTS) Part 3: Oxidation and Mineralization of 2, 4-Dinitrophenol. **Shyam S. Shukla**<sup>1</sup>, Paul Anastas<sup>2</sup>, Julie B. Zimmerman<sup>2</sup>, S. Bhanumati<sup>3</sup>, Mohammad Musaddaq<sup>1</sup>, Kenneth Dorris<sup>1</sup>, and Alka Shukla<sup>4</sup>, (1)Lamar University, (2)Yale University, (3)Chemistry Department, Cargi College, Dehli University, New Delhi, India, (4)Southeast College
- 109** A Mild and Environmentally Friendly  $\alpha$ -Bromo Cycloalkenone In Ionic Liquid Using 1,3-Dibromo-5,5-Dimethylhydantoin(DBDMH) and UHP In  $H_2O$ . **Soon-Uk Chang**, Jong Won Hwang, and Jong Chan Lee, Chung-Ang University
- 110** Controlled Growth and Aggregation of Ferrite Nanoparticles for High Relaxivity MR Imaging. **Jong-Duk Kim**, Bong-sik Cheon, Hee-man Yang, and Won-Hee Hong, KAIST
- 111** Low Cost Green Biochemical Reactor for the Synthesis of Chelating Resins. **Narendar Bhojak**, Neeru Khiwani, D.D. Gudesaria, H.S. Bhandari, and Mona, Green Chemistry Research Centre, Govt Dungar College (A-Grade), MJS University
- 112** A New One Pot, Solvent Free and Microwave Assisted Synthesis of Nickel Porphyrin. **Indu Tucker Sidhwani**, Gargi College, University of Delhi; Gauri Ahuja, Green Chemistry Network Centre; R. K. Sharma, University of Delhi
- 113** Fast and Simple Method for Direct Iodination of Activated Aromatic Compounds in the Presence of Poly(ethylene) Glycol (PEG) Under Microwave Irradiation. **Hee Joong Park**, Insu Kim, and Jong Chan Lee, (1)Chung-Ang University, (2)Chung-Ang University
- 114** Mine Drainage Remediation Using Cactus. **Bryan Bilyeu**<sup>1</sup>, Carlos Barrera-Diaz<sup>2</sup>, Gabriela Roa-Morales<sup>2</sup>, and Patricia Balderas-Hernández<sup>2</sup>, (1)Xavier University of Louisiana, (2)Universidad Autonoma del Estado de México
- 115** Functionalized Biomaterials for Arsenic Removal From Groundwater. **Sarah M. Miller** and Julie B. Zimmerman, Yale University
- 116** Oxidation Desulfurization in Fuel Using Ionic Liquids as Phase Transfer Catalysts. **Dishun Zhao**, Hebei University of Science and Technology; Yanan Wang, School of Chemical Engineering, Tianjin University
- 117** A Novel Deep Eutectic Solvent Prepared by Solid Organic Compounds. **Xingchen Zhang Sr.**, Huiru Liu, and Liqiang Lv, Shijiazhuang University
- 118** 2009 HANCOCK AWARD RECIPIENT: Enzymatic Synthesis in Deep Eutectic Solvents. **Johnathan Thomas Gorke**, Friedrich Srienc, and Romas J. Kazlauskas, University of Minnesota
- 119** The Barriers to the Implementation of Green Chemistry in China. **Xin Xiao**, Institute of Process Engineering, Kira JM Matus, Harvard University

- 120** Design of Gelators based on Amine and Amide Derivatives of (*R*)-12-Hydroxystearic Acid, a Renewable Feedstock obtained from Castor Oil. **V. Ajay Mallia**, Daniel L. Blair, and Richard G Weiss, Georgetown University

## Greenhouse Gas Management and Prevention

2:00 PM – 5:40 PM

### GREENHOUSE GAS MANAGEMENT AND PREVENTION

1105, Marriott Inn and Conference Center

Organizer: Ron R. Chance, Georgia Tech

- 2:00 121** CO<sub>2</sub> Capture on Carbonaceous Sorbents. **Maciej Radosz** and Kaspars Krutkramelis, University of Wyoming
- 2:40 122** Hollow-Fiber-Based Adsorbent System for CO<sub>2</sub> Capture from Flue Gas. **Ryan P. Lively**<sup>1</sup>, Ron R. Chance<sup>1</sup>, Harry W. Deckman<sup>2</sup>, B. T. Kelley<sup>3</sup>, and William J. Koros<sup>1</sup>, (1)Georgia Tech, (2)ExxonMobil Research and Engineering, (3)ExxonMobil Upstream Research Company
- 3:00 123** Management of Green House Gases by Photo-Electrocatalysis. **Alex Omo Ibhaddon**, University of Hull
- 3:20** Break
- 3:40 124** Designer Reversible Ionic Liquids for CO<sub>2</sub> Capture. **Ali Fadhel**, Vittoria Blassuci, Cerag Dilek, Ryan Hart, Hillary Huttenhower, Veronica Llopis-Mestre, Pamela Pollet, Eduarco Vyhmeister, Charles L. Liotta, and Charles A. Eckert, Georgia Institute of Technology
- 4:00 125** A Study of Carbon Dioxide Adsorption Performance by the Ion Exchange of Zeolite-13X. **Kim Hyung Taek**, Young hoon Kim, and Jun mo Koo, Ajou University
- 4:20 126** HCR-188C: An Alternative “Green” High-Efficiency Hydrocarbon Refrigerant. **Gary Keith Whitmyre**<sup>1</sup>, Richard Maruya<sup>2</sup>, Alan Abul-Haj<sup>3</sup>, Roxanne Abul-Haj<sup>3</sup>, and George M. Whitmyre<sup>4</sup>, (1)Whitmyre Research, (2)A.S. Trust, (3)ARA Engineering, Inc., (4)University of Delaware

## Process Design and Optimization

2:00 PM – 5:40 PM

### PROCESS SAFETY & REACTION ENGINEERING

Founders, Marriott Inn and Conference Center

Organizer: David J. am Ende, Pfizer, Inc.

- 2:00 127** Continuous Processes In Small-Scaled Reactors Under cGMP Conditions: Towards Efficient Pharmaceutical Synthesis. **Peter Poechlauer**<sup>1</sup>, Sascha Braune<sup>1</sup>, and Raf Reintjens<sup>2</sup>, (1)DSM

Fine Chemicals Austria Nfg GmbH. & Co KG, (2)DSM Pharmaceutical Products

- 2:40 128** Continuous Microreactor Development: Transport and Biofuel Studies. **Paul Chin**, Brad A. Pindzola, and Arthur D. Schwoppe, TIAX LLC
- 3:20** Break
- 3:40 129** Process Design toward Continuous Manufacturing: a Green Perspective. **David J. am Ende**, Pfizer, Inc.
- 4:20 130** Design, Modeling and Optimization of a Gas-Phase Catalytic Channel Reactor. **Alex Omo Ibhaddon**, University of Hull
- 5:00 131** Integrated Direct Cooling Suspension Crystallization and Absorption Refrigeration Process for PX-Purification. **Min Huang**<sup>1</sup>, De-jin Kong<sup>2</sup>, Jie Cai<sup>1</sup>, Ying Zhu<sup>1</sup>, Yan-zi Guo<sup>1</sup>, Yan Wang<sup>1</sup>, Si-si Guo<sup>1</sup>, and Jun Wu<sup>1</sup>, (1)Tongji University, (2)Shanghai Research Institute of Petrochemical Technology, SINOPEC

2:00 PM - 3:20 PM

### NEW FOCUSES IN GREEN CHEMISTRY

2101/2103/2105, Marriott Inn and Conference Center

Session Chair: Berkeley W. Cue, BWC Pharma Consulting, LLC

- 2:00 67** Systematic Study of C-H Activation/Borylation. **Sean Preshlock**, Michigan State University
- 2:40 68** IMPACT™ Technology: A Greener Polyether Process. **Jack R. Reese II**, Kenneth G. McDaniel, Robert A. Lenahan, Robert G. Gastinger, and D. Mark Morrison, Bayer MaterialScience, LLC

## Renewable Energy Fuels and Feedstocks

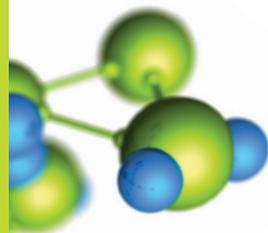
2:00 PM – 5:40 PM

### RENEWABLE FEEDSTOCKS AND MATERIALS

Auditorium, Marriott Inn and Conference Center

Organizer: Richard P. Wool, University of Delaware

- 2:00 132** Renewable Water Soluble Polymer: Polyitaconic Acid. **Yvon Durant**, Itaconix; Mathieu Chirat, University of New Hampshire
- 2:20 133** Chemically Modified Fatty Acids as Styrene Replacement In Vinyl Ester Polymers. **Alejandrina Campanella**<sup>1</sup>, John J. La Scala<sup>2</sup>, and Richard P. Wool<sup>1</sup>, (1)University of Delaware, (2)Army Research Labs
- 2:40 134** Twinkling Fractal Theory of the Glass Transition with Green Chemistry Applications. **Joseph F. Stanzone III** and Richard P. Wool, University of Delaware
- 3:00 135** Enzyme-Catalyzed Conversion of Glycerol to Glycerol Carbonate. **Kerri Cushing** and Steven Peretti, North Carolina State University
- 3:20** Break



# Technical Program continued

- 3:40 136** More Efficient Epichlorohydrin from Glycerin. **Bruce D. Hook Sr.**, John R. Briggs, William J. Kruper, Perry Basile, and Ernesto Occhiello, The Dow Chemical Co.
- 4:00 137** Biogenic Silica for Construction and Industrial Applications. **R. K. Vempati**<sup>1</sup>, Prasad Rangaraju<sup>2</sup>, Elena Pisanova<sup>3</sup>, John Lund<sup>3</sup>, and Jean-Claude Roumain<sup>4</sup>, (1)Southern Methodist University, (2)Clemson University, (3)Harper International, (4)Holcim Cement
- 4:20 138** Performance of Carbon-Neutral Rice Hull Ash as a Supplementary Cementitious Material in Portland Cement Mortars. **Prasad Rangaraju**<sup>1</sup>, K.V. Harish<sup>1</sup>, R. K. Vempati<sup>2</sup>, and Jean-Claude Roumain<sup>3</sup>, (1)Clemson University, (2)Southern Methodist University, (3)Holcim Cement
- 4:40 139** Bio-Composites from Chicken Feathers and Plant Oils for Printed Circuit Boards. **Mingjiang Zhan** and Richard P. Wool, University of Delaware

## Toxicology, Environmental Fate and Effects

3:40 PM – 5:40 PM

### DESIGN SIGNALS FROM ENVIRONMENTAL HEALTH SCIENCES: WHAT EVERY CHEMIST SHOULD KNOW

1123, Marriott Inn and Conference Center

Organizer: *Lin Kaatz Chary, Great Lakes Green Chemistry Network*

- 3:40 140** Design Signals From Environmental Health Sciences: What Every Chemist Should Know. **Lin Kaatz Chary**, Great Lakes Green Chemistry Network

*Moderator: Karen Peabody O'Brien*

*Speaker 1: Linda Birnbaum, Director, National Institute of Environmental Health Sciences, National Institutes of Health*

*Speaker 2: Howard Frumkin, Director, National Center for Environmental Health, Agency for Toxic Substances and Disease Registry*

*Speaker 3: Peter DeFur, President, Environmental Stewardship Concepts, Affiliate Associate Professor, Center for Environmental Studies, Virginia Commonwealth University*

*Speaker 4: Jane Houlihan, Vice President for Research, Environmental Working Group*

## Transforming Green Chemistry and Engineering

3:40 PM – 5:40 PM

### GREEN SYNTHESIS II

2101/2103/2105, Marriott Inn and Conference Center

Organizer: *Topher Buck, GreenBlue*

- 3:40 141** Understanding Enolate Chemistry and the Tishchenko Reaction Under High Speed Ball Milling Conditions. **Daniel C. Waddell**, Indre

Thiel, S. Tyler Marcum, Brandon Smith, and James Mack, University of Cincinnati

- 4:00 142** Pot-In-Pot Reactions: A New Paradigm In 'ad Infinitum' Cascade Reactions. **Martin T. Mwangi**<sup>1</sup>, Michael D. Schulz<sup>2</sup>, Rachel J. Elsey<sup>1</sup>, Anne Beaubrun<sup>2</sup>, and Ned B. Bowden<sup>1</sup>, (1)University of Iowa, (2)Duke University
- 4:20 143** Anchored Homogeneous Catalysts as Environmentally Favorable Alternatives to Homogeneous Catalysts. **Robert L. Augustine**, Setrak K Tanielyan, Gabriela Alvez, and Norman Marin, Seton Hall University
- 4:40 144** Scalable Catalytic Methods for Selective Aerobic Oxidation of Organic Molecules. Xuan Ye<sup>1</sup>, Matthew H. Yates<sup>2</sup>, Martin D. Johnson<sup>2</sup> and **Shannon S. Stahl**<sup>1</sup>, (1)University of Wisconsin-Madison, (2)Eli Lilly and Company
- 5:00 145** Design of Green Recyclable Supported Catalysts for Organic Transformations. **Brindaban C. Ranu**, Indian Association for the Cultivation of Science

## Thursday, June 25, 2009

Thursday, June 25, 7:00 AM – 8:00 AM

### CONTINENTAL BREAKFAST

Main Concourse, Marriott Inn and Conference Center

Thursday, June 25, 7:00 AM – 12:00 PM

### REGISTRATION

Main Concourse, Marriott Inn and Conference Center

Thursday, June 25, 8:00 AM – 3:00 PM

### EXHIBITION

Main Concourse, Marriott Inn and Conference Center

## Thursday Morning

8:00 AM – 9:15 AM

### KEYNOTE ADDRESS

Auditorium, Marriott Inn and Conference Center

Opening Remarks

### STUDENT POSTER AWARDS



#### Jean-Michel Cousteau

*Founder and President, Ocean Futures Society*

*Executive Vice President, The Cousteau Society*

THE CALL OF THE KILLER WHALE

9:15 AM - 9:30 AM

### COFFEE BREAK

## Transforming Green Chemistry and Engineering

9:30 AM – 12:30 PM

### FUNDING GREEN CHEMISTRY & ENGINEERING RESEARCH

Founders, Marriott Inn and Conference Center

*Session Chairs: Rich Engler, US Environmental Protection*

*Agency, Julie B. Manley, Guiding Green, LLC*

- 9:30 147** Using I.P. to Fuel Your Business. **Carlyn A. Burton** and Jeffrey S. Bergman, Osha Liang LLP
- 9:50** **Jeffrey A Smiley**, Office of Research Grants, American Chemical Society
- 10:10** **David H. Brown Ripin**, Drug Access Program, William J. Clinton Foundation
- 10:30** **Mark A. Lester**, Provenance Venture Partners, LLC.
- 10:50** Break
- 11:10** **April Richards**, Office of Research & Development, US Environmental Protection Agency
- 11:30** **John Regalbuto**, Chemical, Biochemical and Biotechnology Systems, National Science Foundation
- 11:50** Pending
- 12:10** Discussion

## Lifecycle Analysis and Green Metrics

9:30 AM – 12:30 PM

### LIFECYCLE ANALYSIS AND GREEN METRICS

1105, Marriott Inn and Conference Center

*Session Chair: Jennifer L. Young, ACS Green Chemistry Institute®*

- 9:30 148** LCA – Making the Sausage. **Paul Chalmer**, NCMS
- 9:50 149** EPA's Green Racing Initiative. **John C. Glenn**, US Environmental Protection Agency
- 10:10 150** Life Cycle Pollution Prevention Utilizing Automated, Web-Based Assessment of "Green" Chemicals, Products, Munitions and Processes. **George R. Thompson**, Chemical Compliance Systems, Inc.
- 10:30 151** Glaxosmithkline's Experiences with Life Cycle Assessment. **Concepción Jiménez-González**, GlaxoSmithKline
- 10:50** Break
- 11:10 73** Standards for Green Solvents: An Example Using Ionic Liquids. Guy A. Hembury, Neil Sullivan, Lauern Tate, Gayle Fairless, and **Robert Newton**, Bioniqs Ltd.
- 11:30 152** Using Life Cycle Assessment to Develop Environmental Leadership Standards.

**Christine Chase**, Cheryl Baldwin, and Nana Wilberforce, Green Seal

- 11:50 153** Standards, Metrics, and Measures – Do We Need Them? **Lin Kaatz Chary**, Great Lakes Green Chemistry Network

## Renewable Energy Fuels and Feedstocks

9:30 AM – 12:30 PM

### RENEWABLE FUELS

2101/2103/2105, Marriott Inn and Conference Center

*Session Chair: Liz Gron, Hendrix College*

- 9:30 154** Upgrading of Bio-Oil for Fuel Production. **Luc Moens**, Stuart K. Black, Michele D. Myers, and Stefan Czernik, National Renewable Energy Laboratory
- 10:10 155** A Novel Ionic Liquid Process for Conversion of Renewable Biomass into Petrochemical Intermediate. **Wei Liu**, Pacific Northwest National Lab
- 10:30 156** Hydrolysis of Lignocellulosic Biomass In Subcritical Water and Catalytic Gasification of Hydrolysates to Produce Hydrogen Rich Gas. **Sibel Irmak**, Bahar Meryemoglu, Ilker Ozturk, Mehtap Kurtulus, Tugba Balin, Arif Hesenov, and Oktay Erbatur, Cukurova University
- 10:50** Break
- 11:10 157** Sensitized TiO<sub>2</sub> for Catalytic Solar Fuel Generation: A Combined Molecular and Materials Based Approach. **Amanda J. Morris** and Gerald J. Meyer, Johns Hopkins University
- 11:30 158** Conversion of Biomass Resources into Chemicals with Integrated Catalytic Technologies. **Anders Riisager**<sup>1</sup>, Thomas S. Hansen<sup>1</sup>, Tim Ståhlberg<sup>1</sup>, Søren K. Klitgaard<sup>1</sup>, Jacob S. Jensen<sup>1</sup>, John M. Woodley<sup>1</sup>, Astrid Boisen<sup>2</sup>, and Sven Pedersen<sup>2</sup>, (1)Technical University of Denmark, (2)Novozymes A/S
- 11:50 159** Cavitation-Enhanced Intensification and Optimization of the Synthesis of Biofuels from Edible and Non-Edible Biomass. **Yusuf G. Adewuyi** and Naresh N. Mahamuni, North Carolina A&T State University

## Process Design and Optimization

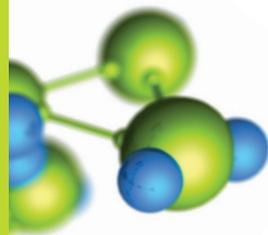
9:30 AM – 3:30 PM

### TECHNOLOGIES FOR THE GREEN TOOLBOX

Auditorium, Marriott Inn and Conference Center

*Organizer: Thomas Roper, GlaxoSmithKline*

- 9:30 160** NonCovalent Derivatization: Physical Properties and Formulation Design at the Molecular Level. **John C. Warner**, Warner Babcock Institute for Green Chemistry



# Technical Program continued

**10:10 161** Use of an Electronic Lab Notebook (ELN) for Green Science at Eli Lilly and Company. **Michael E. Kopach**, Eli Lilly and Company

**10:50** Break

**11:10 162** Explore C-C Bond Formations Beyond Functional Group Transformations. **Chao-Jun Li**, McGill University

**11:50 163** Copper-Catalyzed C-H Amination with Unactivated Amines. Raymond T. Gephart III<sup>1</sup>, Yosra M. Badiei<sup>2</sup>, Mae Joanne Aguila<sup>2</sup>, and **Timothy H. Warren<sup>2</sup>**, (1)University of North Carolina at Wilmington, (2)Georgetown University

## Thursday Afternoon

### Process Design and Optimization

12:30 PM – 1:30 PM

#### LUNCH

Chesapeake/Ft. McHenry, Marriott Inn and Conference Center

#### TECHNOLOGIES FOR THE GREEN TOOLBOX (continued)

Auditorium, Marriott Inn and Conference Center  
Organizer: *Thomas Roper, GlaxoSmithKline*

**1:30 164** Green Chemistry Techniques for Small-Scale Organic Synthesis. **Wei Zhang**, University of Massachusetts Boston

**2:10 165** Environmentally Friendly Routes for the Selective Oxidation of Alcohols. **Robert L. Augustine** and Setrak K. Tanielyan, Seton Hall University

**2:50 166** Transforming Catalytic C-H Borylations Into a Pharma Friendly Synthetic Tool. **Robert E. Maleczka Jr.**, Nathan J. Gesmundo, Venkata A. Kallepalli, Hao Li, A. Monica Norberg, Sean M. Preshlock, Philipp C. Roosen, Luis Sanchez, Clarissa L. Turton, and Milton R. Smith III, Michigan State University

### Transforming Green Chemistry and Engineering

1:30 PM – 3:50 PM

#### DRIVERS AND STRATEGIES FOR GREEN CHEMISTRY AND ENGINEERING

Founders, Marriott Inn and Conference Center  
Organizer: *Topher Buck, GreenBlue*

**1:30 167** The National Conversation On Public Health and Chemical Exposures. Howard Frumkin and **Ben Gerhardstein**, US Centers for Disease Control and Prevention

**1:50 168** The Business Value of GC/GE. **Andrea Larson**, Darden Graduate School of Business, University of Virginia

**2:10 169** Facilitating Implementation of Green Chemistry in Industry. **Emily Reichert** and John C. Warner, Warner Babcock Institute for Green Chemistry

**2:30 170** CleanGredients®: Challenges and Opportunities in the Development of an Open, Multi-Attribute Information Platform for Green Formulation. **Topher Buck**, GreenBlue

**2:50 171** Biomimetic Green Chemistry Solutions: Achievements and Outlook. **Mark H. Dorfman**, Biomimicry Guild

**3:10 172** Policies and Tools for States to Promote Green Chemistry. **Lin Kaatz Chary**, Great Lakes Green Chemistry Network

1:30 PM – 3:50 PM

#### GREEN SYNTHESIS II

(continued)

2101/2103/2105, Marriott Inn and Conference Center  
Organizer: *Liz Gron, Hendrix College*

**1:30 174** Electroless Cr(VI) Reduction. **Carlos Barrera-Diaz<sup>1</sup>**, Bryan Bilyeu<sup>2</sup>, Violeta Lugo-Lugo<sup>1</sup>, Víctor Sánchez-Mendieta<sup>1</sup>, and Patricia Balderas-Hernández<sup>1</sup>, (1)Universidad Autonoma del Estado de México, (2)Xavier University of Louisiana

**1:50 175** Switchable Ionic Liquids — a Benign Paradigm for Coupling Reactions and Separations. **Hillary Huttenhower**, Ejae John, Vittoria Blasucci, Cerag Dilek, Veronica Llopis-Mestre, Ryan Hart, Eduardo Vyhmeister, Ali Fadhel, Pamela Pollet, Charles Eckert, and Charles Liotta, Georgia Institute of Technology

**2:10 176** Green Pathways for Synthesis and Reductive Ring Cleavage of Bioactive 5-Methyltetrahydropyridopyrimidines Using Eco Friendly Phase Transfer Catalysis. **Rina D. Shah**, M.G. Science Institute,

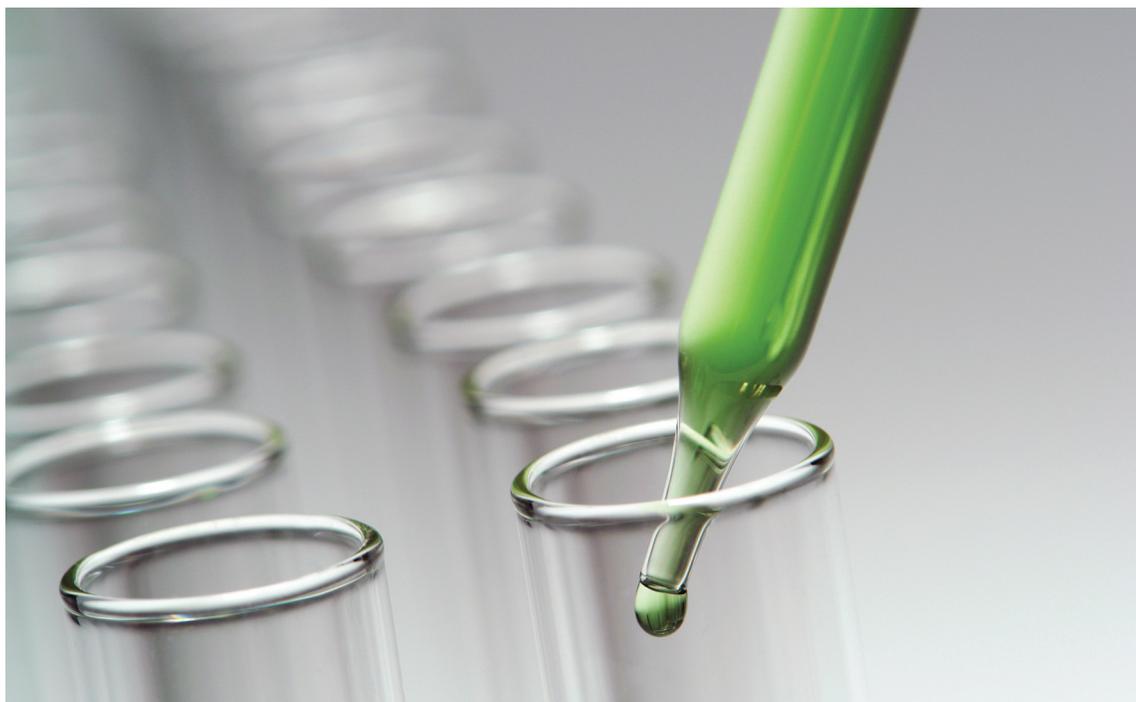
**2:30 177** More Benign Synthesis and Extraction of Ligand-Free Palladium Nanoparticles. **Juncheng Liu Sr.<sup>1</sup>**, Nicholas Ruffini<sup>1</sup>, Christopher B. Roberts<sup>1</sup>, Pamela Pollet<sup>2</sup>, Veronica Llopis-Mestre<sup>2</sup>, Charles L. Liotta<sup>2</sup>, and Charles A. Eckert<sup>2</sup>, (1)Auburn University, (2)Georgia Institute of Technology

**2:50 178** Using High Speed Ball Milling (HSBM) to Maximize Efficiency in Multi-Component Reactions. **William C. Shearouse** and James Mack, University of Cincinnati

**3:10 173** Biofunctionalized Silver Nanoparticles: Synthesis and Characterization. Ranjana Dixit<sup>1</sup>, **Nityananda Agasti<sup>2</sup>**, and Narender Kumar Kaushik<sup>2</sup>, (1)Ramjas College, University of Delhi, (2)University of Delhi



# Abstracts



## 1. Conversion of Racemic Ibuprofen to (*S*)-Ibuprofen

David Chavez and James Salvador, Chemistry, University of Texas at El Paso, El Paso, TX

A *Candida rugosa* lipase-catalyzed enantioselective esterification process under *in situ* racemization of the remaining (*R*)-ibuprofen substrate with NaOH as the catalyst was developed for the production of (*S*)-methyl ibuprofen ester from racemic ibuprofen ((*R,S*)-ibuprofen), in an organic-aqueous biphasic system on a continual product removal reactor. Racemic ibuprofen, methanol, and 45°C were selected as the best substrate and temperature, respectively, by comparing the time-course variations for the followed (*S*)-ibuprofen ester hydrolysis reaction and the non-solubility of methanol on the organic phase. Detailed investigations of NaOH concentrations on the enzyme selectivity and activity, and the kinetic behavior of the (*R*)-ibuprofen on the racemization and enzymatic reactions were conducted, in which good agreement between the experimental data and the theoretical results was observed. Finally the highly enantiomer pure product, (*S*)-methyl ibuprofen ester, was enzymatic hydrolyzed in aqueous conditions using the same *Candida rugosa* Lipase.

## 2. Enzymatic Synthesis in Deep Eutectic Solvents

Johnathan Thomas Gorke, Friedrich Sreinc, and Romas J. Kazlauskas, BioTechnology Institute, University of Minnesota, Saint Paul, MN

Enzymes are desirable catalysts because they give high selectivity with minimal byproducts. Often, non-aqueous conditions are required for desired reactions, particularly with industrial hydrolases. These processes commonly use volatile organic solvents (VOS), which are often flammable, toxic, and environmentally harmful. Ionic liquids (ILs) are molten salts that are recyclable, non-volatile, and non-flammable alternatives to VOS that initially

showed promise in enzymatic reactions. ILs offer advantages in enzymatic reactions such as high enzyme stability, ease of product separation, and recyclability, but their high cost is prohibitive and their lack of sustainable, non-toxic materials is undesirable. Deep eutectic solvents (DES's) are physical mixtures of ammonium or metal salts and hydrogen bond donors that are promising, inexpensive replacements for both VOS and ILs. Examples are 1:2 choline chloride (a naturally occurring vitamin used in chicken feed): urea (fertilizer or animal waste product) and 1:2 choline chloride:glycerol (biodiesel byproduct). In addition to offering the recyclability, low volatility, and low flammability of ILs, DES's are composed of non-toxic and inexpensive materials including vitamins, amides, sugars, and alcohols that have costs and production scales comparable to VOS. Many of these components are natural products or can be made from renewable materials, meaning that DES's are potentially sustainable. We have found that DES's are effective solvents for a number of hydrolase-catalyzed reactions, including transesterification, epoxide hydrolysis, and ring-opening polymerization. Enzyme stability and activity in DES's is comparable to those in VOS, despite the presence of potential denaturants such as chloride or urea. We found comparable polymerization activity of *Candida antarctica* lipase B for the production of polycaprolactone from  $\epsilon$ -caprolactone in 1:2 choline chloride:urea compared to in toluene. We also found a 20-fold conversion enhancement of epoxide hydrolase-catalyzed hydrolysis of styrene oxide to styrene glycol in 25% 1:2 choline chloride:glycerol compared to in water or water/organic mixtures.

## 3. Engineering *Candida tropicalis* for conversions of fatty acids to $\omega$ -hydroxyfatty acids.

Wenhua Lu<sup>1</sup>, Jon E. Ness<sup>2</sup>, Xiaoyan Zhang<sup>3</sup>, Wenchun Xie<sup>1</sup>, Jeremy Minshull<sup>2</sup>, and Richard A. Gross<sup>1</sup>, (1)NSF I/UCRC for Biocatalysis and Bioprocessing of Macromolecules, Department of Chemical and Biological Sciences, Polytechnic Institute of NYU, Brooklyn, NY, (2)DNA 2.0, Inc., Menlo Park, CA. Abstract not available at press time.



# Abstracts continued

## 4. A Greener, Biocatalytic Manufacturing Route to Sitagliptin

*John Grate, Emily Mundorff, and Christopher Savile, Codexis, Inc., Redwood City, CA*

Merck and Codexis have collaborated to develop an environmentally benign alternative manufacturing route to sitagliptin, the active ingredient of Januvia®. Using its directed evolution technologies, Codexis discovered and developed transaminases capable of catalyzing the production of the API, a chiral amine, from a ketone precursor, meeting targeted performance parameters for the process contemporaneously developed by Merck.

This joint presentation will feature the biocatalyst evolution conducted at Codexis and the process development conducted at Merck.

## 5. The Development of a Greener, Enzymatic Manufacturing Process to Sitagliptin

*Gregory J. Hughes, Paul N. Devine, Jeffery C. Moore, and Jacob M. Janey, Process Research, Merck & Co., Rahway, NJ*

Merck and Codexis have formed a strategic partnership aimed at significantly expanding the scope of reaction manifolds which can be affected by biocatalytic transformations. This collaboration seeks to enhance efficiencies and capabilities in the areas of:

1. Medicinal chemistry (0.001-100g)
2. Initial large scale GMP campaigns (>1Kg), and
3. Long term manufacturing approaches (multi-ton).

The focus of this presentation will be on the development of an environmentally benign alternative manufacturing route to sitagliptin, the active pharmaceutical ingredient in JANUVIA®. A new enzymatic process has been found to derive environmental advantages resulting in a significant reduction in the number of unit operations and in substantial reduction in the volumes of reaction solvents and waste streams required to complete the synthesis.

This joint presentation will feature a description of both the enzymatic evolution efforts conducted at Codexis and process development efforts conducted at Merck.

## 6. Sustainable Chemical Production Using Engineered Microorganisms

*Mark J. Burk, Genomatica, Inc., San Diego, CA*

Petrochemicals are valuable products that are manufactured from non-renewable hydrocarbon-based raw materials. Petrochemical processes generally are efficient, yet are relatively costly, energy and capital intensive, and release large amounts of waste and greenhouse gases, which are thought to be a major contributor to climate change. Genomatica is developing innovative ways to produce chemicals directly and sustainably from renewable feedstocks. These bio-manufacturing processes are safer, produce little or no harmful waste, release less greenhouse gas, and require less energy relative to petrochemical processes that produce the same chemical. The time has come for feedstock diversification and sustainable production of industrial chemicals through bio-manufacturing.

Genomatica employs an integrated set of computational and experimental tools to design and engineer pathways, microorganisms, and environmentally responsible processes. Through this novel approach, Genomatica has successfully engineered *E. coli* strains that produce 1,4-butanediol (BDO), a large volume chemical used in many polymer applications, directly from glucose and sucrose. Proprietary metabolic models and simulation algorithms were used to test all possible ways

that BDO could be produced inside a cell, and then the optimal paths from sugar were selected on the basis of criteria such as yield and the number of known enzymatic steps. These pathway and strain designs were then implemented in the lab to afford a microorganism and fermentation process for BDO production. Downstream process development has led to optimum separation and purification designs for a fully integrated cost-advantaged, energy-efficient, clean, safe, renewable Bio-BDO production process. Genomatica's technology platform will be described and details surrounding the development of processes for the production of Bio-BDO and other industrial chemicals will be provided.

## 7. Teaching Green Chemistry and Engineering Concepts in the Undergraduate Organic Laboratory via Biginelli and Hantzsch Reactions

*Andrew P. Dicks, Evangelos Aktoudianakis, and Sarah Styler, Department of Chemistry, University of Toronto, Toronto, ON, Canada*

The concept of "Green Chemistry" has existed for nearly two decades yet laboratory experiments showcasing green chemical principles are still just developing - particularly ones that permit comparison between older and modern technologies. The Biginelli synthesis, which facilitates preparation of vasodilatory dihydropyrimidones will be presented as a vehicle to examine how improvements can be made in the environmental profile of an organic reaction. This experiment is appropriately run in mid-level (second- or third-year) undergraduate laboratories and can be performed on a microscale with standard glassware in a total of three hours. Students undertake both a "traditional" and "modern" Biginelli preparation of a dihydropyrimidone with each method practically straightforward and performed individually or in a pair. Emphasis is placed on comparing the two approaches from a green chemistry perspective. The class probe ideas of catalytic reactivity, solvent-free synthesis, atom economy, and energy consumption to assess green improvements made by employing the modern strategy. Significantly, engineering and industrial concepts are introduced within the framework of solvent-free reaction scale-up, thermal process safety considerations, and microreactor design. This methodology can be extended to the Hantzsch synthesis of 1,4-dihydropyridines.

## 8. Designing a Green, Inquiry-Based Organic Chemistry Laboratory to Educate the Next Generation of Scientists

*Loyd D. Bastin and Kaitlyn Gerhart, Department of Chemistry, Widener University, Chester, PA*

When greening an organic chemistry laboratory, redesigning the course to educate students about green chemistry rather than simply greening the individual experiments is crucial. It is imperative to design the laboratory to incorporate the principles of green chemistry through-out the course regardless of whether the experiments have been "greened." Here we describe our process of redesigning the organic chemistry I laboratory from a microscale course into a green chemistry lab. Our approach involved assessing the pedagogical value of current experiments performed in the organic chemistry I and II laboratories. Then, we collaborated with science faculty to determine the skills/knowledge that students should obtain from the laboratories. From this information, we outlined these skills/knowledge and searched the current literature for "green" organic chemistry experiments that met the course goals. As a capstone experiment, we developed a three-step inquiry-based, green synthesis for the organic chemistry I laboratory. The capstone experiment required the students to search the "literature" and find methods for performing a carbonyl reduction, elimination, and bromination. The student-researched

methods are then analyzed for “greenness” as a class exercise before the experiments are performed, and the class chooses the “best” method for each reaction.

### 9. Development of an Organic Chemistry for Engineers with a “Sustainable” Spin

*Montserrat Rabago Smith and Jennifer Aurandt, Chemistry and Biochemistry, Kettering University, Flint, MI*

Educating burgeoning engineers and scientists about chemical processes that diminish or remove hazardous waste is extremely important in present times. Therefore, education in the area of green chemistry is of extreme value, and its integration into the undergraduate engineering curriculum is fundamental to craft responsible engineers and scientists. In response to this need, we have developed a pollution prevention and green chemistry course designed for undergraduate engineering students with no formal background in chemistry. Instead of the option of adding an additional course to a packed curriculum, Industrial Organic Chemistry, a course that is required of all Engineering students, was modified. This course entitled “Green Industrial Organic Chemistry” meets all of the learning objectives for the traditional organic chemistry course for non majors while using the twelve principles of green chemistry as the spine of the course. The students’ understanding of organic chemistry was assessed and compared to other sections taught without the incorporation of the green principles. In addition, understanding of the green chemistry was assessed through both formative and summative assessment tools. Our pedagogy includes the engagement of students in interactive dialog; internet research on the web using such resources as the EPA’s Toxic Release Inventory; engagement of CES software, materials database, to show the application of chemical materials; networking opportunities with industry, government, and academic professionals that are knowledgeable and well-experienced in the field of P2, the twelve principles of green chemistry, and the principles of green engineering. The course and student learning was assessed using formative and summative assessment and compared to other sections that did not incorporate P2 and the twelve principles of green chemistry. Development of this course is supported by the Michigan Pollution Prevention Retired Engineers Technical Assistance Program Internship Program, administered by the Department of Environmental Quality, Environmental Science and Services Division.

### 10. Empowering Student Education in Chemistry with Novel Green Ideas and Tools

*Chandana Mukherjee, Department of Chemistry, Gargi College, University of Delhi, Delhi, India, Malini Rajendran, An NGO Project Roshni, Delhi, India, Poonam Sharma, Department of Zoology, Gargi College, University of Delhi, Delhi, India, and S. Bhanumati, Chemistry Department, Gargi College, University of Delhi, Delhi, India*

Application of renewable feed stock (poultry waste and egg shell) as adsorbent for scavenging mercury from waste water and adsorption studies (Freundlich isotherm) to assess the concentration of metal cation in the effluent using survisometer (a novel tool for measuring surface tension and viscosity) was carried out with great success. The students were inducted to perform and study similar projects to appreciate the theoretical concepts of the phenomenon of adsorptions. The pond water on biosorption responded equally well with the additional result that even the microbes were scavenged successfully. The presentation will project the educational relevance and significance of this valuable aspect of using the cost effective, eco-friendly, and user-friendly green tool while simultaneously enabling the management of waste biomaterials collected from day-to-day life.

### 11. Greener Chemistry in the Automotive Industry: A Collaboration Between Academia and Industry

*Kristi A. Kneas, Department of Chemistry, Elizabethtown College, Elizabethtown College, PA*

Manufacture of electronic components and screen-printing of instrument clusters by automotive manufacturer DENSO MANUFACTURING TENNESSEE, INC. requires washing of equipment such as jigs, screens, and stencils with sizable quantities of organic solvents. Collaborative efforts between the Maryville College Department of Chemistry and DENSO resulted in a reduction in the use of volatile organic compounds and hazardous air pollutants, in accordance with EPA requirements. Necessary research was initiated during an analytical chemistry course when students were introduced by DENSO associates to a pressing research problem. Students performed preliminary experiments and drafted a research proposal that was submitted by the instructor to DENSO. During the summer, funded work was completed under the supervision of the instructor, and recommendations were included in a final report to DENSO. Details of the research problems, experimental approaches developed, results obtained from research conducted at MC and on-site at DENSO, recommendations made, and changes implemented by DENSO will be discussed, as will the nature of the collaboration, the positive impacts of the research on the environment, and the positive outcomes for students and faculty at MC and employees at DENSO.

### 12. The DOE Hydrogen Program: Technology Status and R&D Issues

*Carole Read, Energy Efficiency and Renewable Energy, Office of Hydrogen, Fuel Cells, and Infrastructure Technologies, US Department of Energy, Washington, DC*

The mission of the DOE Hydrogen Program is to reduce petroleum use, greenhouse gas emissions, and air pollution and to contribute to a more diverse and efficient energy infrastructure by enabling the widespread commercialization of hydrogen and fuel cell technologies.

Research supported by the Program has yielded substantial progress in hydrogen production, delivery, storage, and fuel cell technologies. The Program has met its hydrogen cost target of \$3/gas gallon equivalent (gge) for hydrogen produced by distributed natural gas reforming, down from \$5/gge in 2005. While some current fuel cell vehicles have a range exceeding 300 miles, the Program has identified promising materials-based technologies to achieve this range across all vehicle platforms without compromising passenger or cargo space, performance, or cost. In the area of fuel cells, the projected cost for a mass-produced, polymer electrolyte membrane (PEM), automotive fuel cell system has been reduced to \$73/kW from \$275/kW in 2002. Program-funded research has led to improvements in conductivity for high-temperature PEM fuel cell membranes at low relative humidity and to the development of a membrane electrode assembly (MEA) with over 7,300-hour durability.

In addition to a robust R&D effort, the Program facilitates market transformation by validating hydrogen and fuel cell performance in real-world operating conditions, collecting performance data to evaluate and communicate technical progress, and promoting early market demonstration and deployment opportunities.

This talk will give an overview of the DOE Hydrogen Program and highlight the performance status of the key technologies. A synopsis will be provided on the “well-to-wheels” impacts of fuel-cell vehicles versus vehicles on the road today. The speaker will also address continuing R&D issues that are technology barriers to commercial applications for hydrogen storage, renewable hydrogen production, and PEM fuel cell technologies.



### 13. Water Oxidation Using Iridium Catalysts

*Jonathan F. Hull, Chemistry, Yale University, New Haven, CT*

Producing fuel from water using solar power is a viable strategy for a carbon-neutral energy solution. A major obstacle to this strategy is finding robust and active transition metal catalysts that can undergo the 4e/4H<sup>+</sup> steps to oxidize water and produce dioxygen. A highly active and robust Ir catalyst is reported. DFT studies that compliment the experimental data show that the formation of the O-O bond does not require radical oxyl species and is favored by the presence of a  $\pi^*(\text{Ir}=\text{O})$  orbital with oxygen contribution in the LUMO level.

### 14. Hydrogen Storage On Carbonized Chicken Feather Fibers

*Erman Senöz and Richard P. Wool, Chemical Engineering Department, University of Delaware, Newark, DE*

The biggest obstacles to a hydrogen powered energy economy are the production and storage of hydrogen. The Department of Energy's (DOE) 2010 and 2015 hydrogen storage targets are quite challenging in terms of gravimetric capacity (6 wt% and 9 wt% respectively), volumetric capacity (45 and 81 grams H<sub>2</sub> per L), and storage cost (\$4 and \$2 per kWh respectively). In order to solve the H<sub>2</sub> storage problem, various kinds of nano-structured materials have been investigated and produced, none of which could fulfill these targets entirely. Their disposal methods and degradability are still a big question mark. Additionally, the prices of these materials are extremely expensive. It is crucial that the material that will serve as a hydrogen adsorbent in fuel cell vehicles is cheap and is environmentally friendly.

The goal of this project is to develop new low-cost hydrogen storage substrates from a waste material (6 billion lbs/yr in U.S.)-chicken feathers. The results showed that carbonized chicken feathers (CCFF) have the potential to meet the DOE requirements for H<sub>2</sub> storage and are competitive with carbon nanotubes and metal hydrides at a tiny fraction of the cost. When keratin-based chicken feathers are heat-treated by controlled pyrolysis, hollow carbon microtubes are formed with nanoporous walls. Their specific surface area increases up to 450 m<sup>2</sup>/g by the formation of fractals and micropores, thus enabling more hydrogen adsorption than raw (untreated) feather fibers. Experimental hydrogen storage optimization results and surface characterization of CCFF by SEM, XPS, and N<sub>2</sub> adsorption will be demonstrated. Furthermore, recent findings on heat treatment of chicken feather fibers by thermal analysis techniques will be discussed in detail.

### 15. Heterogeneous H<sub>2</sub> Formation Catalyzed by Economical Molecular Coordination Compounds Anchored to High-Surface-Area Metal-Oxide Thin Films

*Shane Ardo, Siah Hong Tan, and Gerald J. Meyer, Department of Chemistry, Johns Hopkins University, Baltimore, MD*

There is general agreement within the scientific community that climate change promoted by anthropogenic greenhouse gases seriously threatens the sustainability of life on Earth. Immediate steps toward worldwide implementation of carbon-neutral power are necessary. The required power input will undoubtedly come from renewable sources; however, the intermittency and locality of most preclude their direct use. By mimicking photosynthesis, an effective solution can be envisioned whereby transient renewable power is transduced into energetic reducing equivalents that are then stored in stable chemical bonds. Whether or not H<sub>2</sub> is the ultimate fuel or an intermediate, there is no mistaking the benefits of its relatively simplistic overall formation reaction. With that being said, efficient carbon-neutral H<sub>2</sub> production often requires bulk platinum catalysts, even though reaction specificity and

optimization are often better achieved via molecular catalysis. In this study, two classes of cobalt-based molecular coordination catalysts are investigated for H<sub>2</sub> production when bound to high-surface-area electrodes capable of storing multiple reducing equivalents. Synthesis of a novel glyoxime-based catalyst from highly abundant tartaric acid was necessary in order to achieve surface binding to nanocrystalline thin films. Overall two-electron reduction to the Co(I) state poises the compounds for controlled, inner-sphere reactivity via a concerted proton-coupled two-electron-transfer mechanism. Towards this end, the Co(I) state of the compounds is accessible at moderate applied potentials, i.e. as favorable as -90 mV vs. NHE. By binding said catalysts to anatase TiO<sub>2</sub>, an additional attribute often results — tunable non-Nernstian redox behavior. Relationships to account for this phenomenon have been developed based on the Gouy-Chapman-Stern model. This feature will be employed to fine-tune the reduction potentials of each catalyst, without demanding synthetic modification, in order to maximize the rate of H<sub>2</sub> production as assessed by spectroscopic chronoamperometry and/or gas chromatography with a thermal-conductivity detector (GC-TCD).

### 16. Copper Oxide Nanoparticles via Flame Spray Pyrolysis for Photoelectrochemical Hydrogen Generation

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Many countries face challenges with respect to energy utilization, specifically reliance on imported and ever costlier sources of fossil energy and thus many are looking towards conversion to a hydrogen-based economy. The potential of zero emissions is another attraction of hydrogen, in particular when coupled with generation using solar energy. In the rush to new solutions, however, it is important to consider the long-term impact of any technology. One class of hydrogen generation materials receiving renewed attention is earth-abundant transition metal oxides, used for photoelectrochemical (PEC) hydrogen generation. These materials are of interest because of their low life-cycle cost as compared to higher efficiency compound semiconductor heterostructures, once raw material costs, manufacturing, lifetime, and disposal considerations are taken into account. Here, a flame spray pyrolysis process is described for preparation of undoped and chromium doped copper oxide (CuO) nanoparticles from copper nitrate and chromium nitrate precursors. Addition of the Cr dopant was expected to increase conductivity of the powder. The particles were crystalline and consisted of aggregates of primary particles with diameter on the order of 20 nm. Particle diameter decreased with increasing amount of dopant. The powders were pressed into pellets, which were used as photoelectrodes in PEC cells, and current voltage characteristics were obtained under dark and illuminated conditions using a 300 W solar simulator. Interestingly, undoped CuO, which has a band gap in the visible light range, was not photoactive, while 5% Cr doped CuO was found to be photoactive. Results of additional characterization and performance testing will be presented with the goal of developing a better understanding of photoactivity in these materials.

## 17. Heterogeneous Catalysis Reactions of Carbon Dioxide

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Though the Fischer-Tropsch (FT) commercial process has been refined extensively since its development in WWII, there is still a need for more favorable and cost-effective methods of synthesizing fuel and other valuable liquid hydrocarbons such as methanol from natural resources such as CO<sub>2</sub>. CO<sub>2</sub> is a greenhouse gas that is readily available in air, seawater, and as a byproduct of many industrial energy producing processes that include gas, oil, and coal power plants and FT processes. One of the many technologies that has been proposed to reduce its impact on global warming is geological sequestration. However, an interesting and attractive alternative would be to recycle the gas into energy-rich molecules. The problem with the use of this abundant resource as a feedstock is its chemical stability. One of the few avenues open for chemical reaction is that with hydrogen. This reaction is not direct, but must be catalytic in nature. This presentation discusses initial efforts to catalytically hydrogenate CO<sub>2</sub> using traditional FT cobalt catalysts and iron-based catalyst. In efforts to improve conversion rates and product selectivity towards higher hydrocarbons, critical parameters such as chemical feedstock ratios (H<sub>2</sub>:CO<sub>2</sub>) and reactor temperatures and pressures, and catalyst composition were evaluated.

## 18. Chlorantraniliprole: Design of Green Chemistry for Insect Control

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The discovery of new pesticides that are highly effective against target pests, work by new modes of action to aid in resistance management, and meet societal demands for safety to humans and the environment, requires a new and different approach than historical processes which have focused primarily on efficacy. In an effort to meet these demands, a redesigned discovery process was developed to focus early optimization on key health and environmental characteristics along with biological efficacy. This talk will focus on the discovery of chlorantraniliprole, which comprised the evaluation of over 2,000 candidate analogs with the redesigned process in search of the optimum balance of pest efficacy, safety, and environmental attributes. Chlorantraniliprole was also found to control insect pests through a new mode-of-action, activation of insect ryanodine receptors (RyRs), with remarkable selectivity for insect over mammalian RyRs. This selectivity is a key attribute of the high safety margins. Known by the trade names Rynaxypyr® and Calteryx™, chlorantraniliprole is one of the least toxic and most active chemical insecticides ever discovered. The chemistry, biology, and site-of-action will be discussed.

## 19. Application of the Concept of Green Chemistry to Pathology Clearing Agents

*A. Moghissi, Regulatory Science, Institute for Regulatory Science, Alexandria, VA; Raymond T. Jones, University of Maryland Baltimore, MD; Susan Breckenridge, Cape Regional Medical Center, Cape May Court House, NJ*

Green chemistry implies that the life cycle of an agent or a process is evaluated and its human health and ecological risks are minimized. In addition, the economics of production, use, and waste disposal must be considered. On occasion it is not possible to perform all of these processes but numerous indicators are used to compare various options to perform a task. A comparative assessment of various options reduces the need for performing life cycle analysis, risk, and cost assessment for each agent or process. This paper uses the latter approach to evaluate three groups of pathology clearing agents:

1. Xylene is an aromatic hydrocarbon regulated by the Environmental Protection Agency (EPA) as hazardous waste primarily because of its flammability. However, xylene also exhibits certain toxic effects.
2. A number of commercial products including AmeriClear use a naturally occurring product (limonene). Limonene has a strong smell (citrus) and at sufficiently high concentrations is an irritant. There are also other potential toxic effects at sufficiently high concentration of Limonene.
3. MicroClear is an isoparaffin hydrocarbon with low vapor pressure. Its ingredients are not covered under hazardous waste regulation.

This paper presents a comparison among these three groups and addresses advantages and disadvantages of each class of these pathology-clearing agents.

## 20. Towards the Development of Green Plasticizers

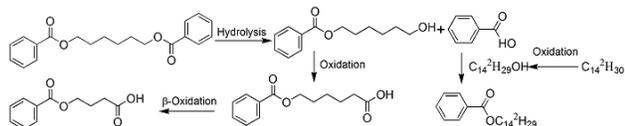
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Widespread use and incomplete biodegradation of plasticizers have led to the presence of these compounds and a number of toxic and stable metabolites in the environment. In order to assess the environmental fate of a potential plasticizer, 1,6-hexanediol dibenzoate, its biodegradation by a common soil microorganism, *Rhodococcus rhodochrous*, was investigated in the presence of hexadecane as a primary carbon source. The following metabolites were detected using GC/MS and FTMS techniques: 1-hexadecyl benzoate, 6-benzoyloxyhexanoic acid, 4-benzoyloxybutanoic acid, 1,6-hexanediol monobenzoate, and benzoic acid.

It is proposed that the formation of 1-hexadecyl benzoate resulted from an enzymatic esterification reaction between the benzoate hydrolyzed from 1,6-hexanediol dibenzoate and hexadecanol, a metabolite of hexadecane. Repetition of the biodegradation experiments using [<sup>2</sup>H<sub>30</sub>]tetradecane as a co-substrate resulted in the formation of 1-[<sup>2</sup>H<sub>29</sub>]tetradecyl benzoate. This confirmed the hypothesis of enzymatic conjugation. The aliphatic chain of all the other metabolites remained intact using [<sup>2</sup>H<sub>30</sub>]tetradecane indicating that these metabolites originated from 1,6-hexanediol dibenzoate (Scheme 1). The metabolism of 1,6-hexanediol dibenzoate is characteristic of hydrolytic, oxidative, and β-oxidative processes. None of these metabolites were persistent as they degraded over the course of the experiment.

Biodegradation of commercial dibenzoate plasticizers, di-ethylene glycol dibenzoate and di-propylene glycol dibenzoate, resulted in

the accumulation of di-ethylene glycol monobenzoate (D(EG)MB) and di-propylene glycol monobenzoate (D(PG)MB), respectively, as a result of incomplete microbial hydrolysis. These two metabolites exhibit significant toxicity. In contrast, metabolism of 1,6-hexanediol dibenzoate does not lead to accumulation of persistent metabolites. The diol fragment of 1,6-hexanediol monobenzoate was processed by a  $\beta$ -oxidation pathway, which was not possible for D(EG)MB and D(PG)MB due to the presence of an ether function in the diols. These results support the consideration of 1,6-hexanediol dibenzoate as a potential green plasticizer.



**Scheme 1.** Biodegradation of 1,6 hexanediol dibenzoate by *Rhodococcus rhodocrous* in the presence of  $[^2\text{H}_{30}]$ Tetradecane as a primary substrate.

## 21. Dissolvine GL: A New, Biodegradable Chelating Agent with an Excellent Safety Profile

*Edwin Bisinger Jr., Regulatory Toxicology, SHERA Americas, Chicago, IL*

Chelates are chemical agents that interact or complex with metal ions, often allowing for increased solubility of the metal ion.

Current chelate substances are based on aminocarboxylic acids (e.g. EDTA) and also on phosphates (tripolyphosphates) and are used in many types of cleaners such as those used in automatic dishwashing (ADW). Unfortunately, because EDTA is not readily biodegradable and because phosphates are known to cause eutrophication in natural waters, the current chelating substances are viewed as environmentally unfriendly.

In response to these concerns, AkzoNobel has developed a readily biodegradable chelating agent that is manufactured principally from a renewable feedstock. This new chelate, tetrasodium L-glutamic acid, N,N-diacetic acid (GLDA), will be replacing phosphates in ADW detergents throughout the United States.

A major advantage of GLDA relates to its demonstrated safety profile. A comprehensive set of toxicity tests reveal that GLDA has excellent safety properties with regard to human health and ecological effects.

GLDA is manufactured from the flavor enhancer monosodium glutamate (MSG). MSG is made from the fermentation of readily available corn sugars and is considered a renewable material. In contrast with the manufacture of EDTA whose carbon content is fossil-based, the carbon source of GLDA is primarily bio-based.

In summary, GLDA is readily biodegradable and will replace phosphates in ADW cleaners in the United States. Moreover, GLDA has an excellent safety profile with respect to both human health and ecological effects.

## 22. Plastics Scorecard: Applying Life Cycle Thinking to Environmental Assessments of Plastics

*Mark Rossi, Clean Production Action, Medford, MA, and Tim Greiner, Pure Strategies, Gloucester, MA*

This paper presents a method, the Plastics Scorecard, for applying life cycle thinking to the evaluation of the environmental preferability of plastic products. Plastic products pose many sustainability challenges across their life cycle. They rely overwhelmingly upon non-renewable resources. They are often

manufactured from hazardous chemicals – including persistent, bioaccumulative, and toxic (PBT) chemicals; carcinogens; endocrine disruptors; and neurotoxicants. Their use may lead to the release of toxic chemicals into homes and offices. They typically contain little to no post-consumer recycled content. And their incineration may lead to the formation of hazardous pollutants like dioxins. Yet, over their entire life cycle, plastics as a class of materials could be significantly more sustainable. Companies, governments, and environmental organizations are in search of an approach that enables them to readily assess the environmental preferability of plastic products. The Plastics Scorecard specifies eight levels on the path to sustainable plastics, moving from “Level 1 - Avoid” to “Level 8 - Prefer.” The criteria for moving from Level 1 - Avoid to each more preferred level are calibrated to progressively increase the sustainability of each stage in a plastics product life cycle: feedstock production, manufacturing, use, and end of life management. The Scorecard develops a set of criteria that simultaneously advances sustainable feedstock practices, green chemistry, and closed loop systems. Overall, Level 8 – the most preferred level – is a challenging level for any plastic product on the market today to attain. That said, it is possible for some plastics to attain Level 8, although it will depend on a number of factors, including agricultural practices, additives, and monomers used and recycling rates. This paper includes the findings of applying the Plastics Scorecard to eight generic polymers: acrylonitrile-butadiene-styrene (ABS), polycarbonate, polyethylene, polyethylene terephthalate (PET), polylactic acid (PLA), polystyrene, and polyvinyl chloride (PVC).

## 23. Collaboration through Green Chemistry Roundtables Can Promote and Commercialize Green Chemistry

*Robert J. Israel, JohnsonDiversey, Inc., David Long, ACS Green Chemistry Institute®, Schubert Pereira, Rug Doctor, Inc., Rob Predale, Johnson & Johnson Consumer Companies, Inc., Herbert Vanderbilt, Bissell Homecare, Inc., Philip G. Sliva, Access Business Group, and Stanley R. Weller, Zep, Inc.*

Green Chemistry Roundtables are one of the newest collaborative partnerships between the ACS Green Chemistry Institute® and industry to promote and commercialize Green Chemistry. The ACS GCI Formulator's Roundtable was developed in 2008 and formally launched in 2009. The mission of the Formulator's Roundtable is to be a driving force in the formulated products industry to use Green Chemistry in creating innovative products that are more sustainable throughout the product life cycle and safer to make and use.

The ACS GCI Formulator's Roundtable has identified strategic priorities to guide the organization's progress. The priorities include:

- Promote transparency and consistency through a set of green chemistry principles for formulated products.
- Drive good science in the development of environmentally preferred products standard/certification.
- Inform and influence suppliers and academia to develop greener alternatives.
- Be recognized leaders in Green Chemistry.
- Incorporate risk-based decision making into green chemistry.

This presentation will summarize the development of the ACS GCI Formulator's Roundtable and provide a status report on 2009 objectives.

## 24. Moving towards Greener Solvents for Pharmaceutical Manufacturing – An Industry Perspective

*Peter J. Dunn, Pfizer, Inc., Sandwich, Kent, United Kingdom, Richard K. Henderson, Cehs, GlaxoSmithKline, Ware, Hertfordshire, United Kingdom, Ingrid Mergelsberg, Chemical and Physical Sciences, Synthetic Chemistry, Schering-Plough, Union, NJ, and Andrew S. Wells, Global Process Research and Development, AstraZeneca, Loughborough, United Kingdom*

The ACS GCI Pharmaceutical Roundtable is a group of 12 pharmaceutical companies and the ACS Green Chemistry Institute® with the objective of promoting Green Chemistry within the pharmaceutical industry. In 2006 and 2008, the group performed some benchmarking exercises where companies submitted blinded data on a number of pharmaceutical processes from all stages of chemical development, from pre-clinical drug candidates to commercial drugs. In 2008, the latest results showed 56% of the waste from these processes was solvents and 32% water. Very similar results were obtained in 2006 and these data reinforce the need for wider use and availability of greener solvents.

The Roundtable companies have identified three critical areas:

1. The need for replacements for chlorinated solvents
2. The need for modified ethers that exhibit low peroxide formation and reasonable flammability
3. Replacements for polar aprotic solvents

Each of these areas will be discussed in detail, looking at the current alternatives and in some cases suggesting some potential alternatives.

## 25. Botanical Drug Products: Sustainable Pharmaceuticals

*Zelleka Getahun, Office of Generic Drugs, CDER / FDA, Rockville, MD*

Can an herbal medicine that is safe and effective be marketed as a Drug Product, with FDA approval? Yes it can. Is market exclusivity granted? Definitely. Can it be patented? Possibly.

It is well known that there are many conventional active pharmaceutical ingredients (APIs) that are based on natural products, either direct isolation, or by semi-synthetic production. Natural product based APIs were either discovered through screening for a targeted biological activity, or were isolated by targeted bioassays, based on knowledge of the therapeutic properties of herbal medicines.

It is also generally accepted that there may be “undiscovered” therapeutic chemical entities in herbal medicines. The technical challenges of natural product chemistry, coupled with absence of pathways to getting market exclusivity, have resulted in lack of any significant interest in what otherwise may have been a promising and sustainable source of drug products.

What is new, and may now bring renewed interest in natural products, is that the FDA has started accepting New Drug Applications (NDAs) for herbal-medicine-based preparations under the category, “Botanical Drug Products” (BDPs), and that the FDA grants market exclusivity for a period certain once a BDP is approved. Moreover, BDPs data requirements are far less complex, compared to requirements for conventional New Chemical Entities (NCE).

The reduced regulatory requirements for BDPs (i.e. in line with the reduced risk associated), and the grant for market exclusivity for BDPs make success in research and development of BDPs feasible. This brings a promise of sustainable and safe production of safe and effective Drug Products (therapeutics and prophylactics).

*Statements and views expressed are those of the author and do not necessarily reflect the policies of the FDA.*

## 26. Working with Suppliers to Manage Total Environmental Footprint of Active Pharmaceutical Ingredient Manufacture

*Cairen R. Hargreaves, Safety, Health and Environment, AstraZeneca, Macclesfield, United Kingdom*

There is generally an increasing level of externalisation within the pharmaceutical industry. The complexity of molecules and therefore synthetic routes means that a number of third parties are involved in the supply chain for launched products. Furthermore, during research and development of new products, process development and/or manufacture of materials may be outsourced.

Since 2005, AstraZeneca have worked with over thirty partner suppliers of intermediates and Active Pharmaceutical Ingredients (APIs) for launched products to understand the external environmental footprint from this outsourced manufacturing activity. In line with our corporate environmental targets for reductions in global warming emissions and amount of waste, data has been collected and reported in these areas to establish a baseline. This will facilitate setting corporate targets for the future and help identify the most significant opportunities for improvement.

AstraZeneca’s SHE (Safety, Health, Environment) Triggers model has been used to drive environmental improvement in the process development of new APIs for a number of years both internally and when working with external partners. A number of recent project case studies demonstrate the prioritisation of improvement actions to ensure effort is focused on the process steps with the greatest environmental impact.

The results of our data collection efforts show that the contribution of external primary manufacture to AstraZeneca’s total environmental footprint is significant and increasing. Pharmaceutical companies can work collaboratively with their supply chain to help achieve a continuous reduction of their environmental footprint.

## 27. The Green Chemistry and Commerce Council

*Ken Geiser, Lowell Center for Sustainable Production, University of Massachusetts Lowell, Lowell, MA*

The Green Chemistry and Commerce Council (GC3) is a project of the Chemicals Policy Initiative at the Lowell Center for Sustainable Production.

The GC3 was formed in 2005 following *Sustainable Business and Safer Chemistry Through the Supply Chain: An Innovators Roundtable* hosted by the Lowell Center for Sustainable Production and the Darden School of Business at the University of Virginia. The GC3 provides an open forum for participants to discuss and share information and experiences relating to advancing green chemistry and design for environment as it pertains to sustainable supply chain management.

The mission of the GC3 is to promote and support green chemistry and the design for environment approach to research and practices nationally and internationally among companies and other governmental and non-governmental entities by:

- Implementing green chemistry, green engineering, and design for environment throughout supply chains and sharing strategies to overcome barriers and reduce environmental footprints;
- Promoting education and information on safer chemicals and products that can increase demand by a broad range of consumers; and
- Identifying existing and needed information on toxics hazards, risks, exposures, and safer alternatives to promote green chemistry as defined in the “12 Principles of Green Chemistry.”



## 28. Feasibility Study for Establishing a Center for Green Innovation & Technology Transfer for the Automotive Industry in Michigan

*Carol Henry<sup>1</sup>, Cindy Reese<sup>2</sup> and Jack Pokryzwa<sup>2</sup>, (1)Chemical Society of Washington, Bethesda, MD, (2)SAE Automotive*

In October 2006, Michigan Governor Jennifer M. Granholm issued an Executive Directive, "Promotion of Green Chemistry for Sustainable Economic Development and Protection of Public Health." Hence, the State of Michigan seeks to garner support and commitments from stakeholders in Michigan to advance green chemistry, green engineering, sustainable chemistry, facilitate research and commercialization of new innovation technology, as well as establish the Michigan Green Chemistry Program as a Model for Green Chemistry Innovation.

SAE Automotive has been awarded a grant from the State of Michigan to develop a workshop devoted to exploring the feasibility of establishing a Center for Green Innovation & Technology Transfer for the automotive industry in Michigan. The importance and difficulty of commercializing new technology cannot be understated, particularly within the automotive community. Attention to the automotive sector as a source and example for green chemistry and green engineering is potentially critical both for the sector itself, the United States, and to the future success of green initiatives.

Focusing on a center for the automotive industry will accelerate the awareness and understanding of green chemistry, green engineering, and green "mobility" products and projects, innovative approaches for new products and processes, standards development in the green arena, as well as identifying new methods for successful technology transfer and sustainable practices. SAE, in partnership with the State of Michigan, is in the process of identifying other partner organizations and a steering committee to guide development of the feasibility study and workshop.

## 29. Incorporating Green Chemistry and Engineering into a Non-Majors Course

*Loyd D. Bastin, Department of Chemistry, Widener University, Chester, PA*

As part of the College of Arts and Science's Values Seminar program, I have designed a course that incorporates Green Chemistry and Engineering into a discussion of environmental pollution. The Values Seminar at Widener University is a capstone experience in our general education program for the Colleges of Arts & Sciences and Engineering. There are a multitude of sections offered each semester on a variety of topics. Students from any discipline within the Arts, Sciences, and Engineering populate the courses. This particular Values Seminar was designed to provide a historical perspective of environmental pollution from a chemist point of view. The course examines the causes, effects, and solutions of environmental pollution. Specifically, we examined the effect of industry on the environment in addition to examining the effect of pollution on communities. The course finishes by examining the steps that society and scientists can take to improve and reverse environmental pollution. Green Chemistry and Engineering is presented as part of the solution. In order to educate the general public and future policy makers, we must incorporate Green Chemistry and Engineering into general education courses. Courses such as the one described here are essential to reach this goal.

## 30. Green Chemistry Education for Chemical Workers

*Paul Renner, Labor Institute, New York, NY*

The Tony Mazzocchi Center for Safety, Health, and Environmental Education (TMC) is working to integrate Green Chemistry education into chemical worker health and safety training programs. TMC is a partnership between the Labor Institute, a non-profit educational institute, and the United Steel Workers union (USW), the largest industrial union in the country. The USW encompasses oil refineries, chemical plants, DOE nuclear weapons sites, paper mills, steel mills, and rubber manufacturers, a non-exhaustive list. Chemical workers may not have a formal education in chemistry but nevertheless they have a stake in the future of Green Chemistry. The goal of the training programs is to provide workers with the scientific background they need to advocate for Green Chemistry in workplaces and communities. The TMC provides thousands of hours of education to workers each year on a variety of health and safety and environmental topics. The Labor Institute has been developing these materials and training workers to deliver them for over thirty years. In collaboration with the Center for Green Chemistry and Green Engineering at Yale University, we have developed a course which introduces workers to the Twelve Principles of Green Chemistry. This course has been presented to workers in California, New Jersey, Texas, and Pennsylvania. TMC hopes these efforts will grow and multiply those who are knowledgeable of Green Chemistry in the chemical industry sector. Expanding and reinforcing the community awareness of, and education about, Green Chemistry will create a better environment for innovative research, healthier workplaces, and safer communities.

## 31. Business Education and GC/GE

*Andrea Larson, Darden Graduate School of Business, Charlottesville, VA*

Abstract—Between 2006 and 2008 cleantech discussion in business moved from the margins to center stage. Today business and political leaders talk about "green" technology as the foundation of the next wave of economic growth. This is not a fad, nor is it an "environmental" agenda item typical of the last 30 years in the United States. Characterized by concerns for national security, resource scarcity, ecological system carrying capacity, pollution levels, and human health, this shift is fundamental. Corporate senior management teams feel the pressure directly from energy price volatility, climate change impacts and associated fiduciary responsibility, and growing buyer demands for safe products. Life cycle assessment of products, efforts to reduce and eliminate hazardous materials in processes and products, and clean supply chain management approaches have become common. Required corporate reporting on social, ecological, and sustainability topics and risks has created more pressure on firms for transparency and accountability, in turn driving investment in "cleaner" operations and strategies. Companies have discovered that eco-efficiency measures reduce costs; the next phase is sustainability innovation in which green design advances create market differentiation and competitive advantage at the same time that performance improves across community, ecological, and health indicators. As companies pay more attention to green and clean solutions for a wide range of challenges, Green Chemistry (GC) and Green Engineering (GE) have become essential tools. For MBA students, awareness of GC and GE is equally essential because these students are future business leaders. They must be educated to lead in a very different future than the industrial revolution that has taken us to this point. This presentation discusses pioneering efforts to develop strategies, curriculum materials, and innovative courses that bridge silos across schools, academic disciplines, and business functional areas to incorporate GC and GE.

### 32. Science Education and Civic Engagement

*Richard D. Sheardy, Cynthia Maguire, and Jennifer DaRosa, Chemistry and Physics, Texas Woman's University, Denton, TX*

Science Education for New Civic Engagements and Responsibilities (SENCER) is a relatively new instructional approach now used at over 330 high schools, colleges, and universities from the US and 13 other countries ([www.sencenr.net](http://www.sencenr.net)). SENCER is a program funded by the National Science Foundation dedicated to improving science education at all levels by: 1) engaging students in science learning through connection with real world issues; 2) supporting the development of science courses (for both science majors and non-science majors) that have a civic engagement component; and 3) providing a platform for student assessment of learning gains. The distinguishing characteristic of this pedagogy is the use of complex, capacious topics of civic importance to lend value to students' acquisition of new science knowledge. Since the fall of 2007, faculty in the Department of Chemistry and Physics at Texas Woman's University have implemented two SENCER courses which cover important science content and have meaningful civic engagement components. These courses are Introduction to Environmental Chemistry, and Climate Change. Students in these courses have shown remarkable comprehension and retention of basic chemical principles when presented in context with social issues they already consider significant. We are now expanding the use of SENCER ideals into courses for both majors and non-majors as a result of our previous success, and developing a minor in Science and Civic Engagement. This presentation will discuss the SENCER approach, how to develop SENCER courses and examples from around the country of SENCER courses which link science to important social issues ranging from renewable environments to nanotechnology to the biomedical issues of HIV/AIDS.

### 33. Green Chemistry at Wilkes University

*R. Gregory Peters and Terri Wignot, Department of Chemistry, Wilkes University, Wilkes-Barre, PA*

The Department of Chemistry at Wilkes University recently established an innovative degree track for its students, a Bachelor's degree in Chemistry with a concentration in Sustainability. The framework for this degree was built upon the ideas outlined in the new ACS Committee on Professional Training (CPT) guidelines and involves a cross-disciplinary overlap with our Earth and Environmental Sciences Department. This talk will outline the degree track, the rationale behind the course selections, and the efforts of our department to incorporate Green Chemistry into our curriculum.

### 34. Green Chemistry Education: Facilitating Transition to Green Technologies and Processes in India

*R.K. Sharma, Green Chemistry Network Centre, Department of Chemistry, University of Delhi, Delhi, India*

The Green Chemistry Network Centre (GCNC) established at Delhi University with the support of IUPAC CHEMRAWN DEN Grant is working for the development and implementation of Green Technologies in India. This presentation will highlight the following activities of the centre:

- *A Real World Case of Green Chemistry in Indian Pharmaceutical Industry:* Development and implementation of Green Technology was exercised through GCNC.
- *Introducing Green Technologies in Metal Handicraft Industry:* A major Project was awarded to GCNC by Ministry of Textiles, Government of India, to pursue this.

- *Reclaiming the wasteland and chromium created by tanning industry:* GCNC successfully completed a project awarded by Department of Biotechnology; Government of India, for developing this technology.

In addition to this, GCNC is designing and organizing various International and National Green Chemistry Workshops and other activities in India for the incorporation of Green Chemistry and engineering into laboratories of educational and research institutes and industries. Various ongoing activities of GCNC (including forthcoming event of Indo-US Workshop on Industrial Chemistry) are discussed.

### 35. Achieving Synthetic Efficiency through New Method Development

*Jeff Song, Chemical Development, Boehringer Ingelheim Pharmaceuticals, Inc., Ridgefield, CT*

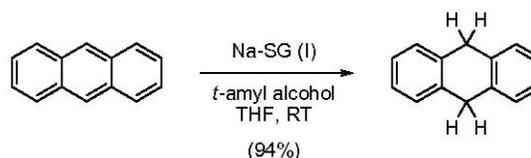
We present an in-depth analysis of several projects from our recent programs to highlight the green chemistry commitment and accomplishments at Boehringer Ingelheim Pharmaceuticals. In all cases, dramatic reductions in E-factors were achieved, mainly by shortening the synthetic routes and by implementing newly developed synthetic methodologies.

### 36. Ammonia-Free Birch Reductions Using Stabilized Sodium In Silica Gel for Safer, More Sustainable Synthesis

*Michael J. Costanzo, Michael Lefenfeld, Mitul N. Patel, Kathryn A. Petersen, and Paul F. Vogt, Process Development Services, SiGNa Chemistry, Inc., Monmouth Junction, NJ*

The Birch reduction of aromatic compounds by alkali metals in liquid ammonia is a synthetically powerful and versatile method that has been in use since its discovery in 1937. It is one of only a few methods that can readily convert aromatic synthons into alicyclic structures. Consequently, the Birch reduction has been widely used in the synthesis of drugs and complex natural products. Despite its great utility, the classic Birch reduction has several undesirable attributes that have limited its use, particularly on a large scale. Primary among these are safety concerns associated with the high toxicity of liquid ammonia, the hazards of cryogenic temperatures, and the dangers of handling of metallic alkali metals.

SiGNa Chemistry, Inc. has discovered and developed proprietary technology for encapsulating alkali metals into nano-structured porous oxides, such as silica gel and alumina. Encapsulation reduces the dangers associated with the handling of alkali metals while retaining the reducing power of the metal. Sodium and sodium-potassium alloys in silica gel (Na-SG, Na<sub>2</sub>K-SG, and K<sub>2</sub>Na-SG) are free-flowing solids that have demonstrated applications in Bouveault-Blanc ester reductions, desulfurizations, and the desulfonylation of secondary amines. This presentation will describe the extension of this technology to the Birch reduction using stabilized sodium in silica gel, Na-SG(I), in place of metallic sodium. The new procedure reduces the danger associated with the handling of metallic sodium and eliminates the risks inherent with liquid ammonia and cryogenic temperatures.





# Abstracts continued

## 37. Recycle Solutions Reduce E-Factor for Pharma Intermediate by 90%

*Nitesh Mehta, Bhadresh Padia, Anand Hunoor, and Hari Ramsubramani, Newreka GreenSynth Technologies, Skillman, NJ*

The paper summarizes the superior economic and environmental performance of a Green Chemistry-based process technology called Newreka Recycle Solutions (NRS) that was recently commercialized to replace a traditional synthetic chemistry-based process. The authors illustrate the application of NRS to four reaction steps in the industrial manufacture of an API intermediate, and share insights on how Green Chemistry and Engineering principles were used to re-engineer traditional processes. The authors of the work are principals at Newreka GreenSynth Technologies, a process technology company with exclusive focus on Green Chemistry and Engineering. The NRS technology outlined herein was awarded the Indo-US Green Chemistry Award for 2008, presented by the Green Chemistry Network Center of India (an affiliate of the ACS-GCI).

NRS technology was successfully applied to four reaction steps in the manufacture of an API involving Diazotization-Hydrolysis, Nitration, Chlorination, and Reduction. NRS technology resulted in the reduction of the combined E-Factor for these steps, from 175 to 17. This improvement in E-Factor (which is defined as the lbs of input materials needed to produce one lb of desired product) represents a 90% reduction in byproducts and a 10x improvement in selectivity. This dramatically superior environmental performance was also accompanied by better economic performance: input costs were lowered by 40%. The strategic business benefits of improved economic and environmental performance were accompanied by several process benefits including: elimination of certain solvents and replacement of others, decreased consumption of fresh water, improved selectivity and conversion to desired product and recycle of aqueous effluent streams. If time permits, the authors will discuss the structured process by which Green Chemistry principles and ideas were used to create NRS technology, including benchmarking process conditions and their impact on selectivity followed by examples of physical and chemical interventions.

## 38. The New Center for Green Chemistry at the University of California, Berkeley: Integrating Approaches

*Michael P. Wilson, School of Public Health, University of California, Berkeley, Berkeley, CA*

The University of California, Berkeley, established a new Center on Green Chemistry, under the aegis of the campus-wide Institute of the Environment. Unique in the United States, the Center is a multidisciplinary unit with participation and faculty involvement from the College of Chemistry, School of Public Health, College of Natural Resources, School of Law, and School of Business. It will conduct research, teaching, and engagement activities in three overlapping spheres: New Chemistries, Health and Environment, and Society and Policy, as they pertain to green chemistry. This presentation will describe the intellectual and institutional development of the Center and its activities to date.

## 39. Green Chemistry In Chinese Higher Education

*Kira JM Matus, Kennedy School of Government, Harvard University, Mclean, VA*

Over the past decade, green chemistry and engineering in China have been growing at an impressive pace. This presentation will look at the position of green chemistry and engineering in the Chinese system of higher education, based on recent visits to a dozen universities and research centers around China. One area of

interest is methods of integrating green chemistry and engineering into the curriculum, including the availability of green chemistry and engineering specific degree programs, and other aspects of green chemistry in the classroom setting. In addition, this presentation will give an overview of academic green chemistry and engineering research. This includes the relationship between academia and industry, and the implications for students at the graduate level.

## 40. Worcester State College: Towards a Green Chemistry Center

*Meghna Dilip, Margaret E. Kerr, and Eihab Jaber, Department of Chemistry, Worcester State College, Worcester, MA*

The chemistry department at Worcester State College in Worcester, Massachusetts, has always been committed to green chemistry. Early successes include the introduction of organic labs with a "green" focus. Recently, with the award of a green chemistry grant, and the hiring of a new faculty member, our green chemistry portfolio is on the rise.

We will report on our efforts in green chemistry via course offerings which include incorporation of green chemistry topics in our environmental chemistry course, a special topics course in green chemistry, and a course proposal submission for a stand-alone green chemistry course. Our faculty members are actively involved in several independent research projects involving undergraduate students with a focus on green chemistry education. A team-taught course dedicated to research has also been proposed with a view to promote inter-area green research. We will also highlight college-wide sustainability efforts.

However, we believe there is a long way to go. We will review the perception of green chemistry among students and their active participation. We will present a five year plan for proposed green chemistry efforts at Worcester State with a view towards starting a green chemistry center on campus.

## 41. Connecting Green Chemistry to the 'TEM' In the K-12 STEM Curriculum

*Rachel Pokrandt, Beyond Benign, Woburn, MA*

Beyond Benign staff will share elements of their new Green Math and Engineering Curricula made possible through program development funding from the Pfizer Foundation. The curriculum units written for the middle and high school classrooms weave concepts of Green Chemistry and sustainability into required content areas with an emphasis on Technology, Mathematics, and Engineering; connecting chemistry to real-world applications; and sustainable life and business models.

## 42. Promoting Green Chemistry Education through Short-Term Courses

*Anju Srivastava and Reena Jain, Green Chemistry Network Centre, Department of Chemistry, University of Delhi, Delhi, India*

The conceptual framework, called Green Chemistry provides exciting opportunities for the chemist community to address the educational and research challenges of sustainability. Students, from schools to Universities, are our next generation scientists who need to be trained in the methodologies, techniques, and principles that take us on the road to sustainability. They should be aware of Green Chemistry and made to practice Green Chemistry, so as to realize that the future does not need to be as bleak as it is portrayed in the world-wide media; that Green Chemistry is something where students really can be a part of the solution rather than part of the overall problem. No doubt, Symposia, Conferences, and Workshops on Green Chemistry, organized on a

regular basis, actively contribute in spreading education and awareness. However, incorporation of the principles of Green Chemistry in the curriculum not only enables a quicker and more effective adoption of changes but also a better understanding. While the integration of Green Chemistry into existing courses without adding to an already over-crowded curriculum is going on, the students can be equipped with strategies and tools of Green Chemistry from short duration courses. We have designed and launched one such state-of-the-art short-term Course on Green Chemistry in the Department of Chemistry at Hindu College, University of Delhi. The course provides participants with an understanding of the principles of sustainability and Green Chemistry. The course comprises of class room lectures, supplemented with laboratory exercises along with real-world case studies, and concludes with assessments and presentations by the students. The course, running successfully for the second consecutive year, has witnessed an interdisciplinary heterogeneous group of students, willing to be homogenized for a greener, healthier, and a sustainable tomorrow.

### 43. Recent Educational Activities by the ACS Green Chemistry Institute®

*Jennifer L. Young, ACS Green Chemistry Institute®, Washington, DC*

The ACS Green Chemistry Institute® (ACS GCI) has partnered with the Education Division at the American Chemical Society (ACS) as well as with green chemistry educators recently to develop several new educational books and case studies. In addition, ACS and ACS GCI have jointly offered a summer school on green chemistry annually since 2003. The summer school, typically a 1-2 week long program of lectures, laboratory experiments, and discussions, has trained over 300 students (graduate students and post-doctoral fellows) studying in the US, Canada, and South America. A recent survey of past participants accessed the impact that the green chemistry summer school has had on their career paths and provides some interesting insights into the directions the students have taken. This presentation will highlight these recent educational activities.

### 44. Non-Acidic Electrochemical Polishing of Some Metals

*Tarek M. Abdel-Fattah, Department of Biology, Chemistry and Environmental Science, Christopher Newport University, Newport News, VA*

In this study, we adapted acid-free electropolishing (AFEP) method for many different metal's surfaces, to eliminate the need for the (~800°C) hydrogen removal and improve the biocompatibility of the surfaces and the ability for surface modifications. We replaced the dangerous acidic mixture simply by using a green material such as vitamin B<sub>4</sub> (2-hydroxyethyl-trimethylammonium) chloride as a medium for the electrochemical process. Quantitative results were produced by using atomic force microscopy (AFM), high-resolution optical microscopy, scanning electron microscopy (SEM), and chronoamperometry for green processed samples and compared with as received samples. The data showed the AFEP method capable of producing very smooth surfaces with average surface roughness below 10 nm.

### 45. RegenSi™: Low Carbon Footprint Alternative Wafer Reclaim Solution for Extending Life Cycle of Silicon Test Wafers

*Michael B. Korzenski and Ping Jiang, Advanced Technology Development, Advanced Technology Materials, Inc., Danbury, CT*

Semiconductor manufacturers typically use test wafers to optimize and monitor their manufacturing processes. A large lab might spend \$2 million/month on test wafers, which cost >\$100 each. Because of the large volumes of test wafers used, silicon remains by

far the greatest material expense in semiconductor manufacturing labs. More than 27 million test wafers are used annually across the industry, and as a result, chip makers are now focusing on extending the usable life of test wafers by attempting to re-use them as many times as possible through a reclaim process.

A wafer reclamation process involves three steps: chemically stripping unwanted films from the wafer surface, mechanically polishing to remove any surface damage, and cleaning to ensure that customers' ultra low defect requirements can be met. Currently, the number of times a wafer may be reclaimed is limited, as the combination of strip and polish steps physically reduces the thickness of the substrate by tens of microns. Eventually, the test wafers become too thin to be reclaimed and are then scrapped and replaced. Therefore, the need for a cost effective method of efficiently reclaiming test wafers is highly desired.

RegenSi™ is a novel all-wet single step process used to strip away most films from the test wafer while limiting damage to the underlying silicon, thus eliminating or reducing the need for wafer surface planarization following the film stripping step, which is both energy intensive, uses high volume of consumables, and is expensive. After implementing RegenSi for internal processing of test wafers, a Taiwanese manufacturer reported that yields rose to 85% and silicon loss was reduced by 75%, enabling them to achieve four times more life from each test wafer. This combination of higher yields, greater productivity, and increased re-use leads to significant overall cost savings, energy savings, and waste reduction.

### 46. Nonisocyanate Polyurethanes: Alternative Nontoxic Process of Polyurethane Coatings Manufacturing

*Oleg L. Figovsky, Leonid D. Shapovalov, Olga V. Birukov, and Dmitry A. Beilin, Polymate, Ltd., International Nanotechnology Research Center, Migdal-HaEmek, Israel*

A recent development in the nonisocyanate process of polyurethane manufacturing results in a better and safer health working environment and expands a field of PU application. The nonisocyanate PU chain is formed as a result of the reaction between oligomeric cyclocarbonates and primary aliphatic amines. The new environment-friendly two-parts product is called Hybrid Nonisocyanate Polyurethane (HNIPU). It is the first-ever chemical platform based on the modified hybrid polyurethane patented concept and processes that allow production of PU using methods which completely eliminate the use of toxic isocyanates resulting in a commercially available substitute for conventional PU. This results in a product that is less toxic than conventional PU, has superior properties, and costs up to 20% less to produce and apply. HNIPU have been developed to the commercial level and can be used as paints, varnishes, adhesives, caulking compounds, flooring/ industrial coatings, rigid foams, and composite materials. HNIPU has unique properties that combine the best mechanical properties of PU and chemical resistance of epoxy binders:

- Absence of harmful and toxic components;
- Absence of sanitizing and irritation effects;
- High durability;
- High moisture resistance and high chemical resistance;
- High adhesion of the coating to any bases;
- High impact and tension strength;
- High wear resistance;
- Hygiene and simplicity of cleaning.



# Abstracts continued

## 47. Water-Based Refractory Coatings with Wet/Dry Color Change Indication

Jörg Kroker, Flavia Duncan, and Lee Horvath, *Casting Solutions, Ashland Performance Materials, Dublin, OH*

The use of refractory coatings in metal casting processes has been common practice in the foundry industry for decades. These coatings are applied to dies, cores, and molds to provide a protective barrier facing the hot liquid metal. When applied to sand cores and molds, refractory coatings prevent casting defects like metal penetration and erosion, improve veining resistance and casting surface finish, or can be used simply to mitigate imperfections resulting from molding media and processes. Traditionally, organic solvent-based refractory coatings have been widely preferred. Drying of these coatings would be accomplished by “torching” the coated substrate. However, workplace environmental, health, and safety concerns, as well as economic considerations stemming from the rapidly increasing costs of petrochemical and bio-based solvents (“fossil fuel alternatives”), continue to spawn the development and use of water-based coating technologies. Ashland Performance Materials has developed a water-based refractory coating technology which features a distinctive color change as the coating dries and transitions from the wet to the dry state. To avoid casting defects resulting from residual moisture at the mold/metal interface that could be expensive to repair or may even require scrapping of the casting, it is necessary to accomplish complete drying of the coating layer to control blows, gas and slag entrapment, porosity, and rough surface finish. Further, optimum drying is critical, as excessive drying wastes energy and may reduce productivity. This technology was successfully introduced to the industry in 2005 and is now widely accepted among metal casters. Typical cost savings are in the 10%+ range, including a 50% reduction in fuel usage from the heaters used to dry coated substrates – an advantage gained simply by the ability to visually determine the coating is dry. The savings are in addition to any reworking cost as a result of coating moisture-related casting defects.

## 48. Novel Biobased Technologies for Coatings Applications

Madhukar (Duke) Rao, *Polymers & Materials Technology, The Sherwin Williams Company, Cleveland, OH*

The tightening VOC regulations, erratic price swings of petroleum derived materials, and a desire in the market for green products is creating challenges and opportunities for coatings companies. Today latex emulsions and various dispersions dominate the waterborne coatings; whereas the solvent-borne coating is dominated by alkyds, various copolymers, polyurethanes, and epoxies. The lower VOC limits enforced by EPA are forcing coatings formulators to seek VOC compliant technologies which meet the performance criteria of currently performing non-compliant technologies.

The talk will briefly cover two novel approaches in polymer technologies developed at The Sherwin Williams Company for low VOC coatings applications.

The first approach was developing a low VOC hybrid dispersion by utilizing the concept of sustainability and green to impart value while meeting performance at low VOCs for Architectural/IM applications. Recycled polyester and a renewable resource material like soy bean oil were used to create the hybrid polymer technology. This can be processed and formulated into value-added VOC compliant performance coating.

The second approach was to develop a high solids vegetable oil-based polyester – this hyperbranched ester was further modified into a solventless high solids hyperbranched ester hybrid. This

renewable resource base was processed and formulated into a low VOC solvent-borne coating.

## 49. Celgard Solvent-Free Microporous Film Technology

Lie Shi and Jill Watson, *Celgard LLC, Charlotte, NC*

Celgard LLC manufactures polypropylene and polyethylene microporous separator membranes using an inventive environmentally friendly solvent-free “Dry stretch” technology, which is unique to the lithium-ion battery separator industry. Competitive separators are made using a wet process, which requires the use of a hydrocarbon solvent / mineral oil plasticizer system to first make a gel-like sheet followed by removal of the plasticizer and solvent to create the microporous structure.

Celgard “Dry stretch” solvent-free technology has the benefit of producing better microporous separators with a reduced environmental footprint and much lower environmental impact when compared to the traditional wet process separators.

The separator is a highly technical component in a battery and functions to prevent contact between the battery electrodes. It serves as an electrolyte reservoir enabling ion flow between the electrodes and in addition, provides a thermal shutdown safety feature. Celgard® separators are widely used in lithium-ion battery applications such as notebook PCs, cell phones, digital cameras, and power tools.

Celgard® dry stretched separators are regarded as enabling technology for energy storage systems in hybrid electric vehicles (HEV) and Plug-in electric vehicles (PHEV) because they provide four key battery performance requirements: 1) high rate capability, 2) high temperature stability, 3) longer battery cycle life, and 4) cost competitiveness. Celgard® separators have the potential to be a ‘win-win’ product for the environment – they are produced using an environmentally friendly manufacturing process and they are a strong candidate for a promising future as the separator of choice for green vehicles.

## KEYNOTE ADDRESS

### 50. P&G’s Environmental Sustainability Journey

Len Sauers, *Vice President, Global Sustainability, The Procter & Gamble Company, Cincinnati, OH*

Abstract not available

### 51. Green Assessment of Chemical Methods

Douglas Raynie and Julee Driver, *Department of Chemistry and Biochemistry, South Dakota State University, Brookings, SD*

A new means for assessing chemical methods relative to green chemistry attributes has been developed in our laboratory. The assessment categorizes risk potential into five categories – health, safety, environmental, energy, and waste – based on toxicity, bioaccumulation, reactivity, waste generation, corrosivity, safety, energy consumption, and related factors. Chemical methods receive a 1-3 score for each attribute using readily available chemical data. The visual presentation of the assessment tool allows individual researchers to make their own value judgments about conflicting green criteria. For example, if a method develops little waste, but the waste is highly toxic, individual flexibility is allowed to compare the method relative to another that generates large quantities of less hazardous waste. Hence, this assessment tool is most valuable in comparing procedures. After discussing the assessment tool, we will present a comparison to similar assessment tools and use the assessment to compare five regulatory methods for the analysis of polycyclic aromatic hydrocarbons in water.

## 52. The Way of Greening Analytical Chemistry

*Mihkel Koel and Mihkel Kaljurand, Institute of Chemistry, Tallinn University of Technology, Tallinn, Estonia*

The first principle of green chemistry – prevention of waste generation – induces the researchers to think about analytical chemistry in info-technological terms to find a strategic approach to its greenness.

An analytical measurement is the presentation of knowledge about the chemical system that can be transferred, interpreted, and processed. The molecule is a source (carrier) of information, and the use of analytical instrumentation or a particular method is the procedure to extract and present this information – an analytical signal – in the precise, most selective and economical way. It is quite clear that the target of analytical chemistry is to get accurate and unambiguous signals directly from the place where something important for a chemist is taking place – be it in the bulk or surface, solid, liquid, or gas.

The greenness of the procedure of extraction of this signal defines that of the analytical method as well. At the same time, it means that one must pay attention to preventing the generation of waste and pollution, using safer solvents, economizing on energy, and using non-hazardous chemicals and processes with the aim to minimizing the risk of accidents. From this point of view the most rational way is down-scaling methods with the use of non-destructive detections. In this presentation possible trends towards green analytical chemistry based on the latter approach, particularly on the miniaturization of sample preparation/separation and application of spectroscopic methods, use of chemometrics, and QSPR methods will be discussed.

## 53. Green Analytical Chemistry

*Ellen R. Campbell and Wilbur H Campbell, NECi: The Nitrate Elimination Company, Inc, LAKE Linden, MI*

Environmental protection requires chemistry. In particular, it requires analytical chemistry. And analytical chemistry involves the use of many reagents and solvents that are inimical to environmental quality and human health. It seems ironic and unfair that the people most closely associated with environmental monitoring and health need to compromise the health of their own environment in order to understand the processes going on around them.

Biotechnology has a role in the future of environmental protection. Chemistry requires harsh environments because energy is required to affect most reactions. Catalysts reduce this activation energy to conditions more in tune to the standard environment (STP). Enzymes are protein catalysts that biological systems use to accomplish the complex chemical reactions that metabolism requires. For most chemical reactions, there is an enzyme that can make it happen efficiently at low energy. NECi is dedicated to the application of enzyme systems to the solution of environmental challenges, especially wet chemical analytical methods. Current focus is on analysis of nitrate.

We have developed two forms of recombinant nitrate reductase (NaR), an enzyme in plants and some microbes that reduces nitrate to nitrite. The enzymes are produced in the *Pichia pastoris* protein expression system by fermentation under tightly controlled conditions, which means that quality is as stable as for any reagent grade chemical. Enzymatic reactions have great specificity and selectivity, as well as being efficient and rapid. NaR reduces nitrate to nitrite in any aqueous solution, from tissue culture media to agricultural runoff to seawater. The resulting nitrite is determined by standard Griess reagent chemistry. The reaction is irreversible and runs to completion (approaching 100% reduction).

NECi has formulated nitrate test kits in many formats. Development of the reagents and methods has been funded by the Small Business Innovation Research (SBIR) programs of NIH and the USDA.

## 54. Extraction Methods That Focus On Green Chemistry

*Fulgentius N. Lugenwa and Eric J. Lawrence, Chemistry, Pennsylvania State University - York Campus, York, PA*

Extractions to isolate natural products from animal and plant materials employ chlorinated and other toxic organic solvents. In order to limit the amount of toxic waste generated in those processes, extractions that minimize toxic solvents have been developed. A mixture of water, ethanol, and ethyl acetate was used at room temperature to extract betulin and betulinic acid from the bark of white birch (*Betula papyrifera*). Using water:ethanol:ethyl acetate mixture (10:45:45, v/v), betulin (13%) was isolated after purification. The same amount of betulin was obtained by extraction using hot toluene. When the aqueous mixture was used to isolate carnosic acid from Rosemary (*Rosemarinus officinalis*), the amount of product obtained was equal or greater than the amount obtained by using either acetone or acetonitrile.

## 55. Thermodynamic Evaluation of the Greenness of Supercritical Fluid Chromatography In the Pharmaceutical Industry

*Geert Van der Vorst<sup>1</sup>, Herman Van Langenhove<sup>1</sup>, Frederik De Paep<sup>1</sup>, Wim Aelterman<sup>2</sup>, Jules Dingenen<sup>2</sup> and Jo Dewulf<sup>1</sup>, (1)Environmental Organic Chemistry, Ghent University, Ghent, Belgium, (2)Johnson & Johnson PRD, Janssen Pharmaceutica, Beerse, Belgium*

In the fine chemical and pharmaceutical industry, preparative supercritical fluid chromatography (Prep-SFC) is often considered a green alternative for Preparative HPLC (Prep-HPLC). However a thorough quantitative assessment of the “greenness” is missing. Taking into account mass and energy requirements at different system boundary levels, Prep-HPLC and Prep-SFC were compared and evaluated for their integral resource consumption. This evaluation was performed on a specific enantiomeric separation from the pharmaceutical company Janssen Pharmaceutica, part of Johnson & Johnson. Based on thermodynamics and exergy analysis, it could be concluded that, when evaluated on a process level, Prep-HPLC requires 26% more resources than the Prep-SFC separation due to its inherent higher use of organic solvents. However, when evaluated on a larger system boundary and quantifying the Cumulative Exergy Extracted from the Natural Environment (CEENE) to deliver all mass and energy flows to the process level system boundary via the overall industrial metabolism, it becomes clear that Prep-SFC requires 34% more resources than Prep-HPLC. The poor score of Prep-SFC in the life cycle approach is partially attributed to the high resource requirements related to the production of liquid carbon dioxide. It can be concluded that for this case, the most sustainable process as for the integral resource consumption is Prep-HPLC. This study also illustrates the possibility and advantages of quantifying both energy and material resource intake for industrial processes. Exergy analysis is here the unique scientifically sound tool that enables to quantify all kinds of resources and products on the same scale and to take into account all the resources for a proper evaluation.

### Acknowledgement

The authors acknowledge the financial support of the Institute for the Promotion of Innovation through Science and Technology in Flanders.



## 56. Sustainable Natural Green Chemistry (NGC) for Cooling Water Treatment

*Dan A. Duke, Water Conservation Technology International, Inc., Temecula, CA*

A natural green chemistry provides a paradigm shift in cooling water treatment, with economical methods to attain source reduction of toxic and persistent chemicals, reduce water and energy use, and support sustainable water ecosystems. Cooling towers evaporate pure water to the atmosphere, but natural minerals in water are concentrated and typically require 20-40% tower discharge to avoid energy-consuming scale or corrosion problems. Chemicals are used to reduce scale and corrosion problems, but low solubility and corrosive minerals still primarily dictate water wastage rates. Towers discharge treatment chemicals that often use inorganic or organic phosphates, heavy metals and organic polymers that are persistent, bioaccumulative, or toxic in the environment along with organic biocides and halogens used to control biological fouling. Biocides are toxic to humans and aquatic life, and also form absorbable organic halides (AOX) and organic derivatives that are toxic, persistent, and bioaccumulative. Approximately 75 million pounds of organic biocides and larger quantities of halogens are discharged annually in the US.

Patented natural green chemistry (NGC) methods use the natural minerals present in water as sustainable feedstock and provides superior corrosion and scale protection that replaces treatment chemicals. NGC permits tower operation with zero discharge, reducing water wastage by 95% and to less than 2% of makeup. NGC permits minerals to concentrate to facilitate natural biostatic chemistry in tower water for 95% or greater reduction in biocide use. NGC chemical replacement and discharge reduction can eliminate US annual discharge of over 400 million pounds of organic and toxic chemicals. US potential for fresh water use reduction with NGC is estimated at 500 billion gallons per year, with over \$1.5 billion in annual incentive to cooling tower operators from reduced water, chemical and energy costs. NGC is equally effective when using recycled waste waters to further reduce fresh water use.

## 57. The Development of Green Corrosion Inhibitors

*Andrea Hansen, Margarita Kharshan, and Alla Furman, Cortec Corporation, St. Paul, MN*

Historically, corrosion inhibitors based on petroleum, calcium nitrate, borate, chromate, or nitrite have been used to prolong the life of metal used in processing systems, metal working operations, water treatment, storage, and reinforced structures. However, tighter environmental regulations continue to put pressure on these old methods and invite green chemistry improvements.

The creation of new Vapor phase Corrosion Inhibitor (VpCI) and Migratory Corrosion Inhibitor (MCI) technologies gives renewable, bio-based products providing a biodegradable, environmentally safe alternative while offering comparable performance and costs

Green chemistry is a process of improvements, wherein the environment is considered along with the chemistry. Green corrosion inhibitors are designed to function effectively, while reducing the impact on the environment by breaking down into innocuous degradation products after use. Different approaches have been used to obtain a required or improved environmental profile:

1. Replacement of solvent- or oil-based carriers in formulations with water-based technology.
2. Replacement of petroleum-based carriers with the solvents, manufactured from renewable resource.
3. The use of biodegradable materials as corrosion inhibitors.

This paper will discuss the different approaches used to obtain the VpCI and MCI chemicals that have been used to replace historical corrosion inhibitors.

## 58. A New Cooling Water Treatment Strategy Significantly Reducing Chemical and Water Usage

*Henry A. Becker, Jon J. Cohen, and Thomas F. Hutchison, R & D, H-O-H Water Technology, Inc, Palatine, IL*

Every year in the United States great quantities of sulfuric acid, phosphorous containing organic compounds, and halogens are used to control calcium carbonate scale and sludge formation in evaporative cooling water systems. The goal of chemical-based strategies is to keep as close as possible to 100% of calcium present in cooling tower make-up in stable or meta-stable solution insuring its transport and removal via bleedoff. Bleedoff is absolutely necessary as it is the only calcium withdrawal sink present.

The amount of bleedoff is dictated by make-up water chemistry, decision to use hazardous acid or less hazardous organic scale inhibitors, along with various cooling system engineering considerations. Bleedoff minimization is most often subservient to maximizing stabilization success and percentage transport. The net environmental effect of chemical treatment is burdening cooling tower discharge with substantial additional sulfate, phosphorous, organic carbon, and possible halogen derivatives such as chloramines and trihalomethanes. While in addition, more make-up water is used than necessary with new technology. There is now a new treatment strategy employing electrochemistry to create an additional cooling system calcium removal sink independent of bleedoff. Side stream electrolysis of cooling water produces in-situ chemistry closely paralleling traditional cold lime softening used to process municipal and large industrial water supplies. No sulfate, phosphorous, or organic carbon is added, cooling water becomes much less supportive of microbial activity so only minimal or no microbicide is required, chemical hazard & supply chain issues are eliminated, and bleedoff discharge is reduced by at least 50% relative to requirements of conventional chemical treatment programs.

## 59. Solar Photo Oxidative Treatment System (SPOTS) Part 4: Treatment of Bacteria in Drinking Water by Induced Oxidation with Transparent Colloidal Systems

*Mohammad Musaddaq<sup>1</sup>, Shyam Shukla<sup>1</sup>, Kenneth Dorris<sup>1</sup>, Paul Anastas<sup>2</sup>, Julie B. Zimmerman<sup>3</sup>, S. Bhanumati<sup>4</sup> and Anh Tran<sup>1</sup>, (1)Department of Chemistry and Center for Green Science and Technology, Lamar University, Beaumont, TX, (2)Chemical Engineering, Yale University, New Haven, CT, (3)Chemical Engineering Department, Environmental Engineering Program, Yale University, New Haven, CT, (4)Chemistry Department, Cargi College, Dehli University, New Delhi, India*

Bacteria and other micro-organisms often act as the source of drinking water contamination making it unfit for drinking. Removal of micro-organisms and bacteria strains from drinking water involves extensive testing and may produce many undesirable byproducts during the application of processes currently being used. In our work, we use a Solar Photo Oxidative Treatment System (SPOTS) to oxidatively destroy E. coli bacteria strain and other micro-organisms present in the drinking water. In this paper we will discuss effectiveness of the SPOTS and will elaborate the simplicity, cost effectiveness, and the safety of this technique, which has been designed and developed over the period of 20 years. We also intend to compare the effectiveness of SPOTS to eliminate E. coli strain from drinking water with other conventional methods currently being employed at various water treatment facilities.

## 60. Novel Biomaterial: Designing, Characterization and Modifications for Decontamination of Metals from Waste Water: A Green Approach

*Man Mohan Srivastava, Shalini Srivastava, and Pritee Goyal,  
Department of Chemistry, Agra, India*

Existing methods of waste water treatments are associated with technical, economical, and other practical constraints. The search for new technologies for the removal of toxic metals, one of the important members of dirty dozen club of pollutants, has directed attention to biosorption phenomenon, which is based on the metal binding capacity of biomaterials. However, the use of biomaterials including agricultural wastes has several drawbacks also related to their less sorption efficiency, specificity, and stability, restricting their commercial use. Constructive efforts towards their modifications leading to novel biomaterials for decontamination of toxic metals from water bodies as economically viable green processes are in great demands.

A laboratory based physico-chemical scheme has been developed, exploring the properties of Agricultural waste- *Saraca indica* leaf powder [SILP] for the removal of metals [Pb (II), Cd (II), Cr (III), Ni (II), and Cr (VI)] from their single and multi metal solutions. Experiments result into the standardization of optimum conditions for sorption of toxic metals ranging from 60 to 90%. The work also addresses handling of percentage sorption efficiency of each metal in terms of thermodynamic feasibility of process and regeneration of metal loaded biomass. Special emphasis is paid on chemical modifications resulting into Tailored SILP novel biomaterial to improve sorption efficiency [5 to 20 %] using synthetic modifications like Acetylation and Succination. Graft Co-polymerized novel biomaterial results into the increase in environmental stability [10°C-30°C] and number of regeneration cycles of modified SILP [3 to 5]. Impregnation of positively charged layer onto the biomaterial results into its enhanced specificity towards anionic metals [Cr (VI)]. The findings open up new avenues in the removal of toxic metals as cost effective, environment friendly, safe, fast pre-treatment step for waste water as green technology.

## 61. A Green Protocol for the Synthesis of Pharmacologically Active Spiro-Indoles and 2-Aryl Benzimidazoles

*Siva Shankar Panda, Rohtash Kumar, and Subhash C. Jain,  
Department of Chemistry, University of Delhi, Delhi, India*

Heterocyclic compounds play a vital role in the search of a new drug candidate and are essential to elucidate the chemistry of living processes. Recent advances in biology have provided the vogue of constructing complex biologically active heterocyclic molecules by molecular modification approach. In continuation to our interest in the development of new bioactive heterocycles, we have recently developed a fast, efficient, clean, and eco-friendly water and microwave mediated synthesis of various heterocycles, viz. Schiff bases, spiro-indoles, and 2-arylsubstituted benzimidazoles each containing different biodynamic moieties. These spiro heterocycles have been prepared via hitherto Schiff's bases, which in turn were obtained by the reaction of indol-2,3-diones with various aromatic and heterocyclic amines, under aqueous condition, in excellent yield. 2-Arylsubstituted benzimidazoles have been synthesized by cyclocondensation of o-phenylenediamines and substituted benzaldehydes in water.

Spiro heterocycles and benzimidazoles are known to possess various biological activities viz. antitumor, anti-inflammatory, antifungal, antibacterial, and anti-convulsant; and therefore all the novel synthetic compounds, prepared using eco-friendly methods above, have been screened for a broad spectrum of biological

activities, in order to discover new pharmacophores for the future. Some of the compounds were found to possess very strong antimicrobial and anti-inflammatory activity *in vitro* and *in vivo* at very low concentration and therefore could be developed as drug candidate(s). Detailed synthetic methodology as well as the bio-activity of these novel compounds will be presented and discussed at the Conference.

## 62. Membrane Separations for Greener Operations in the Chemical Process Industries

*C. Stewart Slater and Mariano J. Savelski, Department of Chemical Engineering, Rowan University, Glassboro, NJ*

Membrane processes represent a green alternative separation to many of the vexing process streams in the chemical process industries. They can be used in product concentration, purification, waste minimization, chemical and solvent reuse and recovery. Their use as a sustainable process alternative is based on their ability to recover water and valuable products from waste streams and save energy. Membrane technology is well suited for direct integration into green manufacturing design for both batch and continuous-based processes. Their scalability makes them well-suited for the fine chemical and pharmaceutical industry as well as the traditional commodity chemical sectors. This presentation will use several case studies to illustrate the potential for membrane technology in green process design. Various industrial examples of membrane separations using reverse osmosis; nano/ultra/microfiltration, and pervaporation will be described along with a focus on green process design applications that the Rowan group has done research on in their engineering clinic program. These applications are drawn from a cross-section of industries such as food and beverage, fine chemical, pharmaceutical, and renewable energy production.

## 63. Benzamide as a Solvent for the Leuckart Reaction

*Mikhail M. Bobylev and Lioudmila I. Bobyleva, Department of Chemistry, Minot State University, Minot, ND*

The Leuckart reaction is a convenient one-step method for the reductive amination of a wide variety of carbonyl compounds via their reaction with formamide. Formamide plays three distinctly different roles in this reaction. First, it serves as a source of amino group for the amination step of the reaction. In this step, formamide and the carbonyl compound react with the formation of a formylimine. Second, it serves as a source of formic acid which functions as a reducing agent in the reduction step of the Leuckart reaction. Formic acid is produced via the hydrolysis of formamide and then reduces the formylimine to formylamine (the final product). Third, the excess of formamide serves as a solvent for the reaction. If the external formic acid is added to the reaction, then formamide is no longer necessary as a source of formic acid and could be replaced by any other amide. The amination by another amide would produce the corresponding acylimine which would then be reduced by formic acid to the respective acylamine. As a result, the Leuckart reaction would turn into a general method for synthesis of various amides. In addition, the replacement of formamide with a less volatile and more benign amide may have a positive environmental impact. Recently, we made an attempt to use acetamide as a solvent for the Leuckart reaction, and to our surprise obtained only the regular formylamine. In this work we tried to use benzamide and again obtained only the respective formylamine. This result raises some interesting questions regarding the mechanism of the Leuckart reaction. At the same time it definitely confirms that both acetamide and benzamide can be used as "greener" solvents for the Leuckart reaction. The project is supported by NIH grant P20 RR016741 from the NCCR.

## 64. Climate Change - How Can Green Chemistry Help?

Peter J. Dunn, Pfizer, Inc., Sandwich, Kent, United Kingdom

This presentation shows how Green Chemistry can save energy and help towards minimizing the impact of climate change. The first part of the presentation covers a brief history of the science of climate change and provides information on how climate change could affect global disease patterns (e.g. Malaria). The second part of the presentation covers the case history of the pregabalin process. Pregabalin is a successful drug for the treatment of pain and fibromyalgia. Pfizer replaced a classical resolution process with an enzymatic process and then subsequently developed an enzymatic process with a recycle operation for the undesired enantiomer. The three processes are analysed in detail and data presented with respect to their waste production and energy usage. The energy usage data is broken down from both a chemistry and engineering perspective to see what energy saving lessons can be learned from this development program. The enzymatic process, which is used for the commercial manufacture of Pregabalin, will eliminate the use of 185,000 metric tons of waste solvent (between 2007 and 2020) and will use 82% less energy than the original classical resolution. In the third part of the presentation, information on Pfizer's Energy and Climate Change program will be given.

## 65. Using Process Mass Intensity (PMI) to Guide Process Development and Design

Aaron S. Cote<sup>1</sup>, Jason G. Dorwart<sup>2</sup>, Paul F. Fernandez<sup>1</sup>, D. Michael Hobbs<sup>1</sup>, Viviane Massonneau<sup>1</sup>, Marguerite A. Mohan<sup>1</sup>, Aaron J. Moment<sup>1</sup>, Anthony W. Moses<sup>1</sup>, Rositza I. Petrova<sup>3</sup>, Debra J. Wallace<sup>4</sup>, and Timothy J. Wright<sup>1</sup>, (1)Chemical Process Development and Commercialization, Merck & Co., Inc., Rahway, NJ, (2)Analytical Development and Commercialization, Merck & Co., Inc., Rahway, NJ, (3)Center for Materials Science and Engineering, Merck & Co., Inc., Rahway, NJ, (4)Department of Process Research, Merck & Co., Inc., Rahway, NJ

In order to increase process efficiency and decrease environmental impact, process development can be guided in part by minimizing Process Mass Intensity (PMI), or the mass of material required to produce one kg of product. In this talk, we will show two ways in which using PMI as a metric served to drive the process development of a coupling reaction and subsequent workup of an Active Pharmaceutical Ingredient (API). First, an evaluation of the PMI for each step was used to identify development opportunities for process optimization, such as unit operations that require large quantities of solvent. Second, calculating the PMI of proposed process changes was used to guide experimental design for development activities, such as solvent selections for the reaction and work up. Drawing on this development work, we will present general scale-up guidelines and applications for incorporating PMI calculations into pharmaceutical process development.

## 66. Surfactants in Green Chemistry Part 1: Their Use as Solvents for Titrations of Water Insoluble Compounds

Shyam Shukla<sup>1</sup>, Paul Anastas<sup>2</sup>, Julie B. Zimmerman<sup>3</sup>, S. Bhanumati<sup>4</sup>, and Mohammad Musaddaq<sup>1</sup>, (1)Department of Chemistry and Center for Green Science and Technology, Lamar University, Beaumont, TX, (2)Chemical Engineering, Yale University, New Haven, CT, (3)Chemical Engineering Department, Environmental Engineering Program, Yale University, New Haven, CT, (4)Chemistry Department, Cargi College, Delhi University, New Delhi, India

Surfactants are amphiphilic molecules containing a long carbon terminated by a polar headgroup. These molecules aggregate together in a spherical structure with a hydrophobic core and an intense surface charge. Water-insoluble molecules can be solubilized in the core and  $pK_a$  of any acid/base group present is

modified. We have employed both of these facts to perform spectrophotometric, thermometric, potentiometric titrations of water insoluble compounds. The results are generally comparable to any traditional titrimetric procedure. It was observed that the  $pK_a$  values of acids became lower in the cationic surfactant aggregates. We also performed non-linear regression analysis to obtain  $pK_a$  values from potentiometric titration data. As an extension of this work, we have utilized o/w microemulsions containing oil, water, surfactant, and butanol as cosurfactant for such analyses with similar accuracy as well. Since surfactants are more benign molecules, their use for analytical determination can play an important role as green solvents.

## 67. Systematic Study of C-H Activation/Borylation

Sean Preshlock, Philipp Roosen, Paul Vogel, Robert E. Maleczka, and Milton R. Smith III, Department of Chemistry, Michigan State University, East Lansing, MI

Based upon the broad utility of Iridium catalyzed aromatic C-H activation borylation, a systematic study of conditions and reagents has been undertaken to assess applicability. The three commonly used precatalysts,  $[\text{Ir}(\text{COD})\text{OMe}]_2$ ,  $[\text{Ir}(\text{COD})\text{Cl}]_2$  and  $(\text{Indenyl})\text{Ir}(\text{COD})$  were investigated with the ligands 4,4'-di-*t*-butyl-2,2'-bipyridine, 1,2-bis(diphenylphosphino)ethane, and 1,2-bis(dimethylphosphino)ethane on a range of electron-poor and electron-rich substrates. The in situ generation of the active catalyst has allowed us to make a general comparison of the overall reactivity and stability of each catalyst by measuring reaction times and conversions. Details of these findings will be presented.

## 68. IMPACT™ Technology: A Greener Polyether Process

Jack R. Reese II<sup>1</sup>, Kenneth G. McDaniel<sup>1</sup>, Robert A. Lenahan<sup>2</sup>, Robert G. Gasting<sup>1</sup>, and D. Mark Morrison<sup>2</sup>, (1)Polyurethanes, Bayer MaterialScience, LLC, South Charleston, WV, (2)Polyurethanes, Bayer MaterialScience, LLC, Pittsburgh, PA

Bayer MaterialScience (BMS) is leading the polyurethane industry in its efforts to continually improve environmental and energy performance in its conventional polyol production processes, which can be considered best in class. A new BMS polyol process, IMPACT™, takes these improvements to a new level with additional energy reductions, carbon dioxide equivalents reductions, and waste elimination along with significant productivity improvements. In our Channelview plant, this technology eliminates about 75 million pounds of wastewater and reduces energy consumption by 80 percent which equates to a yearly reduction of about 54 million pounds of CO<sub>2</sub>. Recent milestones of a billion pounds of production using the continuous process in the U.S. and completion of technology licensing to major competitors has established the IMPACT™ technology as the industry standard for environmental savings and productivity. The technology is being implemented worldwide as plants are being converted or constructed, increasing the positive effects on the environment. The key to this process is a combination of a catalyst invention and an innovative process design. The continuous process developed from these inventions replaces a semibatch process that has been the industry standard for 50 years. The initial invention was the development of a catalyst that is more than ten times as reactive as other catalysts in this class and a thousand times more reactive than conventional catalysts. This catalyst invention was coupled with the design of a novel process based on a unique catalyst characteristic by which low molecular weight materials react preferentially in a mixture of molecular weights. The combination of these two inventions gives a process with little or no waste. The continuous process saves energy by eliminating the heat-up cycle of the semibatch process and further eliminates the energy and waste normally associated with catalyst removal.

## 69. Analysis of the CO<sub>2</sub> and NH<sub>3</sub> Reaction in an Aqueous Solution: Influence of the Operating Temperature

**Bong Gill Choi<sup>1</sup>, Won Hi Hong<sup>1</sup>, Jong-Nam Kim<sup>2</sup>, Kwang Bok Yi<sup>2</sup>, Jong-Duk Kim<sup>2</sup>, and Sungyuol Park<sup>2</sup>,** (1)Chemical and Biomolecular engineering, Korea Advanced Institute of Science and Technology, Daejeon, South Korea, (2)Separation Process Research Center, Korea Institute of Energy Research, Daejeon, South Korea

Among CO<sub>2</sub>-absorption technologies, the aqueous ammonia solution has been attracted for the prevention of global warming and worldwide climate change, due to its lower cost, higher CO<sub>2</sub> absorption capacity, lower decomposition temperatures of ammonium bicarbonate, and a less corrosive environment for the absorber material. Although aqueous ammonia solution has been focused on the removal of CO<sub>2</sub> from flue gas, there have been very few reports regarding the underlying analysis of the reaction between CO<sub>2</sub> and NH<sub>3</sub>. In this report, aqua ammonia process was operated at various temperatures, i.e. 40°C, 20°C, and 5°C. The CO<sub>2</sub> removal efficiencies and the loss of ammonia were influenced by the operating temperatures. Also, infrared spectra and pH measurements were used for the understanding of formation mechanism of ion species in absorbent, such as NH<sub>2</sub>COO<sup>-</sup>, HCO<sub>3</sub><sup>-</sup>, CO<sub>3</sub><sup>2-</sup>, and NH<sub>4</sub><sup>+</sup>, during CO<sub>2</sub> and NH<sub>3</sub> reaction. The reaction CO<sub>2</sub>-NH<sub>3</sub> at 20°C and 40°C has the similar reaction routes. However, the different reaction route was observed at 5°C compared to the other operating temperatures, displaying reaction product of ammonium bicarbonate solid was observed relatively after reaction time of 120 min. The CO<sub>2</sub> removal efficiencies and the formation of carbamate and bicarbonate were strongly influenced by the operating temperatures. In particular, the analysis of the formation carbamate and bicarbonate by infrared spectra and pH measurement provides useful information on the reaction mechanism of CO<sub>2</sub> and NH<sub>3</sub> in aqueous solutions.

## 70. Green Chemistry and Analytical Techniques: Undergraduate Laboratory Experiments

**Keith Dusoe and Meghna Dilip,** Department of Chemistry, Worcester State College, Worcester, MA

Three experiments were used in the undergraduate course of green chemistry (CH 455) at Worcester State College. All three experiments could be easily used in a traditional analytical chemistry/instrumental analysis lab class. The labs were focused on the use of alternative solvents in separations. Experiments conducted include use of aqueous biphasic systems for the spectrophotometric determination of textile dyes, use of supercritical CO<sub>2</sub> for the extraction of caffeine from instant coffee and the use of ionic liquids for the separation and detection of heavy metals using atomic absorption techniques. Design of experiments as well as student outcomes will be presented.

## 71. Reclaiming and Recycling Silver (a precious metal) from Lab Waste of Undergraduate Students

**Chandana Mukherjee, Minakshi Bhardwaj, and S. Bhanumati,** Department of Chemistry, Gargi College, University of Delhi, Delhi, India

A precious metal, silver is widely used in the students' lab as silver nitrate for various qualitative tests and also for quantitative estimations. In inorganic mixture analysis, for testing the halide ions, and in quantitative estimations involving argentometry, the same reagent finds extensive use.

Silver is a mild oxidising agent. In the organic element detection and in functional group tests (aldehydes, reducing sugars, tartaric acid, and alikes) as Tollen's reagent, ammoniacal silver nitrate and

also in its native form, yields silver halides, silver cyanide, silver sulphide, and of course metallic silver.

Due to extensive cost, the use of silver nitrate is extremely limited and hence this calls for looking into procedures, which would reclaim the metal from the reaction products and putting it to use in a profitable way by converting it to the original reagent, i.e., silver nitrate.

We have successfully scavenged silver from the reaction products and prepared silver nitrate in turn. The cost of silver nitrate, 25 gram pack, is around U.S. \$40. The yearly consumption in our undergraduate lab is around 200 gram, incurring a hefty amount from the overall grants sanctioned for chemicals. Recycling process is almost cost free as will be shown in the presentation.

While on one hand, the lab waste is managed meticulously, the pupils benefit from the very idea of reclaiming, recycling, and reusing, giving them a psychological push towards thinking and working green.

## 72. Liquid CO<sub>2</sub> as an Apt Solvent in Undergraduate Labs

**Pragya Sidhwani,** Department of Biochemistry, Sri Venkateswara College, Delhi University, New Delhi, India, **Sunita Dhingra,** Department of Chemistry, Miranda House, University of Delhi, New Delhi, India, and **Indu Tucker Sidhwani,** Department of Chemistry, Gargi College, University of Delhi, New Delhi, India

Supercritical CO<sub>2</sub> is a very good solvent to extract various natural materials. Since specially designed equipment is expensive and intricate, an effective yet affordable alternative in chemistry labs of schools and colleges is liquid CO<sub>2</sub>. About a dozen extractions have been done, including those of turmeric and garlic. The l CO<sub>2</sub> extraction in the lab represents an attractive option for the extraction of garlic oil as it helps retain the fresh flavor of garlic associated with the presence of alkyl thiosulphates and thiosulphonates, which are otherwise lost in harsh extraction processes such as hydro distillation or steam stripping.

It also selectively extracts one or two compounds out of many naturally occurring compounds present in the roots of a medicinal plant, which is used as a natural red dye and to accelerate wound healing.

The use of l CO<sub>2</sub> in the lab is further demonstrated in purification of some inorganic complexes like Ni (DMG)<sub>2</sub> prepared in the undergraduate labs. This work is in progress.

All of the above extractions and purifications show the diversity in the use of l CO<sub>2</sub> as a solvent.

## 73. Standards for Green Solvents: An Example Using Ionic Liquids

**Guy A. Hembury, Neil Sullivan, Lauren Tate, Gayle Fairless, and Robert Newton,** Bioniqs Ltd., York, United Kingdom

Widespread confusion over what constitutes a green solvent has led to a high level of "greenwashing" concerning the purported environmental benefits of many novel solvents, including ionic liquids. This has undoubtedly resulted from the absence of any agreed standard to what constitutes a green solvent.

To address this technical and commercial liability, we have designed a benchmark green solvent certification that we have called *econiqs*. To qualify as a green solvent under the *econiqs* certification, a solvent must satisfy stringent environmentally relevant criteria, including biodegradability within 14 days, sustainability, and low-toxicity towards *Daphnia magna* and green algae. These criteria do not purport to be definitive and are not intended as a substitute for a fully detailed harmonized specification; they are designed



# Abstracts continued

to assure customers of the basic environmental and toxicological performance of products carrying the *econiqs* branding and serve as a reliable set of minimum requirements for assessing the green credentials of a solvent. We have initiated a full assessment of our 200 catalogue materials against the *econiqs* criteria.

CRITERIA	STANDARD
Biodegradable	1. >98% Biodegradable by mixed community of natural soil organisms within 14 days, as determined by HPLC and/or ion chromatography.
Sustainable	2. All precursor materials used in manufacture are available from sustainable, renewable feedstocks.
Non-mutagenic	3. Non-mutagenic as determined by the Ames test (Mutagenicity Index <2, Mutagenic Activity Ratio <2.5).
Low toxicity	4. <i>Daphnia magna</i> EC <sub>50</sub> >250mg/L. 5. Green algae ( <i>Selanstrum capricornutum</i> ) E <sub>r</sub> C <sub>50</sub> >100mg/L.

We will present a worked example of the application of these benchmark criteria to a truly “green” solvent, the ionic liquid – *N,N*-Dimethylethanolammonium acetate.

## 75. Extension of the Environmentally Benign Catecholate Method to the Synthesis of Barium-Based Perovskites

*Heather Sheridan, Samantha DeCarlo, and Anne Marteel-Parrish, Department of Chemistry, Washington College, Chestertown, MD*

Barium titanate (BaTiO<sub>3</sub>), barium zirconate (BaZrO<sub>3</sub>), barium hafnate (BaHfO<sub>3</sub>), and barium stannate (BaSnO<sub>3</sub>), were all synthesized using the environmentally benign catecholate method. This method employs naturally occurring and less toxic precursors, smaller quantities of solvents, and results in the absence of by-products while achieving stoichiometric control over the barium-to-X (X= Ti, Zr, Hf, Sn) molar ratio. The catecholate method was originally applied to the synthesis of barium titanate which is the most well known member of the perovskite family essentially used for multi-layered ceramic capacitors in computers, aerospace, and communication technologies. The goal of this research was to apply this more efficient and environmentally benign synthesis to the production of barium zirconate, barium hafnate, and barium stannate; all three of which are essential components of the electroceramic industry. Barium zirconate is one of the most inert, stable, and corrosion-resistant perovskite utilized in superconducting applications for multi-layer ceramic capacitors. Hafnium based oxides are currently leading components for high temperature hybrid ceramic applications. The most recent focus for barium stannate has been on how to employ this perovskite as a sensor material. Titanium, zirconium, tin, and hafnium all have similar chemical properties: they have four valence electrons, are Curie temperature shifters, are found abundantly in nature, and are able to form alloys, composite materials, and oxides, which suggests that these elements would form complexes in a similar manner. Infrared spectroscopy, X-ray powder diffraction, and inductively coupled plasma optical emission spectroscopy were used to characterize the products. The synthesis, characterization data, and outcomes are detailed in this poster.

## 76. Scalable Green Chemistry: A Catalytic Asymmetric Hydrogenation Case Study

*Stefan G. Koenig, Process Research & Development, Sepracor, Inc, Marlborough, MA*

Recent years have seen the enthusiastic uptake of green catalysis technology by industry. While “sustainable” by definition, catalytic reactions are only truly effective if the entire chemical process is robust. Sepracor scientists have developed a multi-kilo green chemistry synthesis by introducing environmentally favorable transformations in several steps of the sequence. Innovative chemistry is utilized to produce a key enamide intermediate, which is transformed to a chiral acetamide with low loadings of an asymmetric hydrogenation catalyst. Deprotection of the amide is realized by use of creative chemistry to replace an unfavorable reaction. Overall, the new process realizes a notable reduction in E-factor, a key measure of environmental impact.

## 78. Implementation of Green Chemistry and Engineering Principles into Nanomaterial Synthesis and Processing

*Juncheng Liu Sr. and Christopher B. Roberts, Department of Chemical Engineering, Auburn University, Auburn University, AL*

Green chemistry aims toward the design of environmentally-benign products and processes using ecologically friendly materials and solvents, with no or minimal amount waste generation. In this poster, we will present several green chemistry approaches that target advanced synthesis and processing of nanoparticles. These approaches include (1) green synthesis of metal and semiconductor nanocrystals in supercritical CO<sub>2</sub>; (2) metal nanocrystal deposition using CO<sub>2</sub>-expanded liquids and supercritical CO<sub>2</sub> processing for targeting low defect, wide area ordered arrays, and thin films; (3) green synthesis of metal nanostructures with high degree of size and shape control; (4) green synthesis and supermolecular self-assembly of Pt Nanocrystals in aqueous solution; (5) green synthesis of metal nanocrystals for catalytic applications, including ground water treatment and alternative energy synthesis. These research works have each implemented green chemistry principles into the advanced nanomaterials synthesis and processing.

## 79. The Study on the Hollow Titanium Silicalite Zeolite (HTS)

*Min Lin, Bin Zhu, Xingtian Shu, and Xieqing Wang, State Key Laboratory of Catalytic Material and Reaction Engineering, Research Institute of Petroleum Processing, SINOPEC, China, Beijing, China*

The oxidation reactions are very important industrial processes for production of fine chemicals in organic synthesis. The traditional oxidation technology was predominated by its complicated process, harsh operating conditions, and serious pollution caused. The titanium silicate zeolite (TS-1) shows remarkable catalytic properties in oxidation reactions. The selective oxidation of organic substrates by H<sub>2</sub>O<sub>2</sub> in the presence of TS-1 has been an interesting area of high potentiality for the development of new environmentally friendly technologies. However, it is the instability of activity and the production repeatability that affects the wide application of the catalytic material.

In order to synthesize hollow titanium silicate zeolite (HTS), the <sup>29</sup>Si-NMR and <sup>1</sup>H-NMR were used to follow up the trace of basic hydrolysis of tetraethyl orthosilicate (TOES) and the results show that species of monomer, dimer, trimer, cyclic, and polymer silicate are formed. The monomer and/or dimer are more favorable the zeolite synthesizing. The XRD, <sup>13</sup>C CP/MAS, and <sup>29</sup>Si NMR were used to trace the HTS crystallization process. The results show that the induction period of HTS is 80 min, subsequently, it takes next 10 min to form HTS and the remaining time of the crystallization

period maybe acts as cleaning up the pore and/or washing off the impurity in HTS zeolite. The synthesized HTS samples were characterized by XRD, FT-IR, UV-Vis, and Raman spectra.

The commercial HTS samples show good repeatability and high oxidation catalytic activity. The commercial HTS samples have been used to the commercial catalyst for the manufacture 10,000 ton/a catechol and hydroquinone from phenol and 100,000 ton/a cyclohexanone ammoximation processes on industrial scale in China.

*Project supported by the National Science Foundation of China (2006CB202508).*

## 80. Epoxidation of Propylene and Hydrogen Peroxide

*Min Lin<sup>1</sup>, Hua Li<sup>2</sup>, Bin Zhu<sup>1</sup>, Wei Wang<sup>2</sup>, Shunxian Huang<sup>1</sup>, Xingtian Shu<sup>1</sup>, Chijian He<sup>2</sup>, Jizao Gao<sup>2</sup>, and Xiaoju Wu<sup>2</sup>, (1)State Key Laboratory of Catalytic Material and Reaction Engineering, Research Institute of Petroleum Processing, SINOPEC, Beijing, China, (2)China Petroleum & Chemical Corporation Changling Company, Yueyang, Hunan, China*

The propylene oxide is a very important bulk chemical in the petro-chemical and chemical industry. The convention route for propylene epoxidation involves serious pollution, stiff reaction condition, large investment, and the lower selective. The new convention route of propylene epoxidation by hydrogen peroxide with the presence of titanium silicalite-1 (TS-1) catalyst has been put forward, recently. It is an environmentally friendly technology. The atomic utilization ratio in this new process is 76.3%, that much more than the chlorhydrin process (31.2%) or co-products routes (37.7~38.7%). The hollow titanium silicate sieve (HTS) has been synthesized in the paper, and then it has been used to catalyze the propylene epoxidation. The selectivity, effectively, and stability of the HTS catalyst has been studied. The propylene was epoxidized with dilute methanol solutions of hydrogen peroxide in a fixed bed reactor has been investigated. The experimental results show that when the reaction pressure is 0.5 MPa, reaction temperature is 40°C, liquid mass space velocity is 12.5 h<sup>-1</sup>, the conversion of hydrogen peroxide and selectivity of propylene oxide are more than 95% and 95%, respectively.

*Project supported by the National Science Foundation of China (2006CB202508).*

## 81. A Study on Noble Metal Modified Titanium Silicalite\*

*Min Lin, Chunfeng Shi, Bin Zhu, and Jun Long, State Key Laboratory of Catalytic Material and Reaction Engineering, Research Institute of Petroleum Processing, SINOPEC, Beijing, China*

Propylene oxide (PO) is an important chemical intermediate used in the production of polyurethane, polyester resins, and surfactants. The new convention route of PO by hydrogen peroxide with the presence of titanium silicalite-1 (TS-1) catalyst has received much attention in the past decade. It is an environmentally friendly technology. Recent developing technologies involving onsite hydrogen peroxide production followed by hydrogen peroxide conversion to organic oxides without refining (namely direct oxidation technology) are being looked over as promising technologies with good potentials for ulterior savings in capital and production costs. The key point of the direct oxidation technology is the design and preparation of the bi-functional catalysts used therein. Here present such bi-functional catalysts, a new titanosilicate, noble metal modified titanium silicalite (NMTS, modified titanium silicalite with noble metal being incorporated in). The samples have been characterized by various instruments such as powder X-ray diffraction (XRD), fourier transform infrared spectrometry (FTIR), UV-visible diffuse reflectance spectroscopy (UV-visible DRS), transmission electron microscopy (TEM), and

X-ray photoelectron spectroscopy (XPS). Activity and selectivity for the epoxidation of propylene with H<sub>2</sub> + O<sub>2</sub> of NMTS have also been investigated. The result has shown that NMTS is one of excellent catalysts for the preparation of PO using propylene with H<sub>2</sub> + O<sub>2</sub> as oxidant in one-pot process.

*\* Project supported by the National Science Foundation of China (2006CB202508).*

## 82. Development of Safe and Environmentally Friendly Halogenation Reagents

*Rodrigo Cristiano, Kefeng Ma, George Pottanat, and Richard G. Weiss, Department of Chemistry, Georgetown University, Washington, DC*

We describe two strategies for safe and environmentally friendly halogenation reactions that employ phosphonium-based ionic compounds. In one strategy, polystyrene beads with appended triphenylmethylphosphonium tribromide groups (**R-TPP1Br<sub>3</sub>**) are the bromination reagent. The tribromide anion is made from the monobromide (**R-TPP1Br**) and is regenerated after each reaction. A protocol will be described in which **R-TPP1Br<sub>3</sub>** is regenerated and several structurally diverse unsaturated substrates are brominated while the beads remain in the same flask; **R-TPP1Br** can be separated easily from the liquid containing the products. These bromination reactions are stereoselective, giving almost exclusively anti-addition products. The other strategy employs room temperature ionic liquids (RTILs) based on tetraalkylphosphonium salts with trihalide anions (Br<sub>3</sub>, BrCl<sub>2</sub>, and ClBr<sub>2</sub>). The reactions can be conducted in solvent-free conditions when the substrates are liquids. Both strategies avoid the need to work with volatile dihalogen molecules during the reactions and work-up. The yields and stereo- and regio-selectivities from the brominations, chlorinations, and bromochlorinations of several substrates will be presented.

*We thank the Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES, Brazil) for a postdoctoral scholarship to RC and the National Science Foundation for its support of this research.*



## 84. Homogeneous Modification of Cellulose in Ionic Liquid Using Iodine as a Catalyst

*Run-Cang Sun, Institute of Biomass Chemistry and Technology, Beijing Forestry University, Beijing, China*

The homogeneous succinylation of sugarcane bagasse cellulose with succinic anhydride (SA) in solvent system containing 1-butyl-3-methylimidazolium chloride ([C<sub>4</sub>mim]Cl) ionic liquid and dimethylsulfoxide (DMSO) using iodine as a catalyst was investigated. The results showed that the degree of substitution (DS) of all succinylated cellulosic derivatives was in the range of 0.56 to 1.54, which noticeably increased compared with the products without any catalysts, indicating that iodine was an effective catalyst for cellulose succinylation in ionic liquids. The succinylated cellulosic derivatives were also characterized with FT-IR and solid-state CP/MAS <sup>13</sup>C-NMR spectroscopies. The results indicated that the iodine catalyzed succinylation efficiency increased, and the reaction of hydroxyl groups at C-6, C-2 and C-3 positions in cellulose occurred. The thermal stability of the succinylated cellulose was found to decrease upon chemical modification.

## 85. Plants as Factories; Enzymes, Electricity, and Light as Transformative Reagents

*Ian D. Brindle, Brock University, St. Catharines, ON, Canada*

This presentation will outline the work at our university that depends upon our biologists and chemists, who are active in the field of green chemistry. I shall describe our programs underway to develop non-food plants as factories for the production of value-added materials, including drugs, nutraceuticals, and industrial products. In addition, I shall describe the work of our chemists, who are combining oxygenase enzymes, electrochemistry, and light to achieve syntheses of valuable pharmaceutical products. Our use of computer modeling as an aid to efficient synthetic pathways will also be described.

## 88. Properties and Characterization of a Renewable Water Soluble Polymer: Polyitaconic Acid

*Mathieu Chirat, Materials Science, University of New Hampshire, Durham, NH, and Yvon Durant, Principal, Itaconix, Hampton Falls, NH*

Polyitaconic acid is a renewable polymer produced by Itaconix. It is produced from the itaconic acid monomer, itself produced by fermentation of carbohydrates. Various samples have been characterized and some of their properties are reported.

Proton nuclear magnetic resonance (<sup>1</sup>H NMR) shows residual monomer content between 0.5 and 5%. Number average molecular weight was determined by aqueous size exclusion chromatography (SEC) and was found to be between 2,500 to 300,000 with polydispersity indexes between 2 to 11. Peak assignments of carbon NMR were performed with samples in D<sub>2</sub>O after adjusting the pH between 0 and 1. Fourier Transform Infrared Spectroscopy showed evidence of anhydride acid traces. Thermo Gravimetric Analysis (TGA) shows a polymer remaining stable below 100°C, water loss above 100°C extends to 250°C with significant thermal degradation beyond that number.

High molecular weight polyitaconic acid has been confirmed as thickening agent by viscosity measurements of polyitaconic acid aqueous solution using an AR2000 dynamic rheometer. Polyitaconic acid can inhibit the precipitation of salt from divalent cations such as calcium, barium, or magnesium, making it useful as a dispersant and an antiscaling agent for water treatment.

## 89. Evaluation of Different Combinations of *E. Coli* Strains and Cellulase Genes for Cellulosic Substrate Degradation

*Angelica Cavalett, André L. Rodrigues, Larissa G. Paludo, Filipe A. T. Paulo, and Andre O. S. Lima, Laboratorio de Microbiologia Aplicada, Universidade do Vale do Itajaí, Itajaí, Brazil*

The use of biofuels is an alternative to reduce the greenhouse effect. Cellulose is a linear glucose polymer; this carbohydrate is the most abundant polysaccharide in plant biomass and represents a renewable energy resource. Several types of cellulolytic enzymes, including endoglucanases, β-glucosidases, and exoglucanases, have been cloned from bacteria to degrade cellulosic feedstock and, therefore, produce bioethanol. In order to evaluate the efficiency of a cellulases mix over cellulosic substrates hydrolysis, we describe the obtainment of 35 different recombinant cellulolytic strains of *Escherichia coli*. Each strain received by electroporation an expression vector, which carries one or two cellulase genes. A total of seven different plasmids, covering four cellulase genes (*EglA-Bacillus pumilus*; CelB and CelE-*Cellvibrio japonicus*, BglA-*Ferriobacterium* sp.) were introduced in five distinct *E. coli* strains. Once obtained, it was determined the growth curve for all constructs. Samples from initial (14h) and later (24h) stationary phase were collected and evaluated for enzyme activity (endoglucanase - reducing sugar - Somogyi Nelson; beta-glucosidase - p-nitrophenyl-glucopyranoside). The results allowed the determination of the best strain/plasmid combinations for each enzyme. Then, a mixture of those combinations was cultivated in LB media and a pool of concentrated (10X by ultrafiltration) secreted cellulase was evaluated for carboxy-methylcellulase (CMC) and cotton degradation. Preliminary results indicated that our cellulase mix released four times more reducing sugar ends from CMC than commercial cellulase (1mg/mL, Blue Super LT - Novozymes). Future assays include the evaluation of our recombinant cellulase mix over other substrates (sugar cane bagasse, corn straw, etc), as well the investigation of each enzyme separated over the same substrates. We aim by this way to determine which combination plasmid/strain or mix is more appropriate for each cellulosic residue and, consequently, contributes in the development of bioethanol production from cellulosic residues.

## 90. 2009 HANCOCK AWARD RECIPIENT: Chemical Transformation of Lignocellulosic Biomass into Fuels and Chemicals

*Joseph B. Binder, Energy Biosciences Institute, Berkeley, CA, and Ronald T. Raines, Department of Chemistry, University of Wisconsin-Madison, Madison, WI*

Lignocellulosic biomass is a plentiful, renewable, and largely untapped resource for fuels and chemicals. Despite this potential, nearly all renewable fuels and chemicals are now produced from edible resources, such as starch, sugars, and oils; the challenges of non-food lignocellulosic feedstocks have made their conversion inefficient and uneconomical. We have found that N,N-dimethylacetamide containing lithium chloride and chloride-containing ionic liquids are privileged solvents that enable the synthesis of soluble sugars and renewable chemicals in a single step from untreated lignocellulosic biomass. Sugars may be fermented into bioproducts such as ethanol, while other products like 5-hydroxymethylfurfural may be converted into fuels and chemical intermediates. The simplicity of our chemical transformation of lignocellulose contrasts markedly with the complexity of extant bioprocesses, and provides a new paradigm for biomass as a raw material for renewable energy and chemical industries. This work was supported by the Great Lakes Bioenergy Research Center, a DOE Bioenergy Research Center. J.B.B. was supported by an NSF Graduate Research Fellowship.

## 91. Fate of *Jatropha curcas* Phorbol Esters in Soil

*Rakshit K. Devappa, Harinder PS Makkar, and Klaus Becker, Institute for Animal Production in the Tropics and Subtropics (480b), University of Hohenheim, Stuttgart, Germany*

*Jatropha curcas* seeds contain 30-40% oil, which can be converted to biodiesel of high quality. The nitrogen rich seedcake is currently used as a fertilizer. Phorbol esters (PE) are the main toxins present in the oil and seedcake. These are co-carcinogens and exhibit antibacterial, antiviral, and insecticidal activities and are toxic to animals. This study reports the fate of PE in soil and determines its bioactivity during the process of degradation.

Two approaches for incorporation of PE in soil were used. In the first approach, silica bound to PE; and in the second approach, seedcake were used. The degradation studies were conducted at temperatures: room temperature, RT, 22-23°C; 32°C and 42°C, and moistures: 13% and 23%. At zero day, concentration of PE in soil was 2.6 and 0.37 mg/g for approach 1 and 2 respectively. When silica bound to PE was used, 100% degradation was observed after 19, 12, 12 days at RT, 32°C and 42°C at 13% moisture, and after 17, 9 and 9 days at 23% moisture. Similarly when the cake was incorporated in soil, 100% degradation was found after 21, 17 and 17 days at 13% moisture, and after 23, 17, and 15 days at 23% moisture level at RT, 32°C and 42°C. The rate of degradation (%/day) increased with increase in temperature and moisture content (Approach 1: 2.91, 21.77 and 22.42, and 4.13, 23.00 and 23.25 at 13% and 23% moisture, Approach 2: 2.58, 7.07 and 8.67, and 7.94, 10.44 and 14.17 at 13% and 23% moisture; at RT, 32°C and 42°C). Snails (*Physa fontinalis*) and brine shrimp (*Artemia salina*) assays were used to determine activity of PE in soil. With decrease in PE concentration in soil, the mortality decreased. In conclusion, PE are biodegradable in soil and their degraded products appear to be innocuous.

## 92. Web-Based Toxic Information Clearinghouse

*George R. Thompson, Chemical Compliance Systems, Inc., Lake Hopatcong, NJ*

Centralized chemical toxic information databases have become of worldwide interest. The Canadian Environmental Protection Act (CEPA) of 1999 established their centralized Pollution Prevention Planning database. The European Registration, Evaluation, Authorization of Chemicals (REACH) regulations were promulgated in December 2006 and included a provision to create a centralized database under the European Chemicals Agency in Helsinki. Under the California Green Chemistry Initiative, Senate Bill 509 of 2008 required the establishment of their Toxic Information Clearinghouse. Other states in the U. S. are also considering legislation that would require a centralized chemical toxic information database.

Chemical Compliance Systems, Inc. (CCS) began compiling our Web-based, holistic Relational Chemical and Product Database (R-CPD) in 1985. We estimate R-CPD currently contains 75 million data elements for 260,000 chemicals and over 350,000 munition and nonmunition products compiled from over 1,000 sources. The relational design of R-CPD greatly increases the flexibility of both its expansion and its application to innumerable user requirements.

R-CPD is composed of four primary data tables: Chemical, Regulatory, Product, and Munition. The Chemical Data Tables are further subdivided into a Cross Reference Dictionary, Physical/Chemical, Health, Safety, Ecological, "Green" Criteria, and Alternative Chemical fields. The Regulatory Data Tables encompass over 700 local, state, federal, international, nongovernmental, and CCS composite chemical regulatory lists, with all of their associated data. The Product Data Tables include Manufacturer, Composition, Description, Generic Category, Inventory, and Alloy Constituent fields. The Munition Data Tables are compiled by the U.S. Army Defense Ammunition Center and include munition composition from the Component, Part, Material, Chemical, and Elemental levels, as well as demilitarization and live-fire emissions data.

R-CPD can be readily customized for unique customer applications and can be remotely demonstrated.

## 93. Oligonucleotide-Based Fluorescence Probe for Sensitive and Selective Detection of Mercury(II) in Aqueous Solution

*Huan-Tsung Chang and Cheng-Kang Chiang, Chemistry, National Taiwan University, Taipei, Taiwan*

In this paper we unveil a new homogeneous assay—using TOTO-3 and the polythymine oligonucleotide  $T_{33}$ —for the highly selective and sensitive detection of  $Hg^{2+}$  in aqueous solution. The fluorescence of TOTO-3 is weak in the absence or presence of randomly coiled  $T_{33}$ . After  $T_{33}$  interacts specifically with  $Hg^{2+}$  ions through T- $Hg^{2+}$ -T bonding, however, its conformation changes to form a folded structure that preferably binds to TOTO-3. As a result, the fluorescence of a mixture of  $T_{33}$  and TOTO-3 increases in the presence of  $Hg^{2+}$ . Our data from fluorescence polarization spectroscopy and capillary electrophoresis with laser-induced fluorescence detection confirm the formation of folded  $T_{33}$ - $Hg^{2+}$  complexes. Under optimum conditions, the TOTO-3/ $T_{33}$  probe exhibited a high selectivity ( $\geq 265$ -fold) toward  $Hg^{2+}$  over other metal ions, with a limit of detection of 0.6 ppb. We demonstrate the practicality of this TOTO-3/ $T_{33}$  probe through its use for the rapid determination of  $Hg^{2+}$  in pond water and in batteries. This approach offers several advantages, including rapidity (<15 min), simplicity (label free), and low cost.

## 94. Catalytic Activity of Ce MgO Catalyst in the Oxidation of Cumene to the Cumenehydroperoxide

Biaohua Chen, Shuai Xu, Chongpin Huang, and Jie Zhang, State Key Laboratory of Chemical Resource Engineering, Beijing University of Chemical Technology, Beijing, China

Peroxidation of cumene to cumenehydroperoxide (CHP) is the key reaction of industrial phenol-production processes. In this paper, the alkali liquor in the traditional process was replaced by the solid bases, which was environmentally friendly. The effect of the constitute of the solid bases was investigated and the relevant mechanism was discussed.

Ce MgO was prepared by coprecipitation method and characterized by BET surface area, XRD, H<sub>2</sub>-TPR, and XPS. Cumene was oxidized in a 100 ml three-necked flask supplied with a mechanical stirrer with a rotation counter, the bubbler, reflux condenser, and the oil bath. Cumene (50 ml) was placed in the reactor, heated up to 90°C. Then, the catalyst was added and the air was passed through. The air flow was 160 ml/min. The stir speed was above 1000 r/min.

The yield of CHP in 10 h, which was 8% without catalyst, and was 13% under the catalysis of MgO. The yield of CHP increased with the content of Ce of the Ce MgO in the first stage, and it reached 22% in the presence of 10% Ce MgO. Then the yield started to decrease with the content of Ce of Ce MgO. The yield decreased to 14% when the content of Ce in the Ce MgO was 30%.

Alkylbenzene hydrocarbons with an isopropyl group are oxidized with O<sub>2</sub> in the liquid-phase according to the widely known free-radical mechanism. The rate-determining step is the propagation step. The tertiary C-H of cumene could be activated via the interaction between cumene with solid basic catalyst MgO. So, the yield was increased in the presence of MgO. The yield was first increased with the content of Ce because the CeO<sub>2</sub> acted as oxygen storing component. However, the active site of MgO was covered by CeO<sub>2</sub> with the further increasing of Ce content, leading to the decrease of the yield.

## 95. The Concept of a Green Drug, Curcumin and its Derivatives as a Prototype

Krishnaswami Raja, Department of Chemistry, Department of Chemistry, College of Staten Island, CUNY, Staten Island, NY

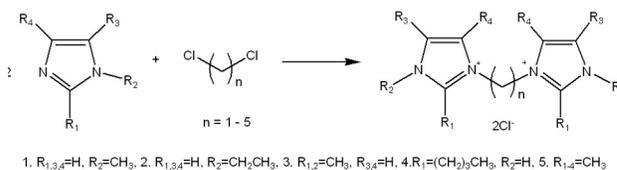
Only 5-15% of the ~25,000 existing species of plants have been examined for the presence of biologically active compounds. The ancient medical systems use a much larger palette of herbs for therapy. Systematic drug discovery involving using cues provided from traditional medical systems is bound to produce a new generation of green drugs. Curcumin, the primary active ingredient in *Curcuma longa*, is used as a model to enunciate the concept of green drug development. Synthetic- and formulation-based approaches to optimize the bioactivity of curcumin are presented.

## 96. Synthesis of Ionic Liquids under Ultra-High Pressure

Dora Lucia Sousa<sup>1</sup>, Laurence Harwood<sup>1</sup>, and Janet L. Scott<sup>2</sup>, (1)Department of Chemistry, University of Reading, Reading, United Kingdom, (2)School of Chemistry, Monash University, Melbourne, Australia

Ionic liquids are receiving increasing attention as solvents for organic synthesis. This interest stems from their potential as 'green' solvents. Their non-volatile character and thermal stability makes them potentially attractive alternatives for the volatile organic solvents.

Synthesis of a series of bisimidazolium chloride ionic liquids with polymethylene spacers ranging from 1 to 5 carbons has been compared using substituted imidazoles with the requisite  $\alpha,\omega$ -dichloroalkanes at ambient pressure and ultra-high pressure (19 kbar).



Bisimidazolium salts, with short linking chains and the chloride counterion, are difficult to prepare efficiently and a range of different strategies has been applied, including: microwave irradiation, ultrasonication, and high temperature synthesis in PEG.

The ultra-high pressure conditions we have introduced minimize the use of solvents and results in faster and cleaner reactions with improved yields of material, particularly when n=1,2 with little or no product obtained at ambient pressure. All solids were purified to a crystalline form.

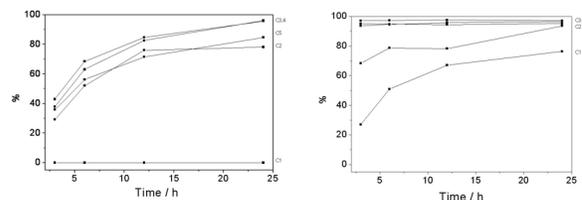


Figure 1. 1-methylimidazole, left) ambient pressure; right) 19 kbar.

## 97. A Green Pathway: Investigation of Corrosion Inhibitors and Inhibitive Effect of Some Novel Organic Dyes on the Corrosion of 2S Aluminium in Alkaline Media

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Some novel organic dyes like acid yellow 23, acid red 52, acid blue 1, acid yellow 36, phenolphthalein, methylene blue, ponceau 4R, bismark brown R are found to be corrosion inhibitors of 2S aluminums in alkaline media. In the present study of corrosion inhibitors, the parameters like alkali concentration, period of exposure time, and temperature are studied. From the inhibitive effect of above dyes in sodium hydroxide solution shows that inhibition efficiency increases with inhibitor concentration but decreases with increases in alkali concentration or with rise in temperature.

Aluminum is used in many industries and different fields. It is used for making alloys, which find extensive application in industries and arts. It is used in manufacture of aeroplanes and airships. It is used for making utensils, frames, coils for motors, wire for electrical transmission and electrical cables. These applications of aluminum are due to its properties like high electrical and thermal conductance, malleable and ductile nature, and its low cost.

Due to above application, aluminum is used in many industries and units. But aluminum is a highly reactive metal according to thermodynamic point of view.  $E^{\ominus}Al^{+3}/Al = -1.67$  V and standard free energy of formation of  $Al^{2}O^3$  is  $-368.8$  Kcal/mole. So, aluminum reacts with oxygen to form  $Al^{2}O^3$ . Therefore, the surface of aluminum is covered with oxide film. Generally, this film is stable in the solutions having pH 4.5 - 8.5. The film is not stable in strongly acidic or alkaline solutions. Thus aluminum and its alloy are attached in alkaline media.

### 98. Highly Efficient and Practical Selective Monohydrolysis of Symmetric Diesters

*Satomi Niwayama, Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, TX*

The development of environmentally friendly and cost-effective organic reactions has been of central importance in both academia and industry. Water is the least expensive and the most environmentally friendly solvent because it generates no hazard during chemical conversion processes. Water-mediated organic reactions thus represent a typical "green chemistry." Among various synthetic conversions, desymmetrization of symmetric compounds is one of the most cost-effective reactions, because the starting symmetric compounds are typically obtained easily on a large scale from inexpensive sources, or commercially available inexpensively. Therefore, water-mediated desymmetrization of symmetric organic compounds would be of tremendous synthetic value, and would make a significant contribution to creating greener reaction processes. To this end, we have been developing highly efficient and practical monohydrolysis of symmetric diesters with remarkable success. Half-esters, which are produced by such monohydrolysis of symmetric diesters, are very versatile building blocks in organic synthesis, and have a commercial value. Since the two ester groups in the symmetric diesters are equivalent, chemically distinguishing these ester groups has been challenging. Classical saponification usually affords slurry complex mixtures, yielding a large amount of undesirable dirty waste. Enzyme reactions provide no basis for prediction of the reactivity. Ring-opening reactions of cyclic acid anhydrides require hazardous organic solvents. However, with our selective monohydrolysis reaction, in which aqueous base is added to a symmetric diester suspended in water that may contain a small amount of a polar aprotic co-solvent at 0°C, pure half-esters are obtained in high to near-quantitative yields without producing dirty waste and without requiring hazardous organic solvents. While successful water-mediated organic reactions are still limited, this reaction takes advantage of the fact that organic compounds are not well-soluble in water and thus unique in this regard. This reaction is anticipated to significantly contribute to green chemistry useful in both industry and academia.

### 99. An Exploratory Study of Propargylation of Aromatics in Ionic Liquids Employing Metallic Triflates as Catalysts

*Viorel D. Sarca<sup>1</sup>, Levente Fabry-Asztalos<sup>1</sup>, Kelley Brown<sup>2</sup>, Casey Kellar<sup>1</sup>, and Kenneth K. Laali<sup>2</sup>, (1)Department of Chemistry, Central Washington University, Ellensburg, WA, (2)Department of Chemistry, Kent State University, Kent, OH*

The propargylic group is a useful and versatile building block in organic synthesis. Many traditional organic solvents have been implicated as environmental contaminants and are often toxic, volatile, and difficult to work with. Room temperature ionic liquids (ILs) have attracted a great deal of worldwide interest as more acceptable, environmentally friendly "green" solvents because of their low melting point, minimal vapor pressure, low toxicity, and recyclability. In continuation of our earlier studies on electrophilic

chemistry in ionic liquids, the aim of this project is to develop a mild and selective synthetic method for the propargylation of aromatics with propargylic alcohols in imidazolium ILs. We employ readily available metallic triflates [bismuth triflate  $Bi(OTf)^3$ , scandium triflate  $Sc(OTf)^3$ , and ytterbium triflate  $Yb(OTf)^3$ ] as catalysts, and 1-butyl-3-methylimidazolium trifluoromethanesulfonate [BMIM][OTf] and 1-butyl-3-methylimidazolium hexafluorophosphate [BMIM][PF<sub>6</sub>] as our IL solvents. Our preliminary studies in this area will be presented.

### 100. New Binary Mixture Ionic Liquid Based on $(C_4H_9)_4NHSO_4$ and Caprolactam

*Dishun Zhao<sup>1</sup>, Hongyan Cui<sup>1</sup>, and Erhong Duan<sup>2</sup>, (1)College of Chemical and Pharmaceutical Engineering, Hebei University of Science and Technology, Shijiazhuang, China, (2)School of Chemical Engineering and Technology, Tianjin University, Tianjin, China*

In recent years, ionic liquids are attracting increased attention worldwide because they have been shown to function as novel green reaction media. As far as we know, ionic liquids typically consist of organic nitrogen-containing heterocyclic cations and inorganic anions. Abbott has reported quaternary ammonium salt/amide type eutectic mixture. Here, a novel room-temperature binary mixture ionic liquid based on  $(C_4H_9)_4NHSO_4$  and caprolactam has been synthesized and characterized by differential scanning calorimetry (DSC), pH, liquid-solid phase diagram, solubility, conductivity and cyclic voltammetry. This molten salt appears as a liquid at  $<100^\circ C$ , though it is composed of two solids. The melting points of the binary ionic liquid vary with the different content of  $(C_4H_9)_4NHSO_4$ . According to the analysis of its liquid-solid phase diagram, the eutectic point is about  $23^\circ C$  with the mass percentage of  $(C_4H_9)_4NHSO_4$ , 25%. This work has shown that mixtures of caprolactam with quaternary ammonium salts form low melting point binary mixture ionic liquid that have unusual solvent properties.

### 101. Hydrolysis of Nitriles to Amide in Water under Microwave Irradiation

*Joo Ho Kim, Ui Yong Kim, and Jon Chan Less, Department of Chemistry, Chung-Ang University, Seoul, South Korea*

The hydrolysis of nitriles to amides is very important transformation in organic synthesis as well as chemical industry as excellent intermediates and raw materials. Various methods have been developed for the hydrolysis of nitriles to amides. However, the majority of known methods commonly have one or more disadvantages such as difficulty in manipulation, high temperature, and utilization of toxic reagents. Therefore, it is still desirable to develop a new mild, selective, and efficient method. Sodium percarbonate, green alternatives to toxic and expensive organic reagents, is a cheap and easily handled reagents which was shown to be a highly effective for conversion of a variety of functional group. In our work, the hydrolysis nitriles to amides by sodium percarbonate in aqueous solution at 150W,  $120^\circ C$  is smoothly achieved under mono mode microwave irradiation. We have accomplished new hydrolysis of nitriles to amides by using sodium percarbonate in water under mono mode microwave irradiations.



## 102. Delineation of More Environmentally Benign Pathways for the Synthesis of Doped Barium Titanate

*Samantha DeCarlo, Heather Sheridan, and Anne Marteel-Parrish, Department of Chemistry, Washington College, Chestertown, MD*

In the electroceramic industry, perovskites are used in applications such as capacitors and transducers. One of the most thoroughly studied perovskites is barium titanate ( $\text{BaTiO}_3$ ). In order for barium titanate to be used in industry as a capacitor or transducer, it must have a high dielectric constant at room temperature. To achieve this goal, barium titanate must be doped. The goal of this research was to develop a greener method of doping barium titanate. The dopants used in this project were strontium oxalate ( $\text{SrC}_2\text{O}_4$ ) and strontium carbonate ( $\text{SrCO}_3$ ). Strontium and barium exhibit similarities in size and charge. The barium precursor doped was barium titanyl catecholate  $\text{Ba}[\text{Ti}(\text{cat})_3]$  produced via the catecholate route. Two environmentally benign methods of doping were investigated: one based on the microwave-assisted route and the other using a centrifuge-assisted process. Both of these methods used water as the main solvent and allowed for thermodynamic control over the molar stoichiometric ratio between barium and strontium. Characterization methods used to analyze the final doped products were infrared spectroscopy, X-ray powder diffraction, and inductively coupled plasma optical emission spectroscopy. These two doping methods combine green and materials chemistry in that they are more economically and environmentally friendly. The synthesis, characterization data, and results are detailed in this poster.

## 103. Surfactants in Green Chemistry Part 2: The Use of Surfactant-Modified Clays for Removal of Traces of Organics from Aqueous Systems

*Shyam S. Shukla<sup>1</sup>, Paul Anastas<sup>2</sup>, Julie B. Zimmerman<sup>3</sup>, S. Bhanumati<sup>4</sup>, and Mohammad Musaddaq<sup>1</sup>, (1)Department of Chemistry and Center for Green Science and Technology, Lamar University, Beaumont, TX, (2)Chemical Engineering, Yale University, New Haven, CT, (3)Chemical Engineering Department, Environmental Engineering Program, Yale University, New Haven, CT, (4)Chemistry Department, Cargi College, Dehli University, New Delhi, India,*

Surfactants are amphiphilic molecules containing a long carbon chain terminated by a polar headgroup. Clays are generally inorganic materials consisting of layered structure. Clays have been used for ages as cosmetic products for removal of oily or hydrophobic materials. However, the capacity of the clays for adsorption of hydrophobic material is limited because of limited hydrophobicity. However, it has been known that the Ca or Mg ions in clays can be substituted by quaternary ammonium salts. Many cationic surfactants are quaternary ammonium salts, which contain one or more long carbon chain. When clays are mixed with these cationic surfactants, they displace Ca or Mg cations by surfactants. Thus, intercalated layers of hydrophobic carbon chain of surfactants greatly enhance Clay's hydrophobicity. In our work, such surfactant modified clays have been examined for removal of traces of organics (such as water disinfection byproducts formed upon chlorination). The clays can be filtered after partitioning of unwanted organic molecules and can be washed to recover these molecules. This could constitute a simple way of removing chlorination disinfection by products from water.

## 104. Phase Transfer Catalysis with Microwaves: Green Synthetic Approaches to Metal Carbonyl Complexes

*Kurt Birdwhistell, Brian E. Schulz, and Kathryn Conroy, Department of Chemistry, Loyola University New Orleans, New Orleans, LA*

Traditional syntheses of Group VI metal carbonyls require 5 to 48 hours of reflux, this novel use of microwave energy coupled with a two-phase catalytic system has significantly reduced synthetic time and temperature. The use of a phase transfer catalyst and a biphasic system allows us to operate at lower reaction temperatures than other microwave methods. This method has shown to be effective for phosphine ( $\text{PPh}_3$ , dppe, dppm) as well as tertiary amine ligands. Characterization was done with NMR and FT-IR spectroscopy. Details of reaction conditions, times, phase transfer catalysts, and yields will be presented.

## 105. Extraction of Toxic Metal Ions Using Aqueous Biphasic System

*Sushmita Chowdhury and Indu Tucker Sidhwani, Department of Chemistry, Gargi College, University of Delhi, New Delhi, India*

Chemistry affects the environment in various ways and the effects are more lethal than benign. A challenge to chemists is to redress the past mistakes and to prevent their repetition. Knowledge of Green Chemistry provides a solution to many chemistry related environmental problems. The toxicity of mercury, lead, chromium and cadmium is well known and they have to be removed or sequestered before their incorporation into the food chain. Solvent extraction is a widely used technique for metal extraction; however, the traditional organic solvents used are often toxic and it is pointless to remove a toxic substance by using another toxic one. The use of aqueous two-phase systems as a separation technique is known in biotechnology. Such systems are formed when water-soluble, ecofriendly polymers are combined with inorganic salts over a specific concentration range. In certain cases water-soluble complexants are added whereby the metal forms a chelate and is extracted into the upper layer. The distribution coefficient can be controlled by using different chelants. The method has an excellent potential as an alternative technique for removal of metal ions from aqueous solutions. The polymer can be recycled. A variety of ligands have been used to selectively extract metal ions. Soil and water samples from industrial areas in and around Delhi have appreciable concentrations of toxic metals and this technique will be valuable for detoxification of our resources.

## 106. 1,3,5-Triisopropylbenzene Synthesis by Alkylation of Benzene with Propylene Using Chloroaluminate Ionic Liquids as Catalysts

*Biaohua Chen, Chongpin Huang and Jie Zhang, State Key Laboratory of Chemical Resource Engineering, Beijing University of Chemical Technology, Beijing, China*

1,3,5-Triisopropylbenzene (1,3,5-TIPB) is mainly used to synthesize 1,3,5-trisphenol, which is an important organic intermediate for flavonoid pharmaceutical product to cure angiodiopathy, cancer, and HIV. It is believed that oxidation of 1,3,5-TIPB to 1,3,5-trisphenol is the preferred and "green" route among all of the 1,3,5-trisphenol synthetic methods because of high yield, low cost, and minor environmental hazards. At present, 1,3,5-TIPB is commercially obtained by the alkylation of benzene with propylene using  $\text{H}_2\text{SO}_4$ , HF, or  $\text{AlCl}_3$  as catalysts. The disadvantages of these catalysts, such as unsafety, corrosion, and acid sludge treatment, are notorious. Therefore, it is very necessary to develop the new catalysts with good activity, high selectivity, and minor environmental hazard for preparation of 1,3,5-TIPB.

Room temperature chloroaluminate ionic liquids have been recognized as novel and “green” solvents and catalysts for synthetic chemistry. The main advantages arising from the use of chloroaluminate ionic liquid catalysts are high catalytic activity, high selectivity for target product, simpleness of product separation, and negligible environmental hazard. To the best of our knowledge, synthesis of 1,3,5-TIPB through alkylation of benzene with propylene using chloroaluminate ionic liquids has not been reported in any publication.

In this work, 1,3,5-TIPB was synthesized by the alkylation of benzene with propylene using chloroaluminate ionic liquids as catalysts. The effects of different catalysts and reaction factors on the product composition were investigated. High selectivity of 1,3,5-TIPB and ratio of 1,3,5-TIPB/1,2,4-TIPB were obtained at the proper reaction conditions. Furthermore, a novel method to reduce the content of 1,2,4-TIPB in the product was also studied. Addition of other alkylation agent such as butene-1 and hexene-1 at a suitable stage of synthesis obviously decreased the content of byproduct 1,2,4-TIPB and facilitated the purification of 1,3,5-TIPB. Chloroaluminate ionic liquid is also good catalyst for the transalkylation reaction to utilize the main byproduct, i.e. tetraisopropylbenzene efficiently.

### 107. Adsorption and Reduction of Cr(VI) Using Orange Peels

*Bryan Bilyeu<sup>1</sup>, Carlos Barrera-Díaz<sup>2</sup>, Patricia Balderas-Hernández<sup>2</sup>, and Gabriela Roa-Morales<sup>2</sup>, (1)Department of Chemistry, Xavier University of Louisiana, New Orleans, LA, (2)Environmental Engineering, Universidad Autónoma del Estado de México, Toluca, Mexico*

Waste orange peels from an orange juice processing plant were evaluated for effectiveness in batch and continuous modes. Batch processes were used to optimize conditions like pH, while the continuous mode determined capacity. Both Cr(VI) and Cr(III) concentrations were monitored. The continuous capacity was 18 mg Cr(VI)/g sorbent. There was significant reduction of the Cr(VI) to Cr(III) even beyond the sorbent capacity.

### 108. Solar Photo Oxidative Treatment System (SPOTS) Part 3: Oxidation and Mineralization of 2,4-Dinitrophenol

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Treatment of drinking water is becoming a growing concern around the globe. Many chemicals including organics and inorganics find their way to drinking water supplies. The cost of treating the water to make it fit for drinking comes with a high price tag including the processes that involve complex machinery and high energy input. Many of the contaminants can still not be removed effectively after applying expensive treatment techniques. In this research we plan to show that a Solar Photo Oxidative Treatment System (SPOTS) developed by us (during our work of over 20 years) to treat 2,4-dinitrophenol. The reason behind using the 2,4-dinitrophenol as the model molecule for this research is that it is one of the contaminants from the dyeing industry and it also serves as a

precursor for waste materials largely disposed off or dumped by the defense industry. With the use of an effective technology like SPOTS we were able to mineralize the product 2,4-dinitrophenol at high and low concentrations effectively by inducing a photocatalytic reaction. In this paper we would also present that how this technology can be used for the treatment of water in bigger bodies of water with the least involvement of energy intensive processes thus bringing the treatment cost to the lowest.

### 109. A Mild and Environmentally Friendly $\alpha$ -Bromo Cycloalkenone in Ionic Liquid using 1,3-Dibromo-5,5-Dimethylhydantoin (DBDMH) and UHP in H<sub>2</sub>O

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Evolution of environmentally benign synthesis is an ultimate goal of the present day synthetic chemistry. In recent years, ionic liquids have been acknowledged as green alternatives to the toxic and volatile organic solvents for various chemical reactions. Bromination of organic compounds is one of the important synthetic implements in organic syntheses. The drawbacks of many known bromination methods associated with the use of organic solvents and toxic reagents lead us to develop more and more environmentally friendly bromination systems. In this context, an environmentally friendly bromination protocol has been developed. In our work, an efficient and selective  $\alpha$ -bromo cycloalkenone by use of 1,3-dibromo-5,5-dimethylhydantoin (DBDMH) and UHP in H<sub>2</sub>O in ionic liquid at 50-60°C is smoothly achieved. Bromination with 1,3-dibromo-5,5-dimethylhydantoin (DBDMH) as a source of bromine cation have been accomplished a mild and environmentally benign UHP in H<sub>2</sub>O and provides selective bromination in excellent yields in the presence of catalytic ionic liquids.

### 110. Controlled Growth and Aggregation of Ferrite Nanoparticles for High Relaxivity MR Imaging

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Ferrite nanoparticles of uniform distribution were synthesized within the microdroplets by replacing the organic solvents to water and prepared a magnetite encapsulated polymer nanocomposite by an emulsification-diffusion technique. We found that the encapsulation efficiency could be precisely controlled according to the portion of magnetite and the capping ligand that covers the surface of the magnetite nanoparticles. The field-dependence and temperature dependence on magnetization, was measured by a superconducting quantum interference device. The size distribution and T<sub>2</sub> relaxivity of encapsulated composite particles were measured using magnetic resonance imaging for analysis of the effect of aggregation, and aggregates of the magnetite nanoparticles showed enhanced relaxation ability. In fact, we successfully replaced the organic and high temperature process to a water-based and low temperature process with equal uniformity of size distribution.



## 111. Low Cost Green Biochemical Reactor for the Synthesis of Chelating Resins

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In the present research we have designed and prepared a low-cost Green Biochemical Reactor (GBR) using microwave as per the principles of Green Chemistry. A series of chelating resins have been prepared by the use of this reactor. In this paper extraction of metal ions in various biological samples is described. The metal ions extracted are: iron, chromium, nickel, and palladium. Investigations were carried out either by batch method or by column method. Three different modified sepharose have been used for investigations: N-salicylaminoethylsepharose (NSAES), N-salicylaminopropyl sepharose (NSAPS), and N-salicylaminoethylsepharose (NSAHS). The best results were obtained with the use of NSAES. Effects of different parameters like pH, amount of modified sepharose, flow rate, inert electrolyte, temperature, and adsorption time were also investigated. The distribution coefficient has been calculated for all metals and these are as Fe:  $3.6 \times 10^2$ ; Ni:  $3.9 \times 10^2$ ; Cr:  $3.8 \times 10^2$ ; Pd:  $2.8 \times 10^2$ . The results of preconcentration and recovery of the metal ions using column method are found to be 98.7% for iron, 97.5% for chromium, 98.4% for nickel, and 97% for palladium. The methods have been developed to determine iron in various samples of cereals, milk, and medicine tablets, and nickel in the samples of vegetable oils. The working conditions are very easy and modified; sepharose can be regenerated and can be reused. This GBR will be significant for low-cost process development in industry, particularly in developing countries like India.

## 112. A New One Pot, Solvent Free and Microwave Assisted Synthesis of Nickel Porphyrin

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Porphyrins and metalloporphyrins are well known optoelectronic as well as biological materials and have been applied in light-emitting diodes. They are also synthetically important compounds due to their aromatic character, inner chelating pockets, and varying peripheral carbon chains. These have allowed scientists to discover new and unique chemical reactions. Porphyrins and their metal complexes have also stirred interdisciplinary interest due to a multitude of their intriguing physical, chemical, and biological properties. A one pot, solvent free, and microwave-assisted method for the preparation of nickel porphyrin complex is reported. This method allows higher yields, lesser times, and follows many principles of green chemistry. The same complex is also prepared by an alternative route: first, the preparation of porphyrin and then the insertion of metal ion. This method is also solvent-free and uses microwave heating.

## 113. Fast and Simple Method for Direct Iodination of Activated Aromatic Compounds in the Presence of Poly(ethylene) Glycol (PEG) under Microwave Irradiation

**Hee Joong Park**, Insu Kim, and Jong Chan Lee, Department of Chemistry, Chung-Ang University, Seoul, South Korea

Aromatic iodination reactions are important reactions and the resultant iodo products are useful intermediates in organic synthesis as they can be easily involved in the metal-catalyzed cross-coupling reaction. Generally iodination of organic substrates by simple application of molecular iodine is not possible because of its least reactive nature. Therefore, an oxidant is used along with

diiodine to get more reactive electrophilic species. In contrast with already reported methods, our methods have developed the fast, simple, and efficient method that does not need any additives by using poly(ethylene) glycol. Poly(ethylene) glycols were developed as recyclable liquid phase reagents. The use of these poly(ethylene) glycols for the iodination of activated anisole, naphthol, amines derivatives such as anilines and phenols is described. The spent poly(ethylene) glycols after the synthetic reaction were easily regenerated for further use.

## 114. Mine Drainage Remediation Using Cactus

**Bryan Bilyeu**<sup>1</sup>, Carlos Barrera-Diaz<sup>2</sup>, Gabriela Roa-Morales<sup>2</sup>, and Patricia Balderas-Hernández<sup>2</sup>, (1)Department of Chemistry, Xavier University of Louisiana, New Orleans, LA, (2)Environmental Engineering, Universidad Autonoma del Estado de México, Toluca, Mexico

Mining and ore processing produce very toxic and complex metal ion wastewater. The metals of concern are Cd, Cr, Cu, Fe, Ni, Pb, and Zn. Adsorption onto cellulose is effective and agricultural wastes are a cheap source. We evaluated the residue (ectodermis) from processing *Opuntia* (Prickly Pear Cactus) for biosorption effectiveness with Cr(VI) and Cr(III), then with actual mine drainage containing Cd, Cr, Cu, Fe, Ni, Pb, and Zn. The sorbent removed 99% of cationic Cr(III), but only 77% of anionic Cr(VI), and showed similar effectiveness for cations in the mixed metal mine drainage.

## 115. Functionalized Biomaterials for Arsenic Removal From Groundwater

**Sarah M. Miller** and Julie B. Zimmerman, Chemical Engineering Department, Environmental Engineering Program, Yale University, New Haven, CT

In the 1970s, governmental and non-governmental agencies joined forces to install hand tube wells in Bangladesh so that the residents there would have access to drinking water free of microbial contamination. Since then, the incidence of diarrheal disease has decreased. However, the discovery of extremely high levels of arsenic in the groundwater of southern Asia has resulted in the "largest mass poisoning of a population in history" (World Health Organization). The arsenic in Bangladeshi groundwater is of geogenic origin and has been measured at levels:  $>1,000 \mu\text{g As/L}$ ; WHO recommendation and US EPA regulation are  $<10 \mu\text{g As/L}$ . Unlike organic contaminants, arsenic is not degradable, so other types of point-of-use strategies, such as disinfection, are not relevant. High arsenic concentrations in the groundwater of southern Asia are expected to persist for some time, and a long-term sustainable treatment solution is needed for those who drink untreated groundwater. In this research, chitosan, a biopolymer, is used as a scaffold on which to attach specific chemical functionalities. In aqueous solution, these chitosan complexes form hydrogels, materials that do not dissolve in water but are able to interact with dissolved species. Batch experiments have been carried out to determine the As(III) and As(V) sorption capacity of these various hydrogelling materials.

### 116. Oxidation Desulfurization in Fuel Using Ionic Liquids as Phase Transfer Catalysts

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Ionic liquids based on dialkylimidazolium and N-alkyl-pyridinium cations were employed as phase-transfer catalysts (PTCs) for phase-transfer catalytic oxidation of thiophene (TS) dissolved in n-heptane, with H<sub>2</sub>O<sub>2</sub> (30%) used as oxidant. The results show that without the IL as the PTC, the oxidation desulfurization rate of thiophene was only about 12.6% with H<sub>2</sub>O<sub>2</sub>. The partition coefficients of thiophene in ILs and n-heptane were researched. The partition coefficients ranged from 0.28 to 1.04 with different ILs, while PTCs and H<sub>2</sub>O<sub>2</sub> were introduced together, the desulfurization rate of thiophene was increased. Apparently, the influence of different factors such as temperature and time bases on desulfurization was studied as well. When the IL([BPy]HSO<sub>4</sub>) was used as PTC, the remove ratio reached the maximum (94.2%). Ionic liquids as PTC can be recycled for 4 times after regenerated.

### 117. A Novel Deep Eutectic Solvent Prepared by Solid Organic Compounds

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A deep eutectic solvent or DES is a type of ionic solvent with special properties composed of a mixture which forms an eutectic with a melting point much lower than either of the individual components. The first generation eutectic solvents were based on mixtures of quaternary ammonium salts with hydrogen donors such as amines and carboxylic acids and it is able to dissolve many metal salts. This study developed a new area of DES prepared by solid organic compounds. The novel DES were synthesized by urea/caprolactam, urea/acetamide and caprolactam/acetamide at the optimal molar ratios. The physical characters such as melt point, conductivity and solubility were investigated. The melt pointing of urea/caprolactam at the molar ratio of 1:3 was about 30°C, which was much lower than raw materials. It was deduced that two organic molecules combined by hydrogen bond and formed super-molecules. Due to the formation of hydrogen bond among the molecules, the electrostatic attraction between hydrogen and organic molecules was decreased, thus the melt point decreasing. The conductivity was low, about 10<sup>-5</sup> S/m. The low conductivity may be not produced by ion, but the moving of super-molecules. The solubility of DES displayed that it was miscible with organic solvent and heterocycles organic compounds, which made it possible to instead the organic solvent and become "green solvents." Most of inorganic salts and transition metal salts were insoluble. The potentially very useful application of DES would be to use as a medium for converting compounds, such as fructose. What could be predicted was that the characteristic property of DES may be related to the H-bond among molecules. The DES would play an important role in separation and purification of organic compounds, in biocatalysis and organic reaction. The "task-specific" DES can be synthesized to use in specific solvent.

### 118. 2009 HANCOCK AWARD RECIPIENT: Enzymatic Synthesis in Deep Eutectic Solvents

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Enzymes are desirable catalysts because they give high selectivity with minimal byproducts. Often, non-aqueous conditions are required for desired reactions, particularly with industrial hydrolases. These processes commonly use volatile organic solvents (VOS), which are often flammable, toxic, and environmentally harmful. Ionic liquids (ILs) are molten salts that are recyclable, non-volatile, and non-flammable alternatives to VOS that initially showed promise in enzymatic reactions. ILs offer advantages in enzymatic reactions such as high enzyme stability, ease of product separation, and recyclability, but their high cost is prohibitive and their lack of sustainable, non-toxic materials is undesirable. Deep eutectic solvents (DES's) are physical mixtures of ammonium or metal salts and hydrogen bond donors that are promising, inexpensive replacements for both VOS and ILs. Examples are 1:2 choline chloride (a naturally occurring vitamin used in chicken feed):urea (fertilizer or animal waste product) and 1:2 choline chloride:glycerol (biodiesel byproduct). In addition to offering the recyclability, low volatility, and low flammability of ILs, DES's are composed of non-toxic and inexpensive materials including vitamins, amides, sugars, and alcohols that have costs and production scales comparable to VOS. Many of these components are natural products or can be made from renewable materials, meaning that DES's are potentially sustainable. We have found that DES's are effective solvents for a number of hydrolase-catalyzed reactions, including transesterification, epoxide hydrolysis, and ring-opening polymerization. Enzyme stability and activity in DES's is comparable to those in VOS, despite the presence of potential denaturants such as chloride or urea. We found comparable polymerization activity of *Candida antarctica* lipase B for the production of polycaprolactone from ε-caprolactone in 1:2 choline chloride: urea compared to in toluene. We also found a 20-fold conversion enhancement of epoxide hydrolase-catalyzed hydrolysis of styrene oxide to styrene glycol in 25% 1:2 choline chloride:glycerol compared to in water or water/organic mixtures.

### 119. The Barriers to the Implementation of Green Chemistry in China

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In China, the barriers to implementation of green chemistry vary from those found in the United States. In China, there appear to be more challenges arising from competing priorities between economic growth and environmental protection, along with the technical challenges from possessing a smaller base of experienced scientists and engineers. China, where rapid growth in production capacity presents an important opportunity for green chemistry implementation, is still catching up with the United States in terms of the education, training, and experience of its scientists and engineers. Overall, the research found six major challenges facing green chemistry innovators in China. They are economic and financial barriers, competing agendas between growth and environmental sustainability, training barriers, research funding barriers, barriers that arise from the system of bureaucratic incentives, and engineering capacity barriers. Despite the challenges, there is growing attention of the need to integrate green chemistry throughout the Chinese chemical enterprise. Understanding the nature of these barriers is important, because it allows for policy-makers to intervene in ways that will help to remove or mitigate them.



## 120. Design of Gelators Based On Amine and Amide Derivatives of (*R*)-12-Hydroxystearic Acid, a Renewable Feedstock Obtained From Castor Oil

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(*R*)-12-Hydroxystearic acid (*R*)-HSA is a natural product from castor oil, a renewable feedstock. It is known to gel many organic liquids. Here, we describe amine and amide derivatives of (*R*)-HSA in which the nitrogen atom (at a chain terminus) is unsubstituted or is appended with an alkyl chain (methyl, ethyl, propyl, butyl and octadecyl). Less than 1 wt % of several of these gelators gel a variety of organic liquids at room temperature. Polarizing optical micrographs show that the self-assembled fibrillar networks of the gels consist of spherulitic objects whose dimensions depend on the protocol employed to cool the precursor sol phases. Scanning electron micrographs of the xerogels reveal their helical nature. X-ray studies, conducted on silicone oil gels also show the fibrous networks that are responsible for immobilization of the liquid components. Some of the organogels exhibit thixotropic properties and they recover a large part of their viscoelasticity within seconds of being destroyed by excessive strain shearing. This recovery is an order of magnitude faster than any other organogel with a crystalline fibrillar network reported to date. Structure-gelation efficiency correlations will be discussed.

We thank the National Science Foundation for its support of this research.

## 121. CO<sub>2</sub> Capture on Carbonaceous Sorbents

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A Carbon Filter Process (CFP) is a low-pressure adsorption process aimed at separating carbon dioxide and other pollutants from combustion flue gas. CFP captures CO<sub>2</sub> on a dry carbonaceous sorbent that requires no compression or refrigeration. Such a sorbent is selective at near ambient temperatures, easy to regenerate with steam or vacuum, and does not heat up much during sorption, because its heat of sorption is low. CFP allows for flexible recovery (up to at least 90%) and flexible purity (up to at least 95%). Compared to the cost of recovered CO<sub>2</sub> using the amine process, which is about \$40-50/ton, the cost of recovered CO<sub>2</sub> using CFP can be reduced by a factor of 2 or more. The CFP technology is being scaled-up for pilot tests at two coal-fired power plants in 2009/2010. An overview of recent science, engineering, and economic data will be presented for CFP and compared to amine absorption, zeolite adsorption, and membranes. An example of previous data for separating CO<sub>2</sub> on carbonaceous sorbents is available in reference.

## 122. Hollow-Fiber-Based Adsorbent System for CO<sub>2</sub> Capture from Flue Gas

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We describe a rapid temperature swing adsorption (RTSA) system based on hollow polymer fibers impregnated with CO<sub>2</sub> sorbents and designed for the capture of CO<sub>2</sub> from the flue gas streams of coal-fired power generation facilities. This post-combustion capture system relies on a two-bed configuration, each bed being composed of hollow fibers with sorbent particles dispersed in the porous polymer matrix. The system takes advantage of the hollow fiber morphology by passing cooling water through the bores during sorption to maximize sorption capacities, and steam through the bores during desorption to release CO<sub>2</sub> to the collection system. The thin-walled hollow fibers offer the advantage of rapid heat and mass transport, with less than 1 second response times expected for both under anticipated operating conditions. To explore the economic viability of this system and provide research guidance, an economic analysis of the system is being conducted, including capital expenditures, operating costs, and compression to a sequestration-ready stream. Though the details of the economic analysis are being continually refined, it is clear that the system has the potential for a carbon cost on CO<sub>2</sub>-avoided basis that is significantly less than systems based on liquid sorbents. This potential is enabled in part by the low pressure drop across the bed and rapid cycles, both of which are made possible by the thin fiber sorbents. Our current estimate for the parasitic load on a 400MW power station is about 120MW, with about half being consumed for CO<sub>2</sub> compression. This hollow-fiber-based adsorbent system has many potential advantages over conventional and competing technologies, including low cost, no waste products, and applicability to retrofit scenarios. The system should also be applicable to many pre-combustion CO<sub>2</sub> capture scenarios.

## 123. Management of Green House Gases by Photo-Electrocatalysis

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It is well known that photocatalysts can be used to both oxidize nitrogen oxides to, for example, nitric acid and to reduce nitrogen oxide to, for example, nitrogen. In the case of photocatalytic reduction, species such as formic acid are used to act as hole scavengers to prevent electron-hole recombination. Electrocatalysis can also be used to reduce nitrites in aqueous solutions; but this usually occurs with oxidation of water to oxygen or by the use of hydrogen to generate protons. The process is quite energy intensive and uses expensive electrode materials such as Pd. In this programme, we propose to combine the photo-oxidation and photo-reduction processes in one reactor configuration by using photo-electrocatalysis.

Heterogeneous photocatalysis employs wide band-gap semiconductors such as TiO<sub>2</sub> (titania) that are subjected to UV light while contacted with the contaminant. As a result of illumination, electrons and holes are generated on the TiO<sub>2</sub> surface to initiate for example an oxidation reaction. Although TiO<sub>2</sub>, as a wide band-gap semiconductor ( $E_g = 3.1$  to  $3.3$  eV), absorbs near-UV and shorter wavelengths of the electromagnetic spectrum, TiO<sub>2</sub> has been favoured in this regard because it is abundant, inexpensive, and resists photo-corrosion.

## 124. Designer Reversible Ionic Liquids for CO<sub>2</sub> Capture

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We have reported the development of reversible ionic liquids (Rev-ILs) and demonstrated their superior capabilities in capturing and releasing CO<sub>2</sub>. Rev-ILs combine chemical and physical absorption of CO<sub>2</sub>. The precursor molecule reacts with CO<sub>2</sub> to generate the Rev-IL, which further absorbs CO<sub>2</sub> via physisorption. The captured CO<sub>2</sub> is released upon elevating the temperature, and the precursor is regenerated and recycled. Further, we are optimizing these solvents by tuning the structure. Structure-property relationships enable the design of CO<sub>2</sub> capture solvents with large capture capacity, low heat requirements for regeneration, favorable equilibrium temperature for capture and release, minimal cycling losses, and low operating cost.

Previously, we have designed and tested two-component Rev-ILs based on amines and guanidines. Now we have synthesized and tested single-component Rev-ILs, which provide simplified chemistry, lower energy penalty, and minimal processing losses. In addition, we are using silanes to enhance CO<sub>2</sub> capture capacity and reduce viscosity to improve mass transfer. We report the thermodynamic properties and reaction rates of these Rev-ILs measured using a high pressure ATR FT-IR cell.

## 125. A Study of Carbon Dioxide Adsorption Performance by the Ion Exchange of Zeolite-13X

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To utilize the gasification product of waste material, CO<sub>2</sub> must be separated from the gas mixture of CO<sub>2</sub>, CO, H<sub>2</sub> to produce medium-Btu syngas mainly composed of CO and H<sub>2</sub>. The syngas can be utilized as fuel in the gas engine for electricity generation, which has higher efficiency or feedstock in C-1 chemistry to produce useful chemical raw materials. In the present investigation, the possible recipe of candidate sorbents are designed and manufactured with various manufacturing methods as well as different composition of Zeolite and inorganic/organic binders. Prepared sorbents are conducted with CO<sub>2</sub> adsorption/desorption experiments in the lab-scale heater in the various reaction condition. Sorbent manufactured with hydro-thermal synthesis showed higher CO<sub>2</sub> adsorption than that with extrusion molding. Resulting sorbent samples are analyzed by XRF, XRD and BET to determine the compositional and physical properties. Zeolite samples of ion exchange with Li<sup>+</sup>, Na<sup>+</sup>, K<sup>+</sup>, Ca<sub>2</sub><sup>+</sup> are also experimented adsorption/desorption and found that Na<sup>+</sup> exchanged sorbent showed higher absorption compared to others.

## 126. HCR-188C: An Alternative “Green” High-Efficiency Hydrocarbon Refrigerant

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A.S. Trust has developed a hydrocarbon formula, HCR-188C, that has been ranked as having zero ozone depletion potential (ODP) and a global warming potential (GWP) of less than 5 over the standard 100-year time horizon. HCR-188C is a low-cost mixture of C<sub>1</sub> to C<sub>7</sub> hydrocarbons. The proprietary mixture of isomers yields the specific application for peak cooling performance. HCR-188C has

been listed by the USEPA (December 15, 2008) under the Significant New Alternatives Policy (SNAP) program as approved for use in household refrigerators and window air conditioners. The optimal charge rate for HCR-188C has been tested to be 1/4<sup>th</sup> that of R-12 and R-134a. Because of the low charge rate and low operating pressures, there is considerable savings in terms of the reduced amount of energy required to operate air conditioning and refrigeration systems with HCR-188C, as shown by test data. For systems where the condenser and bulk of the refrigerant lines are isolated from areas of human exposure (e.g., automotive systems, central air conditioning systems, commercial refrigeration split systems), a safety valve has been designed to vent any sudden unexpected releases of HCR-188C to the outdoors. Because of the low charge rates, low toxicity, and the safety valve for certain applications, the risk to humans from use of HCR-188C has been determined to be very low. The cooling efficiency tests, exposure modeling, fault tree analysis, and risk assessment results will be presented for selected applications.

## 127. Continuous Processes in Small-Scaled Reactors under cGMP Conditions: Towards Efficient Pharmaceutical Synthesis

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To meet quality requirements of their products, the pharmaceutical industry has historically almost exclusively used batch processes even where continuous processes are superior in terms of chemical selectivity, safety, and process control. Margins were high and volumes were frequently small. Therefore the drivers to increase the economy and the ecological footprint of processes have been small compared to the drivers to produce high quality material reliably.

The key element of pharmaceutical batch synthesis has been the “in-spec batch produced by a well-understood process in a qualified plant.” The U.S. FDA’s Process Analytical Technology (PAT) initiative now strongly encourages producers of active pharmaceutical intermediates and ingredients to consider continuous processes more seriously, encouraging their use whenever possible. Apart from their potential to apply “quality by design” principles, these processes offer possibilities for continuous improvement over the life cycle of a pharmaceutical. Their superior selectivity allows reducing waste drastically.

As a technology-driven company, DSM has already developed continuous processes based on microreactor technology to improve selectivity and throughput of fine chemicals synthesis involving hazardous materials. Following the principle to “have each phase of a chemical reaction proceed in the ideally suited environment” we have been able to increase yields of various processes considerably. Recently we have shown that continuous processes based on dedicated micro reactors can also be advantageously used in a cGMP regime.

The advantages of continuous processing in micro-structured reactors, its implications for pharmaceutical synthesis and the consequences for process development are discussed.



## 128. Continuous Microreactor Development: Transport and Biofuel Studies

Paul Chin, Brad A. Pindzola and Arthur D. Schwope, TIAX LLC, Cambridge, MA

Since the publication of the *Twelve Principles of Green Chemistry* in 1998, industries have slowly begun to push for development of green chemistry and engineering. Towards the latter goal, the concept of process intensification is used to change process technologies, yielding improved product quality, throughput, and energy efficiency. With this design philosophy in mind, and drawing on decades of experience and investment, TIAX has developed a proprietary microreactor technology platform that overcomes many challenges limiting their use in the chemical industry.

The TIAX microreactor enables flexible, real-time control over a range of process conditions. The reactor operates continuously, enabling “high-throughput” experimental screening (modifying process conditions in real-time and over wide ranges, e.g., residence time, concentration, temperature, pressure). Thus, chemical processes can be optimized at the bench in a fraction of the time needed using batch systems.

The microreactor is capable of high rates of mass transfer and mixing, even with viscous liquids and multi-phase systems. The reactor can be equipped with distributed energy sources or sinks beyond heating and cooling to provide the freedom to explore novel, or previously impractical, reaction conditions. This presentation will focus on experiments in the TIAX microreactor to elucidate the heat and mass transfer characteristics, and a study of biofuel production by plant oil transesterification.

## 129. Process Design toward Continuous Manufacturing: a Green Perspective

David J. am Ende, Chemical R&D, Pfizer, Inc., Groton, CT

Facing increased cost pressures in the pharmaceutical industry, the need for increasing efficiencies and driving down costs is evident. These include process development as well as manufacturing costs. With these challenges bring new opportunities for integrating chemical engineering science and process design into Process R&D with the aim to develop and launch lower-cost, safe, green, and well-understood processes, while continuing to deliver high quality API. The presentation will illustrate a few of the technology areas within Process R&D such as predictive modeling, process design, and continuous processing aimed, in general, toward enhancing process understanding, delivering green processes, and ultimately toward reducing costs.

## 130. Design, Modeling and Optimization of a Gas-Phase Catalytic Channel Reactors

Alex Omo Ibhaddon, Department of Environmental Sciences/ Chemistry, University of Hull, Hull, United Kingdom

Experimentally validated design of a Channel Gas-Phase reactor with photo-electrochemical enhancement (PE) is reported. Modeling studies involving kinetic, mass transfer parameters, surface reactions, the effect of light absorption on the reactions as well as reactor geometry, indicate that the reactor can be used for gas-phase heterogeneous oxidation reactions, for example, in the detoxification of volatile organic compounds in enclosed atmospheres. The Channel reactor is characterized in terms of the permeability and gas to solid mass transport. This is achieved by performing limiting current techniques using a liquid with the same Reynolds number as for the gas phase system. A mathematical model brings together the transport and mass transport behaviour of the reactor with the kinetics of the photo-

catalytic reactions as determined experimentally and the fluid flow behaviour enabling the simulation of the effect of temperature, concentration of contaminants, pressure, wavelength, and light intensity on reactant conversion. The fluid flow distribution is modeled two-dimensionally to allow the determination of fluid residence time distributions through the catalyst microstructure and any potential inactive zones.

The Channel reactor is optimized by varying the residence time, channel dimensions and the characteristics of the catalyst used including the thickness. A novel feature of the Channel reactor is the introduction of photo-electrochemical (PE) enhancement to suppress electron-hole recombination. This first attempt to carry out gas phase photo-electrochemical oxidation required the optimization of the electrode structure, thickness and ionomer content, achieved both by modeling the current distribution and experimentation. Results indicate that varying the structural parameters, measuring photocurrent and electrode response in a solid-state cell enabled the simulation of the actual photo-electrochemical channel reactor.

## 131. Integrated Direct Cooling Suspension Crystallization and Absorption Refrigeration Process for PX-Purification

Min Huang<sup>1</sup>, De-jin Kong<sup>2</sup>, Jie Cai<sup>2</sup>, Ying Zhu<sup>1</sup>, Yan-zi Guo<sup>1</sup>, Yan Wang<sup>1</sup>, Si-si Guo<sup>1</sup>, and Jun Wu<sup>1</sup>, (1)Chemistry, Tongji University, Shanghai, China, (2)Shanghai Research Institute of Petrochemical Technology, SINOPEC, Shanghai, China

A continuous direct cooling suspension crystallization process with integrated absorption refrigeration unit was studied. The propane-hydrocarbon absorption refrigeration unit was powered by the waste heat generated from the top of the distillation towers within the disproportionation process preparation unit. Pure liquid propane from the generator in the absorption refrigeration unit was directly introduced into the suspension crystallizer. After evaporation and providing cooling power to the crystallization unit, the propane gas was separated then absorbed by the liquid phase hydrocarbon to complete the refrigeration cycle.

Xylene isomer ternary solid-liquid phase equilibrium was investigated experimentally, mathematical equations were derived. The continuous direct cooling suspension crystallization process was optimized by calculating material and energy balance of the process. A propane-hydrocarbon absorption refrigeration unit with COP around 10% will be sufficient to convert the waste heat from the top of the distillation towers to the cooling power for the crystallization unit. The optimized first and second stage temperatures were found to be at 276K and 248K~265K, which agrees well with the industrial operation conditions.

Current industrial crystallization process utilizes compression refrigeration system which, based on the Selective Toluene Disproportionation xylenes, consumes up to 50 kWhr electricity for one metric ton of PX product. This paper describes a new energy efficient process that uses waste heat to power absorption refrigeration, which would save a significant amount of electricity, therefore, indirectly reducing large amount of CO<sub>2</sub> green house gas emission.

## 132. Renewable Water Soluble Polymer: Polyitaconic Acid

Yvon Durant, Itaconix, Hampton Falls, NH, and Mathieu Chirat, Materials Science, University of New Hampshire, Durham, NH

Itaconic acid (IA) is commercially produced by the fermentation of carbohydrate, primarily glucose, using *Aspergillus Terreus*. Consequently it is a fully renewable material. Itaconic acid has been extensively copolymerized but has been recalcitrant to homopolymerization. Only very recently it has been homopolymerized into polyitaconic acid using a process developed

at the University of New Hampshire. The process requires no solvent, generates no materials waste and produces a water soluble polymer with low residual monomer(s), at high polymerization rates. This water soluble polymer has intrinsic properties that rivals the ones found for polyacrylic acid and other carboxylic acid polymer and copolymers. Polyitaconic acid has superior performance advantages in some specific areas when stabilization, dispersion, and chelation of calcium, barium, and manganese are needed. Applications are evolving in the area of detergents, dispersants, and water treatment, especially where sustainability and renewability is needed.

### 133. Chemically Modified Fatty Acids as Styrene Replacement in Vinyl Ester Polymers

*Alejandrina Campanella<sup>1</sup>, John J. La Scala<sup>2</sup>, and Richard P. Wool<sup>1</sup>, (1)Department of Chemical Engineering, University of Delaware, Newark, DE, (2)Army Research Labs, Aberdeen Proving Grounds, MD*

Vinyl ester (VE) resins that are employed in many commercial applications need diluents to allow the resins to be molded using liquid molding techniques. These diluents are typically volatile organic compounds that should be avoided to reduce health and environmental risks. Therefore, two different bio-based reactive diluent modified fatty acids (MFAs), acrylated fatty acid methyl esters (AFAME) and methacrylated lauric acid (MLA), were employed to replace styrene. The viscosity, mechanical properties of the resulting polymers were measured and analyzed. Resins were prepared with various VE:MFA mass ratios. The glass transition ( $T_g$ ) values were predicted using the Twinkling Fractal Theory of  $T_g$  and were found to be in good agreement with the experimental results. Time-temperature superposition experiments were also conducted in this work, and we found that as the MFA content increased the loss modulus master-curve became broader and shifted to higher frequencies, thereby exhibiting more rubber-like behavior. The resins employed in this work were also compared to the VE resins copolymerized with 30 wt.% of styrene.

### 134. Twinkling Fractal Theory of the Glass Transition with Green Chemistry Applications

*Joseph F. Stanzione III and Richard P. Wool, Department of Chemical Engineering, University of Delaware, Newark, DE*

A fundamental understanding of the nature and structure of the glass transition in amorphous materials is currently seen as a major unsolved problem in solid-state physics. In order to solve this problem, we propose a conceptual approach to understanding the glass transition temperature ( $T_g$ ) of glass forming liquids called the Twinkling Fractal Theory (TFT). The development of dynamic percolating fractal structures near  $T_g$  in amorphous polymers is the main element of the TFT. The key concept of the TFT derives from the Boltzmann population of excited states in the anharmonic intermolecular potential between atoms, coupled with percolating solid fractal structures near  $T_g$ . The percolating fractal *twinkles* with a frequency spectrum that is a function of both temperature and time as solid and liquid clusters interchange. The twinkling fractal spectrum at  $T_g$  predicts the dynamic heterogeneity behavior via a spatio-temporal thermal fluctuation autocorrelation relaxation function. We present an experimental dielectric atomic force microscopy technique to validate the TFT with preliminary data of traditional petroleum-based polymers. Currently, we are extending this work to include bio-based materials such as acrylated epoxidized soybean oil. The ultimate goal of this research is to gain greater knowledge of the physical properties of amorphous materials from the TFT such that desired characteristics of materials are predicted accurately while eliminating the need to spend time, money, materials, and energy by conducting costly experiments.

### 135. Enzyme-Catalyzed Conversion of Glycerol to Glycerol Carbonate

*Kerri Cushing and Steven Peretti, Chemical and Biomolecular Engineering, North Carolina State University, Raleigh, NC*

The recent growth of the biodiesel industry has resulted in an excess of glycerol for which there is no market. This surplus glycerol offers an interesting opportunity to produce biomass-derived raw materials and chemical intermediates that have previously been manufactured from petroleum. If the surplus glycerol can be converted into a higher value product, the economics of the biodiesel production would be enhanced. This project aims to convert glycerol to glycerol carbonate, a versatile chemical that may be used as a solvent or additive by itself, or as a platform chemical for other industries. Lipases, which are able to catalyze ester synthesis reactions in low water environments, were evaluated as biocatalysts for a reaction between glycerol and a dialkyl carbonate. Multiple lipases, dialkyl carbonate reactants, solvents, and reaction conditions were considered. It was found that the conversion of glycerol to glycerol carbonate can be effectively catalyzed by *Candida antarctica* lipase B. A solvent is not required for this reaction, but it can enhance lipase activity. The rate of reaction as well as the product specificity differs for different dialkyl carbonate substrates. The effects of reaction water content, lipase loading, and reactant molar ratios were also investigated. Under the right conditions, nearly 100% glycerol conversion was achieved after 12 hours of reactions time, with the primary product being glycerol carbonate. The effect of these various reaction conditions on lipase activity and product selectivity will be presented.

### 136. More Efficient Epichlorohydrin from Glycerin

*Bruce D. Hook Sr.<sup>1</sup>, John R. Briggs<sup>2</sup>, William J. Kruper<sup>2</sup>, Perry Basile<sup>1</sup>, and Ernesto Occhiello<sup>1</sup>, (1)Epoxy R&D, The Dow Chemical Co., Freeport, TX, (2)Research and Engineering Sciences, The Dow Chemical Co., Midland, MI*

The Dow Chemical Company is currently the world's largest producer of epichlorohydrin, a key building block in the synthesis of liquid epoxy resins. In 2006, Dow announced its intent to manufacture epichlorohydrin in China (150 kTpa) via a novel, acid-catalyzed hydrochlorination process using glycerin. The increased availability of glycerin stems from the production of biodiesel. The process not only utilizes a renewable feedstock, but it allows for an economically attractive alternative to the incumbent process.

This paper will discuss the advantages of the Dow glycerin-to-epichlorohydrin process (GTE) over that of existing process routes. These include much faster reaction kinetics, the ability to produce a more concentrated dichlorohydrin stream, high regioselectivity to 1,3-dichloro-2-propanol, formation of very low levels of RCI byproducts, and the fact that this process, run in either batch or continuous operation, may operate without a solvent. All of these advantages make this process more sustainable by reducing unit operations, the environmental footprint, and overall manufacturing costs. The focus of this presentation will be on environmental and energy costs.



## 137. Biogenic Silica for Construction and Industrial Applications

R. K. Vempati<sup>1</sup>, Prasad Rangaraju<sup>2</sup>, Elena Pisanova<sup>3</sup>, John Lund<sup>3</sup>, and Jean-Claude Roumain<sup>4</sup>, (1)Department of Chemistry, Southern Methodist University, Dallas, TX, (2)Civil and Environmental Engineering, Clemson University, Clemson, SC, (3)Harper International, Lancaster, NY, (4)Holcim Cement, Louisville, CO

The United States generates 7.1 million tons of this biomass and it is an added cost to the farmers for its disposal. For instance, the rice mill owners in Texas are being paid \$8 per ton for their rice hulls, which in most cases does not even pay for its freight. Hence, rice hulls are a definite expense to most rice mill owners in Texas and throughout the country. The United States Environmental Protection Agency (USEPA) restricts open heap burning of this product as it generates undesirable smoke. In addition, dumping rice hulls in a landfill site is undesirable because the anaerobic decomposition results in the subsidence of the landfill site. Rice hulls contain 18 to 20% amorphous SiO<sub>2</sub> by weight. We have developed a patented green and sustainable technology where the 80% of the organic component can be burnt off maintaining the resulting off white SiO<sub>2</sub> in amorphous state. The CO<sub>2</sub> emission is "Carbon Neutral;" therefore, there is no need to capture and treat it. Further, except for particulate scrubber, there is no need for SO<sub>x</sub> and NO<sub>x</sub> scrubbers. The process of making the RHA will be discussed along with the physical, chemical and mineralogical properties. This residue can be used to make several other value-added products, e.g., high performance concrete (HPC), and zeolite syntheses. This presentation will focus on manufacturing the material and its applications to the HPC industry.

*This research was funded by the National Science Foundation under the SBIR Phase II Grant No. 0724463 to ChK Group, Inc., Plano, TX.*

## 138. Performance of Carbon-Neutral Rice Hull Ash as a Supplementary Cementitious Material in Portland Cement Mortars

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This presentation is the second of the two presentations that focus on rice hull ash (RHA). In this presentation, the performance of a carbon-neutral RHA as a supplementary cementitious material for use in portland cement composites will be discussed. The RHA used in this study was developed through an improved combustion technique that resulted in very low unburnt carbon content in the RHA. Also, with its very high levels of amorphous biogenic silica, the RHA has a significant potential for use as a supplementary cementitious material in portland cement composites. Various tests conducted in this study focused on investigating the influence of RHA on selected properties of portland cement pastes and mortars. In specific, effort was focused on studying its microstructure, pozzolanic reactivity, and the effect of grinding RHA on its pozzolanic reactivity. In addition, the effect of RHA dosage on the workability (flow) and mechanical properties of cementitious mortars was studied. Based on the results from these studies, it was found that RHA was highly pozzolanic in nature. Also, the use of RHA as a cement replacement level at dosage levels up to 20% by mass of cement yielded significant improvement in compressive strength of mortars. Grinding RHA to a finer size further improved the performance of RHA as supplementary cementitious material. However, the use of RHA as a supplementary cementing material resulted in substantially increased water demand of the mortars, regardless of the dosage level. The increased water demand was easily alleviated by the use

of adequate amounts of high-range water reducing agent in the mortars. Further investigations on the impact of RHA on durability of portland cement composites are being investigated. It is anticipated that with further evaluation and refinement, the biogenic silica from rice hull can be a valuable resource in developing environmentally sustainable construction materials.

## 139. Bio-Composites From Chicken Feathers and Plant Oils for Printed Circuit Boards

Mingjiang Zhan and Richard P. Wool, Department of Chemical Engineering, University of Delaware, Newark, DE

For decades, more than 90% of printed circuit boards (PCB) are based on fiberglass reinforced polymer composites. Today, the most successful and widely used resin systems for PCBs are epoxy resins, which are petroleum-based and non-renewable. The process of manufacturing woven fiberglass cloth begins with melting the various inorganic components, which requires a large amount of energy. Flame retardancy of PCBs has commonly been achieved by brominating the epoxy resin, which brings environmental and health concerns.

To decrease environmental impact and health concerns, we presented new bio-based composites from modified plant oil, halogen-free flame retardants, and chicken feather fibers for printed circuit applications. Epoxidized soybean or linseed oils and different types of polycarboxylic anhydrides were used with presence of catalysts. Chicken feather fibers are all natural and these fibers are compatible with several modified plant oil resins. The hollow, light weight fibers innately contain a significant volume of air which made their dielectric constants lower than e-glass fibers. The feather fibers are tough enough to withstand both mechanical and thermal stress. Chicken feathers are abundant and cheap since the U.S. poultry industry generates more than one billion kilograms of feathers annually as byproducts. Alternatively, epoxidized plant oils were also functionalized with acrylate groups, guided by the newly developed Twinkling Fractal Theory. The halogen-free diethylphosphinic acid aluminium salt and/or melamine polyphosphate were added to the system as flame retardants.

The bio-composites were optimized to meet the requirements of IPC 4101B specifications. The peel strength, dielectric properties, resistivity, flexural strength, and flammability of the resultant materials met or were close to the requirements.

The new bio-based PCBs from plant oils and chicken feathers, which potentially can replace the conventional FR-4 laminates, had much less carbon dioxide footprint and were more sustainable.

## 140. Design Signals from Environmental Health Sciences: What Every Chemist Should Know

Lin Kaatz Chary, Great Lakes Green Chemistry Network, Gary, IN

With over 80,000 chemicals in commercial use and a rapidly growing scientific literature documenting the negative environment and health effects of many chemicals in common use, the public is increasingly demanding safer products. Environmental Health Sciences and Green Chemistry are two fields of science that collectively promise to have significant – and growing – impact on public health. The degree to which these two fields are able to communicate across disciplinary boundaries will profoundly affect the efficacy of both. Moreover, such cross-fertilization will advance Green Chemistry's mission to minimize or eliminate inherent hazard. In this special session, some of the key leaders in the Environmental Health Sciences will define the field and its relevance for chemists.

- Speaker 1: Linda Birnbaum, Director, National Institute of Environmental Health Sciences, National Institutes of Health
- Speaker 2: Howard Frumkin, Director, National Center for Environmental Health, Agency for Toxic Substances and Disease Registry
- Speaker 3: Peter DeFur, President, Environmental Stewardship Concepts, Affiliate Associate Professor, Center for Environmental Studies, Virginia Commonwealth University
- Speaker 4: Jane Houlihan, Vice President for Research, Environmental Working Group

#### 141. Understanding Enolate Chemistry and the Tishchenko Reaction under High Speed Ball Milling Conditions

*Daniel C. Waddell, Indre Thiel, S. Tyler Marcum, Brandon Smith, and James Mack, Department of Chemistry, University of Cincinnati, Cincinnati, OH*

Due to increased interest in the development of more environmentally benign synthetic methods, there is a strong effort to revolutionize the manner by which chemists conduct organic reactions. One method is the use of a novel, high energy, solvent-free technique known as high speed ball milling (HSBM). Since conducting chemical reactions under these conditions is a new area, many of the fundamental rules that govern these reactions need to be understood. We report our ability to generate regio- and stereoselective enolates of 2-methyl cyclohexanone. Our results show that we can selectively create kinetic vs thermodynamic products utilizing HSBM. Using sodium hydroxide we observe a thermodynamic: kinetic product ratio of 13.5:1. Alternately, using lithium hexamethyldisilazide we observe thermodynamic:kinetic product ratio of 1:2. We also discovered NaH, which is typically a non-nucleophilic base in solution, acts as a nucleophile under HSBM conditions. We were able to conduct the Tishchenko reaction, a transformation of an aldehyde to its dimeric ester, for a variety of aryl aldehydes. For example, benzyl benzoate, used in flavorings and fragrances, can be prepared under these conditions in >99% yield. The Tishchenko reaction is particularly environmentally friendly because it makes use of a catalyst and is 100% atom economic.

#### 142. Pot-In-Pot Reactions: A New Paradigm in 'ad Infinitum' Cascade Reactions

*Martin T. Mwangi<sup>1</sup>, Michael D. Schulz<sup>2</sup>, Rachel J. Elsey<sup>3</sup>, Anne Beaubrun<sup>4</sup>, and Ned B. Bowden<sup>1</sup>, (1)Department of Chemistry, University of Iowa, Iowa city, IA, (2)Department of Chemistry, University of Iowa, Iowa City, IA, (3)College of Pharmacy, University of Iowa, Iowa city, IA, (4)Duke University, Durham, NC*

Many excellent examples of homogeneous catalysts have been developed that elegantly and efficiently catalyze one reaction at a time. Although the use of catalysts is ubiquitous in chemical synthesis, reactions must be carried out sequentially; else the catalysts/reagents may poison one another or require incompatible reaction conditions. These limitations make organic synthesis a tedious, expensive, and wasteful process. The process of multi-step synthesis is also not environmentally benign based on the sheer volume of waste generated per step. To overcome some of these limitations, catalysts have been site-isolated from each other therefore facilitating several steps in one reaction pot. However, available site-isolation methods have major shortcomings. Therefore, a general approach that works via already known chemistry and catalysts, without the need for further modification, is desired.

We report a new approach to catalyst site-isolation. We exploited the advantages of both heterogeneous and homogeneous processes to develop new cascade reaction sequences by employing polydimethylsiloxane (PDMS) thimbles as selective semi-permeable walls. These thimbles allow small organic molecules to diffuse through while retaining polar reagents and/or organometallic catalysts. A felicitous choice of reaction conditions led to the development of pot-in-pot reactions, a new concept in organic catalysis. To demonstrate how dynamic this new technique is, we performed 2- and 3-step cascade reactions. This new approach circumvents the need to isolate intermediates, therefore enabling synthesis of otherwise challenging molecules. The genesis of our work was the occlusion of an organometallic catalyst in PDMS slabs to perform catalysis in aqueous solvents. Also, by simply occluding the catalyst in a polymer matrix, it was possible to dictate whether the Grubbs' catalysts gave a metathesis or an isomerization product. Since our work demonstrates site-isolation of a whole reaction process, there is a need to redefine the term catalysis to accommodate this heterogenization of homogeneous reaction processes.

#### 143. Anchored Homogeneous Catalysts as Environmentally Favorable Alternatives to Homogeneous Catalysts

*Robert L. Augustine, Setrak K. Tanielyan, Gabriela Alvez, and Norman Marin, Center for Applied Catalysis, Seton Hall University, South Orange, NJ*

Even though catalysis, in general, is a mainstay in 'green synthesis' there are some problems in this area, which still need solving. Most important in this regard is the synthesis of pharmaceutical and specialty chemicals using homogeneous catalysts, which are capable of selectively promoting a variety of synthetically important reactions which cannot be catalyzed by the common dispersed metal heterogeneous catalysts. The use of homogeneous catalysts, however, can present environmental problems associated with the commonly used solvents and the separation of the complex, both metal and ligand, from the reaction product. While a number of techniques have been developed to facilitate this separation, one of the most promising is that of immobilizing the complex on a solid support. After being used, these immobilized catalysts are removed from the reaction mixture by filtration.

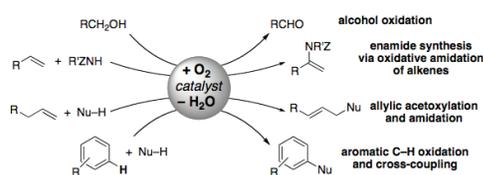
We present here a discussion of our Anchored Homogeneous Catalyst technology by which a catalytically active complex is anchored to a solid support using a heteropoly acid (HPA) as the anchoring agent. The complex is attached to the HPA by an O-Metal bond. These catalysts are generally as active and selective as the homogeneous analogs and can be used in both chiral and achiral reactions as well as in batch or continuous reactors. They are stable at pressures up to 1000 psig and temperatures up to 200°C. Metal leaching is virtually non-existent with, typically, less than 1 ppm of metal detected in the reaction mixture.

The presentation will include a discussion of the Anchored Wilkinson catalyst with which substrate to catalyst ratios of 250,000 have been observed, the use of anchored catalyst precursors from which a number of anchored chiral catalyst have been obtained, as well as the utilization of these catalysts to promote reactions other than hydrogenation.

## 144. Scalable Catalytic Methods for Selective Aerobic Oxidation of Organic Molecules

Xuan Ye<sup>1</sup>, Matthew H. Yates<sup>2</sup>, Martin D. Johnson<sup>2</sup>, and Shannon S. Stahl<sup>1</sup>, (1)Department of Chemistry, University of Wisconsin-Madison, Madison, WI, (2)Eli Lilly and Company, Indianapolis, IN

Molecular oxygen is the most attractive oxidant available for chemical synthesis from the perspective of cost and waste minimization. In recent years, academic researchers have discovered a wide range of synthetically useful catalytic aerobic oxidation methods (see Scheme 1), most of which proceed effectively in non-chlorinated organic solvents. The first part of this presentation will survey recent advances in this field. Despite these new opportunities, however, safety concerns continue to hinder the use of these reactions in large-scale applications within the pharmaceutical and fine-chemical industries. The second part of this presentation will describe the results of an academic-industrial collaboration that has led to a safe and scalable method for the implementation of catalytic aerobic oxidation methods. Our approach utilizes a continuous-flow, rather than batch, process that minimizes the reaction volume exposed to elevated pressures of O<sub>2</sub>.



## 145. Design of Green Recyclable Supported Catalysts for Organic Transformations

Brindaban C. Ranu, Department of Organic Chemistry, Indian Association for the Cultivation of Science, Kolkata, India

The heterogeneous supported catalysts are of much current interest because of their primary advantages such as, ease of separation, reusability, improved efficiency due to stable active site and better steric control of a reaction intermediate, compared to their homogeneous counterparts. These qualities made them very promising for applications in industry. Recently, we have developed a number of heterogeneous supported catalysts, which showed improved efficiency for several important reactions. These include hydroxyapatite supported palladium for Heck reaction towards synthesis of en-yne carboxylic esters, molecular sieves (4 Å) supported palladium for Suzuki coupling, copper oxide supported Pd(0) nanoparticles for shape selective Suzuki and cyanation reactions, alumina supported copper sulfate for arylation of thiols, amines and phenols in water, and polyacrylamide supported Ru nanoparticles for allylation of thiols in water. The significant advantages of these reactions are simple operation, high yields, reusability of the catalysts, and high TON. These advantages make these catalysts suitable for industrial applications. The details will be presented.

## 147. Using I.P. to Fuel Your Business

Carlyn A. Burton and Jeffrey S. Bergman, Osha Liang LLP, Houston, TX

It is without question that intellectual property is an important part of any business's value and success in the marketplace. Like any asset, intellectual property (IP) requires a capital investment; and it should not be sought haphazardly. A regular strategic review of a company's intellectual property policies and portfolio, as well as employee education, will bring clarity to the question of "are we maximizing our potential assets?" With increasing levels of funding in the sustainable energy sector, maximizing potential assets through intellectual property should be at the forefront of any research and development or scale-up efforts. Further, in the course of a commercial viability analysis, consideration of other parties' intellectual property can help minimize the potential asset from becoming a liability rather than an asset. While these considerations are important for any business sector, they are of extreme importance in emerging business sectors, such as the sustainable energy sector. Specifically, outside investors often review and value a company based on its IP portfolio and freedom to operate. Potential challenges and opportunities for IP, in biofuels, for example, include methods of obtaining feedstock, co-products, and the entire processing cycle. From avoiding stepping on a competitor's rights or acquiring one's own, the sustainable energy sector is going to continue to see an increase in activity in the IP arena. This talk will discuss these issues as well as provide an overview of recent developments in IP law that are of significant interest to those in the sustainable energy arena. Understanding these implications and evaluating potential patent filings based on these considerations should be a part of any company's intellectual property strategy.

## 148. LCA — Making the Sausage

Paul Chalmer, NCMS, Ann Arbor, MI

Life-cycle assessment (LCA) should be as straightforward as cost accounting. While it might take special training to audit financial statements, anyone who can operate a cash register should be able to input the required data and understand the totals. By the same token, a product designer or a consumer who is concerned with the environmental consequences of his or her choices should be able to input a few pieces of readily available data about an item they are considering, and receive a good approximation of the energy consumed or greenhouse gas emitted over the life cycle of the item.

LCA as currently practiced does not lend itself to this goal. Everything is connected to everything else, system boundaries are always somewhat arbitrary, and life-cycle questions are inherently complicated. But we can make significant progress, even while leaving standard LCA methodology intact, with a few changes in interpretation. A key idea is to stop treating LCA results as engineering numbers, but as indicators that act more like prices and dollar amounts in balance sheets. The numbers are meaningful, and can be used quantitatively, but they include values choices and cannot be specified in terms of physical measurements. The best LCA number is as much a matter of consensus as "correctness."

In this presentation, we will look at some specific examples of how this approach looks when reduced to practice. In particular we will look at three different LCA tools in spreadsheet format that generate ...

- cradle-to-gate materials impacts for several common commercial materials (including metals, plastics, and wood)

- gate-to-gate manufacturing impacts for selected industry sectors (e.g. furniture manufacture)
- full LCA impacts for a specific product type (paints and coatings)

... from a few items of user input data, applied to stored industry data from a variety of available sources.

#### 149. EPA's Green Racing Initiative

*John C. Glenn, Office of Resource Conservation and Recovery, U.S. Environmental Protection Agency, Arlington, VA*

Auto racing, for the better part of one hundred years, used engine displacement as the primary metric for regulating power. The result has been the development of engines that make a great amount of power per unit of engine displacement. Street engines emulated race engines, which led to today's small, powerful, spark ignition, gasoline engines – engines that maximize power density, but not energy efficiency. If a hundred years ago, racing had used fuel allocation instead of engine size to control the sport, we would all be driving more energy efficient cars today.

EPA in collaboration with the Department of Energy and SAE International approached auto racing in 2005 to discuss the use of energy allocations as the primary way to control power. We felt that this single change would turn motor sports into a laboratory for energy efficiency and accelerate the development of energy efficient technologies. It would force race engineers to get the most power per unit of energy instead of power per unit of engine displacement. It would completely change racing. Diesels and hybrids would become the race engines of choice.

The American Le Mans Series is the first race series to embrace the concept. Our initial step with the ALMS has been to develop "a race within a race." EPA, Argonne National Laboratories, and the International Motor Sports Association developed a sophisticated program measuring wells to wheel energy efficiency, greenhouse gas emissions, and petroleum displacement for each race car. The car that goes the fastest, using the least amount of energy and petroleum while creating the fewest GHGs is the winner of the Green Racing Challenge. Our first race was in October 2008. The winner of the GT class was a Corvette using cellulosic E-85 and a Porsche RS in the Prototype class.

#### 150. Life Cycle Pollution Prevention Utilizing Automated, Web-Based Assessment of "Green" Chemicals, Products, Munitions and Processes

*George R. Thompson, Chemical Compliance Systems, Inc., Lake Hopatcong, NJ*

Individuals involved with the development, manufacture, or procurement of "green" chemical products base their decisions upon one, or more, of four life cycle stages: (1) design/material procurement, (2) manufacturing, (3) usage/ storage/transport, and (4) disposal. Quantitative criteria for "green" chemicals and products have been derived from our relational database (R-CPD) that includes more than 75,000,000 data elements for over 260,000 chemicals and 350,000 chemical products compiled over the past 24 years from over 1,000 sources. We have also developed Web-based "green" product, munition, and process analytical compliance systems (GP-CAS, G-MACS and G-PACS, respectively). All three systems utilize 43 ecological, health, and safety data 43 endpoint criteria. GP-CAS and G-MACS provide assessments for the first and third stages of the LCA. GP-CAS and G-MACS provide automated, objective, and quantitative "green" ratings for a chemical, product, or munition within seconds, and also quantitatively identify the

type of compromising hazard(s), and the contributing hazardous chemical constituent(s) within the product. GP-CAS and G-MACS also provide constituent impacts on over 112 state, federal, international and third party regulations, and can be utilized for "green" assessments of individual products or munitions, or for comparison of the "greenness" of similarly functional products (e.g., spray paints, cleaners, mortars, bombs, etc.). G-PACS can be utilized for green assessments of both the second and fourth LCA stages for a single, or alternate, process. G-PACS quantitatively ranks the process, or wastestream, chemicals from the worst to best "greenness," thereby focusing incremental pollution prevention improvements on the least "green" chemicals first. Each of these three systems can also provide comparative assessments utilizing Alternative Chemicals data from R-CPD. GP-CAS/G-MACS, and G-PACS provide a "green" LCA analysis for any product and munition in any organization or industry that can be applied to individual life cycle stages, or together, across all life cycle stages.

#### 151. GlaxoSmithKline's Experiences with Life Cycle Assessment

*Concepción Jiménez-González, Cehs, GlaxoSmithKline, Research Triangle Park, NC*

GlaxoSmithKline has investigated life cycle impacts in the pharmaceutical supply chain for more than a decade, incorporating life cycle inventory and assessment (LCI/A) within metrics, tools, and decision systems within the organization to drive towards more sustainable business practices. This presentation intends to briefly cover GSK's experiences in developing, applying, and embedding LCI/A concepts, metrics, and tools into business process.

#### 152. Using Life Cycle Assessment to Develop Environmental Leadership Standards

*Christine Chase, Cheryl Baldwin, and Nana Wilberforce, Science and Standards, Green Seal, Washington, DC*

In order for an environmental standard to adequately promote sustainability in the marketplace, it needs to be based on the life-cycle of the product: from raw material extraction, production, and ultimately, use and disposal of the product. Green Seal incorporates life-cycle assessment to help determine criteria in the development of environmental standards for products and services. The presentation will highlight some of the recent life-cycle approaches utilized in the standard-development process for paper products, stains and finishes, and restaurants and food service, focusing on data collection, analysis, and determination of life-cycle performance metrics in the development of a stakeholder-involved environmental standard. The presentation will discuss what life-cycle methods were used, how metrics were developed in the context of the categories and how life-cycle studies influence and are incorporated into an environmental standard. The presentation will conclude by discussing the potential impact and effectiveness of leadership environmental standards in promoting sustainability and green chemistry in the marketplace.



## 153. Standards, Metrics, and Measures - Do We Need Them?

*Lin Kaatz Chary, Great Lakes Green Chemistry Network, Gary, IN*

Much discussion has been generated over the question of standards and metrics for green chemistry and green engineering. How do we distinguish green chemistry from green washing? This roundtable will include both presenters and audience in a discussion on this very current debate from several different perspectives. The focus of the discussion will be on what kinds of policies and tools are needed to inform the effort to assure that processes, substitutions, and alternative products adhere to the principles of green chemistry and green engineering. This session will be an opportunity for panelists and audience to hear a diversity of views on these critical questions about green chemistry and metrics.

Moderator: Lin Kaatz Chary, Great Lakes Green Chemistry Network

Speaker 1: Jennifer Young, ACS GCI ANSI green chemistry standard process

Speaker 2: Lauren Heine/Mark Rossi, Clean Production Action, The Green Screen for Safer Chemicals

## 154. Upgrading of Bio-Oil for Fuel Production

*Luc Moens, Stuart K. Black, Michele D. Myers, and Stefan Czernik, National Bioenergy Center, National Renewable Energy Laboratory, Golden, CO*

Fast pyrolysis of lignocellulosic biomass leads to the formation of a liquid product called bio-oil. Bio-oils are complex mixtures of molecules resulting from thermal depolymerization and fragmentation reactions of the three building blocks of biomass, i.e., cellulose, hemicellulose, and lignin. There is significant interest in using bio-oil for the production of transportation fuels (e.g., gasoline) through hydroprocessing in existing petroleum refinery units. However, the high acidity and chemical instability of whole bio-oils requires the development of cost-effective methods to upgrade the oils before they can be introduced into the infrastructure of a refinery. This presentation will discuss the ongoing R&D efforts at NREL to overcome this technical barrier.

## 155. A Novel Ionic Liquid Process for Conversion of Renewable Biomass into Petrochemical Intermediate

*Wei Liu, Energy and Environment, Pacific Northwest National Lab, Richland, WA*

Most of today's bulk petrochemical and chemical products are manufactured from raw materials that are derived from petroleum oil or natural gas. For example, aromatics - one common feedstock - are produced in refineries through a series of energy and capital-intensive refining process steps. Replacement of such oil-based feedstocks with intermediates derived from renewable biomass material has both energy and environmental benefits by reducing oil consumption and green house gas emissions. In addition, chemical feedstocks typically have a higher value than the liquid transportation fuel. 5-hydroxymethylfurfural (HMF) has been proposed as a flexible platform chemical to make various chemical intermediates that can substitute for today's petroleum-derived feedstock such as paraxylene in manufacturing of polyester and polyamide. A good amount of research has been done for synthesis of HMF from renewable hydrocarbon sources. However, there are no practical processes yet to produce HMF at a cost level competitive with today's petrochemical feedstock. A continuous flow process based on ionic liquids will be described

in this presentation for conversion of sugars, cellulose into HMF. The ionic liquid fluid serves both as a green solvent to dissolve the sugar-type biomass and as a catalyst carrier. Novel catalysis reaction chemistries and HMF/ionic liquid separation technologies will be discussed for development of a low-cost HMF manufacturing process.

## 156. Hydrolysis of Lignocellulosic Biomass in Subcritical Water and Catalytic Gasification of Hydrolysates to Produce Hydrogen Rich Gas

*Sibel Irmak, Bahar Meryemoglu, Ilker Ozturk, Mehtap Kurtulus, Tugba Balin, Arif Hesenov, and Oktay Erbatur, Department of Chemistry, Cukurova University, Adana, Turkey*

The lignocellulosic biomass materials are abundant, cheap, and renewable feedstocks suitable for biofuels production. The present study was designed to hydrolyze lignocellulosic biomass in subcritical water for further gasification by the mild processing technique of Aqueous Phase Reforming (APR) to produce hydrogen rich gas mixture. Wheat straw, an abundant byproduct from wheat production, and kenaf (*Hibiscus cannabinus* L.), a well known energy crop and an annual herbaceous plant growing very fast with low lodging susceptibility, were used as representative lignocellulosics in the present study.

The hydrolysis efficiency of biomass materials was examined with respect to several parameters such as ultrasonication of biomass/water mixture before thermal treatment, changing temperature and pressure of the hydrolysis process, adding carbon dioxide or nitrogen as pressurizing gas. APR experiments were performed using catalysts which were made of Pt, Pd, and Ru doped on carbon (various carbon types) and alumina supports for producing hydrogen-rich gas mixtures.

The biomass exposed to ultrasound before subcritical water treatment were hydrolyzed easily. The total organic carbon (TOC) content of ultrasonically pretreated solutions were significantly higher comparing to untreated ones. In addition, the molar mass of polysaccharide fractions in those solutions notably decreased because of effective degradation. The extent of hydrolysis was more effective at higher temperatures and under carbon dioxide atmosphere rather than nitrogen as the pressurization gas. The gasification (APR) experiments showed that the amount of hydrogen was always higher when the supporting material of the platinum-doped catalyst was carbon compared to other types of supports.

## 157. Sensitized TiO<sub>2</sub> for Catalytic Solar Fuel Generation: A Combined Molecular and Materials Based Approach

*Amanda J. Morris and Gerald J. Meyer, Department of Chemistry, Johns Hopkins University, Baltimore, MD*

Global warming and the production of a carbon-neutral fuel are arguably the most environmentally pressing issues of this decade. The reduction of CO<sub>2</sub> or H<sup>+</sup> with solar photons requires compounds capable of multiple electron transfer (MET) catalysis. Therefore an important first step is to identify conditions where such catalysts can be reduced to their active states with visible light. Toward this goal, we report the visible light sensitized reduction of iron protoporphyrin IX (hemin) and cobalt tetracarboxyphenyl porphyrin anchored to mesoporous nanocrystalline (anatase) TiO<sub>2</sub>. Reduced porphyrins are known to catalyze several important MET reactions including the reduction of protons to hydrogen and carbon tetrachloride to dichlorocarbene. In this paper we conduct experiments to test whether electrons injected into TiO<sub>2</sub> from standard dye molecules, such as Z907 [(4,4'-(CO<sub>2</sub>H)<sub>2</sub>-2,2'-bipyridine)(4,4'-(C<sub>9</sub>H<sub>19</sub>)<sub>2</sub>-2,2'-bipyridine)(NCS)<sub>2</sub>Ru(II)] and

Ru(bpy)<sub>2</sub>(dcb), were capable of reducing co-adsorbed porphyrins to these states on the surface of TiO<sub>2</sub>. Included is a quantitative analysis of the kinetic and thermodynamic properties of the molecularly-sensitized, TiO<sub>2</sub> mediated, reduction of porphyrins.

### 158. Conversion of Biomass Resources into Chemicals with Integrated Catalytic Technologies

*Anders Riisager<sup>1</sup>, Thomas S. Hansen<sup>1</sup>, Tim Ståhlberg<sup>1</sup>, Søren K. Klitgaard<sup>1</sup>, Jacob S. Jensen<sup>2</sup>, John M. Woodley<sup>2</sup>, Astrid Boisen<sup>3</sup>, and Sven Pedersen<sup>3</sup>, (1)Department of Chemistry and Centre for Catalysis and Sustainable Chemistry, Technical University of Denmark, Kgs. Lyngby, Denmark, (2)Department of Chemical and Biochemical Engineering and Center for BioProcess Engineering, Technical University of Denmark, Kgs. Lyngby, Denmark, (3)Novozymes A/S, Bagsvaerd, Denmark*

The projected depletion of fossil resources has in recent years accelerated significant interest in shifting from a fossil-based chemical industry towards a sustainable infrastructure relying on the only accessible renewable carbon-source, namely biomass. In this context, particular focus should be directed towards technologies that facilitate production of carbonaceous chemicals, which presently exclusively are manufactured from a few platform compounds with fossil-based origin. A feasible approach towards obtaining a renewable chemicals industry is based on catalytic conversion of carbohydrates, which comprise a major part of the accessible biomass and therefore an abundant source. The acid-catalyzed dehydration of hexoses (e.g. glucose, fructose, or their polymeric derivatives) yields 5-hydroxymethylfurfural (HMF). HMF is an intermediate platform compound that potentially can be catalytically converted into a range of value-added chemicals applicable as solvents, polymer monomers, bulk chemicals, fuel, and fuel additives by, e.g. isomerization, hydrogenation, or oxidation. In this field, a particularly interesting future direction is to develop integrated technologies, which facilitate multistep catalytic synthesis and combined reactions without intermediate recovery steps. Such methods may increase space-time-yield and reduce operational costs through minimized expenditure of supplementary chemicals and energy. In this presentation, our latest results obtained in catalytic conversion of carbohydrates to furanic chemicals with integrated technologies combining different catalyst types, modes of operation, and reaction media (e.g. ionic liquids) will be highlighted.

### 159. Cavitation-Enhanced Intensification and Optimization of the Synthesis of Biofuels from Edible and Non-Edible Biomass

*Yusuf G. Adewuyi and Naresh N. Mahamuni, Department of Chemical Engineering and Department of Bioengineering, North Carolina A&T State University, Greensboro, NC*

The recent attempts in the applications of ultrasonic and hydrodynamic cavitation for biodiesel synthesis and conversion of lignocellulosic biomass to ethanol present an urgent need to optimize the process to reduce cost of operation and make it economically attractive for large-scale applications. Cavitation is the formation, growth, and implosive collapse of gas- or vapor-filled microbubbles and can be induced acoustically or hydrodynamically in a body of liquid. The collapse of these bubbles leads to local transient high temperatures (<sup>3</sup> 5000 K) and pressures (<sup>3</sup> 1000 atm), resulting in the generation of highly reactive species including hydroxyl (OH), hydrogen (H) and hydroperoxyl (HO<sub>2</sub>) radicals, and hydrogen peroxide. The cavitation event also gives rise to acoustic microstreaming or formation of miniature eddies that enhance the mass and heat transfer in the liquid. However, little fundamental

research has been carried out to date on the catalytic / biocatalytic and enzymatic conversion of lignocellulosic biofuels and biodiesel from esterification/transesterification of vegetable oil via cavitation enhanced homogeneous and heterogeneous catalysis. To aid the cost-effectiveness and commercialization of cavitation-enhanced biodiesel and lignocellulosic conversion processes, the fundamental understanding of the effects of various ultrasonic parameters (e.g., frequency, intensity, etc), the transport behavior and mass transfer parameters, and the mechanistic chemistry and kinetics of the cavitation-enhanced reactions must be understood and quantified. To accomplish these objectives, we have designed and constructed several novel ultrasonic and hydrodynamic reactors to be used to quantify the kinetics and mechanisms of the important catalyzed chemical and enzymatic reactions as they relate to the production of chemicals, biodiesel and lignocellulosic biofuels. This talk will present some of the results of our studies, the current practical limitations of these processes, and future challenges of developing ultrasonic and hydrodynamic cavitation technologies for the production of biofuels.

### 160. NonCovalent Derivatization: Physical Properties and Formulation Design at the Molecular Level

*John C. Warner, Warner Babcock Institute for Green Chemistry, Wilmington, MA*

This presentation will discuss recent advances in the field of NonCovalent Derivatization, as an emerging tool in the Green Chemistry Toolbox. The fundamental basis of materials property control in physiological systems is primarily based on the additive combination of weak molecular forces such as hydrogen bonding, pi-stacking, and lipophilic interactions. By understanding the fundamental principles that govern these interactions, it is possible to create molecular systems that respond specifically to various environments. Dissolution and distribution kinetics, oxidative and hydrolytic stability and other important properties can be precisely controlled by the purposeful manipulation of the weak intermolecular forces surrounding an active pharmaceutical environment. This approach can result in unique chemical entities, and novel formulation compositions that have useful properties.

### 161. Use of an Electronic Lab Notebook (ELN) for Green Science at Eli Lilly and Company

*Michael E. Kopach, Chemical Product Research and Development, Eli Lilly and Company, Indianapolis, IN*

Since the initial deployment of a fully electronic lab notebook at Eli Lilly and Company in 2004, numerous organizational efficiencies have been achieved. For commercial R&D processes, minimization of waste and elimination of hazardous solvents are important environmental objectives. To assist with these green chemistry goals, an electronic lab notebook application has been developed and deployed, which calculates Process Mass Intensity (PMI) for a specific step and an entire process. In addition, the new tool reports Toxic Release Inventory (TRI) chemicals, and classifies all solvents with an environmental rating.



## 162. Explore C-C Bond Formations Beyond Functional Group Transformations

*Chao-Jun Li, Chemistry, McGill University, Montreal, QC, Canada*

The development of novel chemical reactivities and reaction conditions that can improve resource efficiency, energy efficiency, product selectivity, operational simplicity, as well as environmental health and safety, represents both an ideology and an aspiration for synthetic chemists. Carbon-carbon bond formation is a central part of various chemical syntheses, and innovations in carbon-carbon bond formations will profoundly affect overall synthetic efficiency. During the past several years, our laboratory has been investigating the innovative concept of forming carbon-carbon bonds directly from two different C-H bonds under oxidative conditions, termed as Cross-Dehydrogenative-Coupling (CDC), with an eye on more efficient syntheses. These methods provide an alternative to the traditional requirement of separate steps of pre-functionalization and defunctionalization in synthesis design, one that will increase synthetic efficiencies at the most fundamental level.

## 163. Copper-Catalyzed C-H Amination with Unactivated Amines

*Raymond T. Gephart III<sup>1</sup>, Yosra M. Badiei<sup>2</sup>, Mae Joanne Aguila<sup>2</sup>, and Timothy H. Warren<sup>2</sup>, (1)Department of Chemistry, University of North Carolina at Wilmington, Wilmington, NC, (2)Department of Chemistry, Georgetown University, Washington, DC*

Numerous natural and pharmaceutical small molecule targets as well as technologically important materials contain C-N bonds, prompting cost-effective and environmentally benign approaches for their synthesis. The direct conversion of C-H bonds to C-N bonds offers opportunities to streamline syntheses with a resulting savings in cost and reduction in environmental impact. We describe a new catalytic system for C-H amination, which employs unactivated amines such as anilines and aliphatic secondary amines as substrates along with an inexpensive, simple oxidant. In contrast to most C-H amination systems, powerful electron-withdrawing nitrogen substituents, usually discarded in a later synthetic step, are not required. This new catalytic system was conceived through the observation of a series of stoichiometric reactions involving well defined, reactive copper intermediates, later linked together to form a functioning catalytic cycle. We will discuss our approach to outline mechanistic details which are intimately connected with the substrate scope and selectivity for this new C-H amination system under active development.

## 164. Green Chemistry Techniques for Small-Scale Organic Synthesis

*Wei Zhang, Department of Chemistry, University of Massachusetts Boston, Boston, MA*

Described in this presentation is a personal overview on the green chemistry aspects of fluoruous technologies for small-scale organic synthesis. The unique phase separation and broad combinatorial capability of fluoruous technologies have led to the development of fluoruous chromatography-free separations, chemical recycling techniques, atom economic reactions, energy-focused microwave reactions, metal-free organocatalysis, aqueous media reactions, and modified reagents. The utility of these green chemistry tools have been demonstrated in the discovery chemistry, medicinal chemistry, and academic labs. Issues related to the high cost and environment impact of fluoruous chemicals are also discussed.

## 165. Environmentally Friendly Routes for the Selective Oxidation of Alcohols

*Robert L. Augustine and Setrak K. Tanielyan, Center for Applied Catalysis, Seton Hall University, South Orange, NJ*

The selective oxidation of alcohols to the corresponding carbonyl compounds is one of the more important transformations in synthetic organic chemistry. A large number of oxidants have been reported in the literature but most of them are based on the use of transition metal oxides such as those of chromium and manganese. Since most of these oxidants and their reduced compounds are toxic species, their use creates serious problems concerning their handling and disposal, especially in large scale, commercial applications. A common alternative to the use of these metal oxides involves the oxidation of alcohols using NaOCl and TEMPO as described by Anelli. This reaction is carried out in a two-phase ( $\text{CH}_2\text{Cl}_2/\text{H}_2\text{O}$ ) system utilizing TEMPO as a catalyst and NaOCl as the oxidant. The presence of a co-catalyst, KBr, increases the reaction rate. One of the oxidation procedures described here is an extension of this Anelli process, which does not require the use of any organic solvents and replaces the KBr co-catalyst with the more benign,  $\text{Na}_2\text{B}_4\text{O}_7$  (Borax). The next step was to develop an oxidation procedure using the more benign oxidants to replace the NaOCl. There are only a few reports that describe the selective oxidation of primary or secondary alcohols to the corresponding aldehydes or ketones utilizing TEMPO based catalyst systems in combination with clean oxidants such as  $\text{O}_2$  and  $\text{H}_2\text{O}_2$ . These processes commonly use substantial amounts of expensive and/or toxic transition metal complexes as co-catalysts, a factor which makes them unsuitable environmentally. The second procedure described here is an effective aerobic oxidation of primary and secondary alcohols using a catalyst system based on 4-acetamido-TEMPO,  $\text{Mg}(\text{NO}_3)_2$  and NBS in an acetic acid solvent.

Finally, an efficient vapor phase copper catalyzed dehydrogenation applicable for use with relatively low boiling alcohols is described.

## 166. Transforming Catalytic C-H Borylations Into a Pharma Friendly Synthetic Tool

*Robert E. Maleczka Jr., Nathan J. Gesmundo, Venkata A. Kallepalli, Hao Li, A. Monica Norberg, Sean M. Preshlock, Philipp C. Roosen, Luis Sanchez, Clarissa L. Turton, and Milton R. Smith III, Department of Chemistry, Michigan State University, East Lansing, MI*

Over the past several years, we, along with others, have worked to establish Ir-catalyzed C-H borylations as a green and complementary route to aryl and heteroaryl boronic esters and allied molecules. These reactions can be merged with subsequent in situ chemical events and are thus proving quite amenable to diversity-orientated syntheses. Moreover, the functional group tolerance of catalytic borylations facilitates late stage functionalization of drugs and drug candidates.

## 167. The National Conversation on Public Health and Chemical Exposures

*Howard Frumkin and Ben Gerhardstein, National Center for Environmental Health/Agency for Toxic Substances and Disease Registry, U.S. Centers for Disease Control and Prevention, Atlanta, GA*

The National Center for Environmental Health/Agency for Toxic Substances and Disease Registry (NCEH/ATSDR), Centers for Disease Control and Prevention, is launching the National Conversation on Public Health and Chemical Exposures, a stakeholder-engagement process to revitalize the public health approach to chemical exposures. In an effort to build on our nation's successes in protecting public health from harmful chemical exposures, and to modernize our nation's health

protection approach, this conversation will focus on strengthening core public health functions related to chemical exposures. As many have noted, our current approach to chemical exposures has been limited in its ability to assemble needed data, draw conclusions, launch protective actions, and inform stakeholders. Further, the landscape has changed in recent years; scientific methods and understanding have evolved; decision-making tools have advanced; and significant changes have occurred in the policy arena. This talk will outline the National Conversation initiative, goals, and process, and highlight opportunities for involvement.

### 168. The Business Value of GC/GE

*Andrea Larson, Darden Graduate School of Business, Charlottesville, VA*

Green Chemistry and Green Engineering are at a tipping point in business. The pressures on companies for more transparency as well as cleaner and safer products have brought GC/GE into the mainstream. If companies are not aware of the shifting terrain, it is time to pay attention. The forces at work come from both positive and negative directions. First, the negative: Firms are at greater risk than ever before for legal liabilities, fines, and being shut out of markets if they do not focus on redesign consistent with GC and GE protocols. On the positive side, the market shift offers innovative companies the opportunity to differentiate their processes, products, technologies, and brand in ways that can drive revenue and improve competitive position. This presentation discusses the shifting landscape for business as more attention is paid to safety, financial risk, and ability to compete going forward.

### 169. Facilitating Implementation of Green Chemistry in Industry

*Emily Reichert and John C. Warner, Warner Babcock Institute for Green Chemistry, Wilmington, MA*

Most companies and industries have realized that they MUST respond to the growing demand by government, NGOs, and informed consumers for more sustainable products and processes. The Twelve Principles of Green Chemistry provides a framework for meeting these demands at the molecular level, guiding the design of more sustainable chemicals and materials. For a technology to be considered green chemistry, it must demonstrate performance in THREE areas: (1) environment (2) functionality, and (3) cost. If any of these three are missing, the technology will not succeed in the marketplace.

However, despite growing consumer demand and a framework for implementation, many companies and industries have not yet re-designed their products and process. How can the Principles of Green Chemistry be implemented in a practical way within these companies and industries? What skills and mechanisms must be created to facilitate implementation? We will discuss an approach to integrating the Principles of Green Chemistry throughout the R&D of chemicals and materials re-design within companies, based on the Warner Babcock Institute's experience working with industry partners to develop successful and sustainable products.

### 170. CleanGredients®: Challenges and Opportunities in the Development of an Open, Multi-Attribute Information Platform for Green Formulation

*Topher Buck, GreenBlue, Charlottesville, VA*

The push for open and transparent information to facilitate the design and production of safer, healthier, and more sustainable products is gaining momentum. The California Green Chemistry Initiative's nascent Online Product Ingredient Network and Wal-Mart's push for data regarding the ingredients in the products it sells, as well as the growing movement behind "open-source"

LCI data, are some prominent, recent examples. CleanGredients®, a project of the nonprofit Green Blue Institute (GreenBlue®), is a multi-attribute information platform that represents an extensible model framework for chemical alternatives assessment. GreenBlue has developed CleanGredients in close collaboration with the U.S. EPA Design for the Environment (DfE) Program and NSF International. CleanGredients presently encompasses modules for surfactants and solvents, with additional modules for fragrances and chelants nearing completion. More than 300 household, industrial, and institutional (HI&I) cleaning product formulators subscribe to access the information in CleanGredients, and 27 chemical manufacturers subscribe to list their ingredients. From the outset, GreenBlue's goals for CleanGredients have been to foster greater transparency and stimulate the growth of green chemistry and green formulation by allowing companies to share the chemical data needed to make better-informed design decisions while rewarding innovation by protecting proprietary information. One approach involves sharing data at a level of resolution fine enough to support effective alternatives assessment but coarse enough to conceal, and thereby protect, proprietary information. CleanGredients provides standard physical-chemical attribute data and independently verified data on key human and environmental health attributes for listed chemicals, facilitating consideration of human and environmental health along with typical product attributes (e.g., cost and performance) during product formulation. Challenges to be discussed include establishing the proper organizational relationships and incentive structures. Opportunities include the applicability of the CleanGredients model to formulated product categories such as personal care products and inks, coatings, and adhesives.

### 171. Biomimetic Green Chemistry Solutions: Achievements and Outlook

*Mark H. Dorfman, Biomimicry Guild, New York, NY*

This colorful PowerPoint presentation will begin with an overview of a number of current biomimetic green chemistry products and processes, and promising biomimicry research. It will be followed by a discussion of what distinguishes biomimetic green chemistry with a focus on how "life's principles" mesh with the 12 green chemistry principles. The last portion of the presentation will describe intriguing chemistries in the natural world that could, if mimicked, potentially address sustainability challenges.

### 172. Policies and Tools for States to Promote Green Chemistry

*Lin Kaatz Chary, Great Lakes Green Chemistry Network, Gary, IN*

Several states such as Michigan, California, and Maine have moved forward to implement green chemistry initiatives at the state level. Other states are active in banning PBDEs and other hazardous chemicals and are now looking for tools and policies to promote safer substitutes. This panel will present an update on state efforts to implement green chemistry strategies, including informed substitution methodologies.

Moderator: Kira Matus, Harvard University

Speaker 1: Michael Wilson and Megan Swartzman, UC Berkeley

Speaker 2: Tracey Easthope, Ecology Center, Ann Arbor, MI

Speaker 3: Micheal Belliveau, Environmental Health Strategy Center, Bangor, Maine



## 173. Biofunctionalized Silver Nanoparticles: Synthesis and Characterization

Ranjana Dixit<sup>1</sup>, Nityananda Agasti<sup>2</sup>, and Narender Kumar Kaushik<sup>2</sup>, (1)Department of Chemistry, Ramjas College, University of Delhi, Delhi, India, (2)Department of Chemistry, University of Delhi, Delhi, India

Metal nanoparticles have been considered as an area of ever increasing interest in material science, because of their noble properties leading to wide range of applications in the field of catalysts, biological sensors, photonics[1], optoelectronics[2], information storage[3], and surface enhanced Raman scattering (SERS)[4], etc. The intrinsic properties of metal nanoparticle are mainly determined by its size, shape, composition, crystallinity, and structure. Again shape and morphology of metal nanoparticle are dependent on route of synthesis of nanoparticle. The challenge of synthetically controlling the crystal morphology of metal nanoparticle has been met with biomolecule directed nanoparticle synthesis.

We report a single step solution phase synthesis of silver nanoparticles by using small amino acid glycine as capping agent. Particles synthesized were characterized by UV-Visible spectroscopy, FTIR, XRD, TEM, TGA, and DTA. Thermal stability and solid state decomposition pattern of glycine capped silver nanoparticles has been investigated through thermo analytical techniques (TGA/DTA). Effect of concentration of glycine as stabilizing agent, on silver nanoparticle has been discussed. Phase specific adsorption of stabilizing agent glycine on the surface of silver nanoparticle has been explored through UV-Visible, FTIR and XRD techniques.

The synthetic route presented in this paper involves an economical technique as we conduct this at ambient reaction conditions; water has been used as solvent, reaction completes within a very short time period of around 30 minutes and easily reproducible. The prospects of this experiment are good for synthesis of biofunctionalized silver nanoparticles and will certainly be an addition to nanotechnology.

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## 174. Electroless Cr(VI) Reduction

Carlos Barrera-Diaz<sup>1</sup>, Bryan Bilyeu<sup>2</sup>, Violeta Lugo-Lugo<sup>1</sup>, Victor Sánchez-Mendieta<sup>2</sup>, and Patricia Balderas-Hernández<sup>2</sup>, (1)Environmental Engineering, Universidad Autonoma del Estado de México, Toluca, Mexico, (2)Department of Chemistry, Xavier University of Louisiana, New Orleans, LA

Hexavalent chromium Cr(VI) is carcinogenic and mutagenic, a strong oxidizing agent, and irritating to plant and animal tissue in low doses, as well as diffusing readily through soil, water, and even skin. Unlike many metals, Cr(VI) is usually found as oxyanions in aqueous solution, specifically  $\text{Cr}_2\text{O}_7^{2-}$ ,  $\text{CrO}_4^{2-}$ , and  $\text{HCrO}_4^-$ , the relative distribution of which depends on the solution pH and concentration. However, none of them form insoluble species of the pollutant, such that its separation is not feasible from the wastewater through a direct precipitation method. The most widely used industrial treatment method for Cr(VI) removal requires three steps: the addition of sulfuric acid ( $\text{H}_2\text{SO}_4$ ) for adjusting the pH of the wastewater to a value of 2-3, the adding

of an iron compound ( $\text{FeCl}$  or  $\text{FeSO}_4$ ) or sodium bisulphate ( $\text{NaHSO}_3$ ) for the chemical Cr(VI) reduction and finally a pH adjustment up to 8.5-9.0 for a good chemical precipitation. Unfortunately, such methods require energy, chemical reactive, and produce a considerable amount of sludge. A novel approach for Cr(VI) reduction is the use of electrochemical methods, since they provide good reduction yields, requires less addition of chemicals, and less sludge is produced. The use of electrochemical methods could represent an interesting option as many chemical reactions occur simultaneously when they are applied. In fact, electrochemical treatment techniques have attracted a great deal of attention because of their versatility and environmental compatibility, which makes the treatments of liquids, gases, and solids possible. Indeed, the main reagent is the electron, which is a "clean reagent". However, in all these cases the electrolysis requires the energy input into the system to attain the Cr(VI) reduction. Therefore, our objective in the present work is to study the viability to obtain Cr(VI) reduction with no energy input in an electrochemical cell.

## 175. Switchable Ionic Liquids — a Benign Paradigm for Coupling Reactions and Separations

Hillary Huttenhower<sup>1</sup>, Ejae John<sup>1</sup>, Vittoria Blasucci<sup>2</sup>, Cerag Dilek<sup>2</sup>, Veronica Llopis-Mestre<sup>3</sup>, Ryan Hart<sup>2</sup>, Eduardo Vyhmeister<sup>2</sup>, Ali Fadhel<sup>2</sup>, Pamela Pollet<sup>3</sup>, Charles Eckert<sup>3</sup>, and Charles Liotta<sup>1</sup>, (1)Department of Chemistry/Specialty Separations Center, Georgia Institute of Technology, Atlanta, GA, (2)School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, (3)Chemical & Biomolecular Engineering/Specialty Separations Center, Georgia Institute of Technology, Atlanta, GA

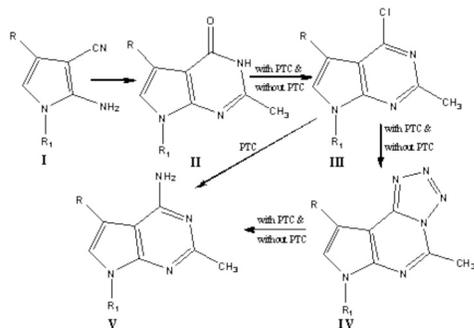
Solvents as they are traditionally known have fixed properties, like polarity. For some applications this can be beneficial, but from a synergistic reaction-separation standpoint it would be useful to have a solvent whose properties can be changed when desired. For example, tunable solvents are solvents that can have a gradual change in properties upon gradual changes of pressure, temperature or other stimuli. In contrast, switchable or reversible solvents can undergo an abrupt change of property by applying a stimulus such as heat. We have developed both two-component and one-component reversible ionic liquids that can be easily switched from a molecular to an ionic state by the addition of  $\text{CO}_2$ . Reversible ionic liquids have all the benefits of ionic liquids, with an extra built in switch that can help solve the separations problem often encountered with traditional ionic liquids. The benefits of the two-components and one-component reversible ionic liquids are many, including the ability to recycle and reuse the solvents and greatly decrease solvent waste. These benefits have been demonstrated for coupling reactions and separations for various applications.

## 176. Green Pathways for Synthesis and Reductive Ring Cleavage of Bioactive 5-Methyltetrazolopyrrolopyrimidines Using Eco Friendly Phase Transfer Catalysis

Rina D. Shah, Department of Chemistry, M.G. Science Institute, Ahmedabad, India

Strategy to involve eco friendly phase transfer catalysis (PTC) with nucleophilic displacements and reductive tetrazole ring cleavage has always been of great interest to study. Therefore, comparative studies of chlorination, azidolysis, and reduction for synthesis and ring cleavage of novel 5-methyltetrazolopyrrolopyrimidines have been undertaken with and without PTC and obtained compounds IV were investigated for their antibacterial activity. Chlorination of 5,7-disubstituted 2-methyl-7H-pyrrolo[2,3-d]pyrimidin-4(3H)-ones II obtained from 1,4-disubstituted 2-amino-3-pyanopyrroles I, followed by azidolysis of 5,7-disubstituted 2-methyl-4-chloro-7H-pyrrolo[2,3-d]pyrimidines III forming 7,9-

disubstituted 5-methyl-7H-tetrazolo[1,5-c]pyrrolo[3,2-e]pyrimidines IV and a chemoselective tetrazole ring cleavage to 5,7-disubstituted 2-methyl-4-amino-7H-pyrrolo[2,3-d]pyrimidines V have been carried out with and without PTC. PTC assisted one pot synthesis of 4-amino compounds V directly from 4-chloro compounds III have also been reported.



### 177. More Benign Synthesis and Extraction of Ligand-Free Palladium Nanoparticles

Juncheng Liu Sr.<sup>1</sup>, Nicholas Ruffini<sup>1</sup>, Christopher B. Roberts<sup>2</sup>, Pamela Pollet<sup>3</sup>, Veronica Llopis-Mestre<sup>3</sup>, Charles L. Liotta<sup>5</sup>, and Charles A. Eckert<sup>6</sup>, (1)Chemical Engineering Department, Auburn University, Auburn, AL, (2)Department of Chemical Engineering, Auburn University, Auburn University, AL, (3)Department of Chemistry/Specialty Separations Center, Georgia Institute of Technology, Atlanta, GA, (4)Georgia Institute of Technology, Atlanta, GA, (5)Department of Chemistry, Georgia Institute of Technology, Atlanta, GA, (6)Schools of Chemical and Biomolecular Engineering and Chemistry/Biochemistry, Georgia Institute of Technology, Atlanta, GA

We demonstrate a more benign synthesis method for small, relatively nondisperse, metal nanoparticles for catalysis. By eliminating separate capping agents and using a recyclable solvent, this technique avoids the massive waste streams associated with current processes.

Metal nanoparticles offer size-dependent optical, electronic, magnetic, catalytic, and other properties. But their syntheses generally require reduction of metal salts in aqueous or organic solutions with capping ligands. These caps serve to passivate the surface of the formed particles and to suppress the growth of the metal clusters that would otherwise aggregate due to the high surface energy of the system. However, the capping ligands may reduce the surface area of the nanoparticles available for catalytic applications. It would be desirable to produce small, uniform metal nanoparticles in a solvent medium without the need for the addition of capping ligands and the resulting purification processes. An ideal solvent medium would not only exhibit favorable solvation of a metal salt (e.g. Na<sub>2</sub>PdCl<sub>4</sub>) and of a reducing agent (e.g. NaBH<sub>4</sub>), but would also exhibit sufficient interaction with the surface of the formed metal nanoparticles to passivate and stabilize the nanoparticle dispersion as created within this solvent medium effectively. Dimethyl sulfoxide (DMSO) is a favorable solvent for ionic solids, as well as both polar and polarizable molecules. In addition, it is relatively inexpensive, stable, and exhibits low vapor pressure and a high boiling point of 189°C. Here we present the first successful synthesis and stabilization of 2.5nm Pd nanoparticles (standard deviation of 0.5nm) within DMSO via a fast, homogeneous reduction of a Pd salt using NaBH<sub>4</sub> in the absence of traditional capping ligands. We have also successfully extracted the Pd metal nanoparticles from the DMSO phase into an organic phase, thereby providing a means of recycling the DMSO solvent.

### 178. Using High Speed Ball Milling (HSBM) to Maximize Efficiency in Multi-Component Reactions

William C. Shearouse and James Mack, Department of Chemistry, University of Cincinnati, Cincinnati, OH

Recently there has been a strong push to minimize waste in the chemical industry. This has triggered a considerable amount of research in greener methodology in organic synthesis. Our research employs High Speed Ball Milling (HSBM) to significantly reduce solvent waste from organic reactions. Where solvents have been used in traditional synthetic methods to achieve homogeneity, HSBM uses mechanical energy to breakdown reagents into small enough particles to the extent where a homogenous mixture is attained. Subsequent collisions of the ball bearing with the walls of the reaction vial result in chemical reactions. One specific class of organic reactions, multi component reactions, has proven to be valuable to many different chemical industries including pharmaceuticals, dyes, conducting polymers, and agrochemicals. This research aims to understand the processes by which multi-component reactions take place under solvent-free, HSBM conditions. More specifically, the Gewald reaction, a multi-component reaction will be discussed. The Gewald reaction involves the reaction of a carbonyl species with an activated nitrile and elemental sulfur in the presence of an amine base. Methods that use a solvent for this reaction make use of long reaction times and tedious reaction methods. HSBM utilizes a one-pot, one-step method while simultaneously producing faster reaction rates in appreciable yields.

### 180. California's Green Chemistry Initiative — Application of Lca in Public Policy

Bob Boughton, California EPA, Department of Toxic Substances Control, Sacramento, CA

The California Green Chemistry initiative comes at a time of growing concern that the federal Toxic Substances Control Act, passed three decades ago, has failed to control an explosion of hazardous materials in commerce. Europe has enacted tougher toxics rules than the United States, forcing many American companies to revamp products sold for export, but the California program would go further in its disclosure requirements. California law passed last fall has jump-started implementation. AB 1879 requires the state to identify "chemicals of concern" and to evaluate safer alternatives by implementing a policy option, "Accelerate the Quest for Safer Products, creating a systematic, science-based process to evaluate chemicals of concern and alternatives to ensure product safety and reduce or eliminate the need for chemical-by-chemical bans." The adopted rules will lay out the process for products with chemicals of concern to be compared to alternatives by assessing the "environmental and economic footprint" of each using a life-cycle perspective. This application of life-cycle thinking for assessing environmental impacts and for assessing total costs will be described within the alternatives analysis process. The background information and progress on the initiative implementation can be accessed at HYPERLINK "<http://www.dtsc.ca.gov/PollutionPrevention/GreenChemistryInitiative>"

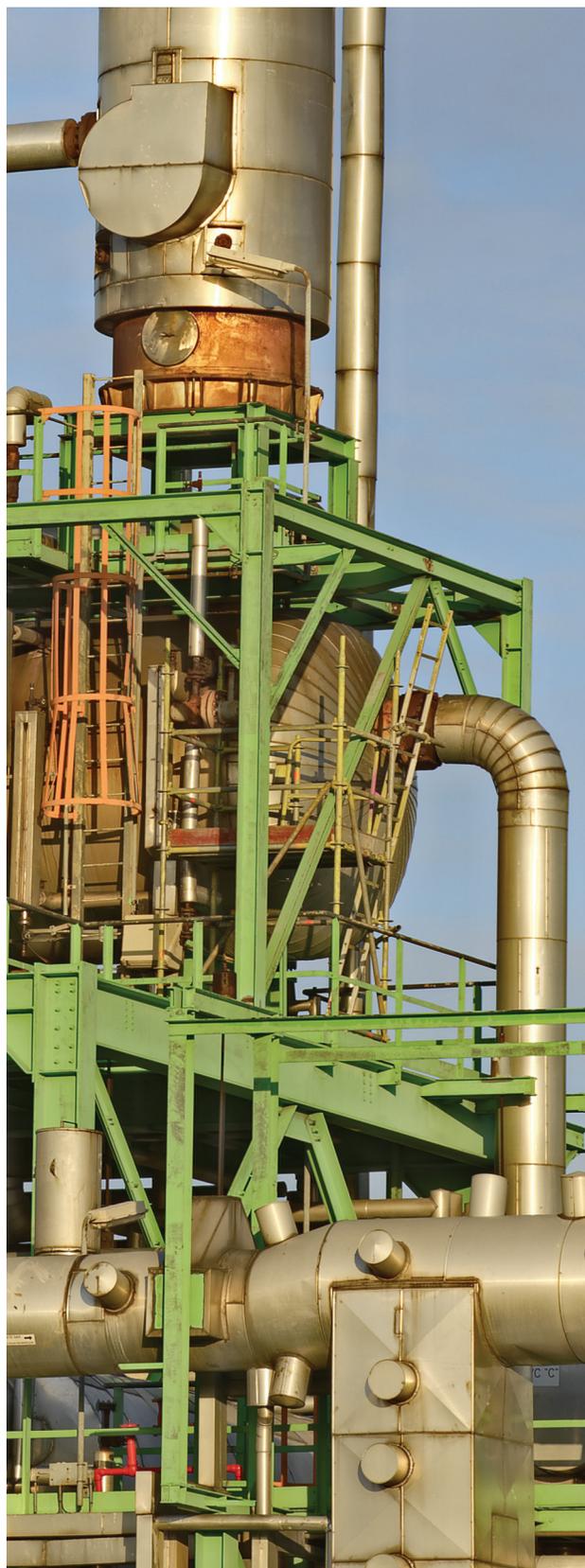


# Abstracts continued

## 181. Solvent-Free Method for Membrane Recoverable Oil and Grease by Infrared Determination

Dean Smith, Engineering, OSS - Orono Spectral Solutions, Old Town, ME

Oil and grease is one of the five conventional pollutants covered by the 1974 Clean Water Act. The measurement of oil and grease is included in all of the National Pollution Discharge Elimination Systems (NPDES) permits, all pre-treatment permits, and all Industrial Effluent Guidelines. It is important to note that it is the 2nd most-enforced-against parameter—2nd only to pH. In 1989, EPA was required to move from a Freon extraction infrared-based determination method to a n-Hexane extraction mass-based determination method, creating four new issues: 1) a flammable liquid is required, 2) n-Hexane is a known neurotoxin, 3) the analytical time is significantly increased, and 4) we are left with a large amount of n-Hexane for disposal. An estimated 1.1 million liters of n-Hexane is used each year for EPA Method 1664A analyses. A new method “ASTM WK23240 – Standard Method for Solvent-Free Membrane Recoverable Oil and Grease by Infrared Determination” being developed by Orono Spectral Solutions will remedy the four issues listed above by removing the use of hexane or any other solvent from the analysis or cleanup. Under EPA Method 1664A the use of solid phase extraction (SPE) is explicitly allowed as long as the laboratory shows the results are comparable to those obtained with liquid-liquid extraction (LLE). In effect, the SPE process determines what could more accurately be termed “membrane extractable – hexane elutable material.” The new method WK23240 is a ‘green’ extension of the SPE process in that it uses a novel extraction membrane that is infrared-amenable so that the oil and grease does not need to be eluted by a solvent for measurement. The new method is an advantageous merging of current and past methods to eliminate most solvent use and shorten the analysis time. The new method is currently undergoing independent validation according to ASTM guidelines.





# Notes

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# Index

- NAME**                      **ABSTRACT**
- A**
- Abdel-Fattah, Tarek M..... 44  
Abul-Haj, Alan..... 126  
Abul-Haj, Roxanne..... 126  
Adewuyi, Yusuf G..... 159  
Adomaitis, Raymond.....16  
Aelterman, Wim..... 55  
Agasti, Nityananda..... 173  
Aguila, Mae Joanne..... 163  
Ahuja, Gauri..... 112  
Aktoudianakis, Evangelos..... 7  
Alvez, Gabriela..... 143  
am Ende, David J..... 129  
Anastas, Paul.....59, 66, 103, 108  
Ardo, Shane.....15  
Augustine, Robert L..... 143, 165  
Aurandt, Jennifer..... 9
- B**
- Badiei, Yosra M..... 163  
Balderas-Hernández, Patricia ... 107, 114, 174  
Baldwin, Cheryl..... 152  
Balin, Tugba..... 156  
Barot, Tushar Gopinath.....97  
Barrera-Diaz, Carlos... 107, 114, 174  
Basile, Perry..... 136  
Bastin, Loyd D.....8, 29  
Beaubrun, Anne..... 142  
Becker, Henry A.....58  
Becker, Klaus..... 91  
Beilin, Dmitry A..... 46  
Bergman, Jeffrey S..... 147  
Bhandari, H.S..... 111  
Bhanumati, S., 10, 59, 66, 71, 103, 108  
Bhardwaj, Minakshi..... 71  
Bhojak, Narendar..... 111  
Bilyeu, Bryan.....107, 114, 174  
Binder, Joseph B.....90  
Birdwhistell, Kurt..... 104  
Birukov, Olga V..... 46  
Bisinger, Edwin.....21  
Black, Stuart K..... 154  
Blair, Daniel L..... 120  
Blassuci, Vittoria..... 124, 175  
Bobylev, Mikhail M..... 63  
Bobyleva, Lioudmila I..... 63  
Boisen, Astrid..... 158  
Boughton, Bob..... 180  
Bowden, Ned B..... 142  
Braune, Sascha..... 127  
Briggs, John R..... 136  
Brindle, Ian D..... 85  
Brown, Kelley.....99  
Buck, Topher..... 170  
Burk, Mark J..... 6  
Burton, Carlyn A..... 147
- C**
- Cai, Jie..... 131  
Campanella, Alejandrina..... 133  
Campbell, Ellen R..... 53  
Campbell, Wilbur H..... 53  
Carver, Richard A..... 18  
Cavalett, Angelica..... 89
- Chalmer, Paul..... 148  
Chance, Ron R..... 122  
Chang, Huan-Tsung.....93  
Chang, Soon-Uk..... 109  
Chase, Christine..... 152  
Chavez, David..... 1  
Chen, Biaohua.....94, 106  
Cheon, Bong-sik..... 110  
Chiang, Cheng-Kang..... 93  
Chin, Paul..... 128  
Chirat, Mathieu.....88, 132  
Choi, Bong Gill.....69  
Chowdhury, Sushmita..... 105  
Cohen, Jon J.....58  
Conroy, Kathryn..... 104  
Cooper, David G.....20  
Cordova, Daniel.....18  
Cote, Aaron S.....65  
Cristiano, Rodrigo.....82  
Cui, Hongyan..... 100  
Cushing, Kerri..... 135  
Czernik, Stefan..... 154
- D**
- Dandekar, Nikhil..... 179  
DaRosa, Jennifer..... 32  
Dass, Sahab.....16  
DeCarlo, Samantha.....75, 102  
Deckman, Harry W..... 122  
De Paep, Frederik.....55  
Devappa, Rakshit K..... 91  
Devine, Paul N..... 5  
Dewulf, Jo.....55  
Dhingra, Sunita..... 72  
Dicks, Andrew P..... 7  
Dilek, Cerag..... 124, 175  
Dilip, Meghna..... 40, 70  
Dingenen, Jules..... 55  
Dixit, Ranjana..... 173  
Dorfman, Mark H..... 171  
Dorner, Robert W.....17  
Dorris, Kenneth.....59, 108  
Dorwart, Jason G.....65  
Driver, Julee.....51  
Duan, Erhong..... 100  
Duke, Dan A.....56  
Duncan, Flavia.....47  
Dunn, Peter J..... 24, 64  
Durant, Yvon.....88, 132  
Dusoe, Keith..... 70
- E**
- Eckert, Charles.....124, 175, 177  
Ehrman, Sheryl..... 16  
Else, Rachel J..... 142  
Emmanuel, Joshua.....16  
Erbatur, Oktay..... 156
- F**
- Fabry-Asztalos, Levente.....99  
Fadhel, Ali..... 124, 175  
Fairless, Gayle..... 73  
Fernandez, Paul F.....65  
Figovsky, Oleg L.....46  
Flexner, Lindsey.....18  
Freudenberger, John H..... 18
- Frumkin, Howard..... 167  
Furman, Alla..... 57
- G**
- Gao, Jizao.....80  
Gastinger, Robert G..... 68  
Geiser, Ken.....27  
Gephart, Raymond T..... 163  
Gerhardstein, Ben..... 167  
Gerhart, Kaitlyn..... 8  
Gesmundo, Nathan J..... 166  
Getahun, Zelleka..... 25  
Glenn, John C..... 149  
Gorke, Johnathan Thomas..... 2, 118  
Goyal, Pritee.....60  
Grate, John..... 4  
Greiner, Tim.....22  
Gudesaria, D.D..... 111  
Guo, Si-si..... 131  
Guo, Yan-zi..... 131  
Gupta, Monika..... 16
- H**
- Hallett, Jason P..... 74  
Hansen, Andrea..... 57  
Hansen, Thomas S..... 158  
Hardy, Dennis R.....17  
Hargreaves, Caireen R..... 26  
Harish, K.V..... 138  
Hart, Ryan..... 124, 175  
Harwood, Laurence..... 96  
He, Chijian.....80  
Hembury, Guy A..... 73  
Henderson, Richard K.....24  
Henry, Carol.....28  
Hesenov, Arif..... 156  
Hobbs, D. Michael..... 65  
Hong, Won-Hee..... 110  
Hong, Won Hi.....69  
Hook, Bruce D..... 136  
Dorner, Robert W.....47  
Huang, Chongpin.....94, 106  
Huang, Min..... 131  
Huang, Shunxian.....80  
Hughes, Gregory J..... 5  
Hull, Jonathan F.....13  
Hunoor, Anand.....37  
Hutchison, Thomas F..... 58  
Huttenhower, Hillary..... 124, 175  
Hwang, Jong Won..... 109  
Hyung Taek, Kim..... 125
- I**
- Ibhadon, Alex Omo..... 123, 130  
Irmak, Sibel..... 156  
Israel, Robert J.....23
- J**
- Jaber, Eihab.....40  
Jain, Reena.....42  
Jain, Subhash C.....61  
Janey, Jacob M..... 5  
Jensen, Jacob S..... 158  
Jiang, Ping.....45  
Jiménez-González, Concepción..... 151  
John, Ejae..... 175  
Johnson, Martin D..... 144
- K**
- Kaatz Chary, Lin.....140, 153, 172  
Kaljurand, Mihkel..... 52  
Kallepalli, Venkata A..... 166  
Kaushik, Narender Kumar..... 173  
Kazlauskas, Romas J..... 2, 118  
Kellar, Casey..... 99  
Kelley, B. T..... 122  
Kermanshahi pour, Azadeh.....20  
Kerr, Margaret E.....40  
Kharshan, Margarita..... 57  
Khiwani, Neeru..... 111  
Kim, Insu..... 113  
Kim, Jong-Duk.....69, 110  
Kim, Jong-Nam.....69  
Kim, Joo Ho..... 101  
Kim, Ui Yong..... 101  
Kim, Young hoon..... 125  
Klitgaard, Søren K..... 158  
Kneas, Kristi A.....11  
Koel, Mihkel..... 52  
Koenig, Stefan G.....76  
Kong, De-jin..... 131  
Koo, Jun mo..... 125  
Kopach, Dr. Michael E..... 161  
Koros, William J..... 122  
Korzenski, Michael B.....45  
Kroker, Jörg.....47  
Kruper, William J..... 136  
Krutkramelis, Kaspars..... 121  
Kumar, Rohtash.....61  
Kurtulus, Mehtap..... 156
- L**
- Laali, Kenneth K.....99  
Lahm, George P..... 18  
Larson, Andrea.....31, 168  
La Scala, John J..... 133  
Lawrence, Eric J..... 54  
Lee, Jong Chan.....101, 109, 113  
Lefenfeld, Michael.....36  
Lenahan, Robert A.....68  
Li, Chao-Jun..... 162  
Li, Hao..... 166  
Li, Hua..... 80  
Lima, Andre O. S..... 89  
Lin, Min..... 79, 80, 81  
Liotta, Charles..... 124, 175, 177  
Liu, Huiru..... 117  
Liu, Juncheng.....78, 177  
Liu, Wei..... 155  
Lively, Ryan P..... 122  
Llopis-Mestre, Veronica ... 124, 175, 177  
Long, David..... 23  
Long, Jun..... 81  
Lu, Wenhua..... 3  
Lugemwa, Fulgentius N..... 54  
Lugo-Lugo, Violeta..... 174  
Lund, John..... 137  
Lv, Liqiang..... 117
- M**
- Ma, Kefeng..... 82  
Mack, James..... 141, 178  
Maguire, Cynthia..... 32  
Mahamuni, Naresh N..... 159

Makkar, Harinder PS .....91  
 Maleczka, Robert E..... 166  
 Mallia, V. Ajay ..... 120  
 Marcum, S. Tyler ..... 141  
 Maric, Milan.....20  
 Marin, Norman ..... 143  
 Marteel-Parrish, Anne.....75, 102  
 Maruya, Richard ..... 126  
 Massonneau, Viviane..... 65  
 Matus, Kira JM.....39, 119  
 McDaniel, Kenneth G..... 68  
 McNally, Mary Ellen.....18  
 Mehta, Nitesh .....37  
 Mergelsberg, Ingrid ..... 24  
 Meryemoglu, Bahar..... 156  
 Meyer, Gerald J.....15, 157  
 Miller, Sarah M..... 115  
 Moens, Luc ..... 154  
 Moghissi, A. .... 19  
 Mohan, Marguerite A. .... 65  
 Moment, Aaron J..... 65  
 Moore, Jeffery C..... 5  
 Morris, Amanda J..... 157  
 Morrison, D. Mark ..... 68  
 Moses, Anthony W..... 65  
 Mukherjee, Chandana ..... 10, 71  
 Mundorff, Emily..... 4  
 Musaddaq, Mohammad ..... 59, 66, 103, 108  
 Mwangi, Martin T..... 142  
 Myers, Michele D..... 154

**N**

Newton, Robert ..... 73  
 Nicell, Jim A.....20  
 Niwayama, Satomi ..... 98  
 Norberg, A. Monica..... 166

**O**

Occhiello, Ernesto..... 136  
 Ozturk, Ilker ..... 156

**P**

Padia, Bhadrash ..... 37  
 Paludo, Larissa G..... 89  
 Panda, Siva Shankar ..... 61  
 Park, Hee Joong ..... 113  
 Park, Sung yuol ..... 69  
 Patel, Mitul N..... 36  
 Patel, Popatbhai kuberbhai ..... 97  
 Patel, Pravinbhai Ranchhodhbhai. 97  
 Pati, Ranjan K. .... 16  
 Paulo, Filipe A. T. .... 89  
 Pedersen, Sven ..... 158  
 Pereira, Schubert ..... 23  
 Peretti, Steven ..... 135  
 Peters, R. Gregory ..... 33  
 Petersen, Kathryn A. .... 36  
 Petrova, Rositza I. .... 65  
 Pindzola, Brad A..... 128  
 Pisanova, Elena ..... 137  
 Poehlauer, Peter..... 127  
 Pokrandt, Rachel.....41  
 Pokryzwa, Jack ..... 28  
 Pollet, Pamela..... 124, 175, 177

Pottanat, George ..... 82  
 Predale, Rob ..... 23  
 Preshlock, Sean ..... 67, 166

**R**

Rabago Smith, Montserrat ..... 9  
 Radosz, Maciej ..... 121  
 Raines, Ronald T..... 90  
 Raja, Krishnaswami ..... 95  
 Rajendran, Malini..... 10  
 Ramsubramani, Hari ..... 37  
 Rangaraju, Prasad ..... 137, 138  
 Ranu, Brindaban C. .... 145  
 Rao, Madhukar (Duke) ..... 48  
 Raynie, Douglas ..... 51  
 Read, Carole..... 12  
 Reese, Cindy..... 28  
 Reese, Jack R. .... 68  
 Reichert, Emily ..... 169  
 Reintjens, Raf..... 127  
 Renner, Paul ..... 30  
 Riisager, Anders ..... 158  
 Ripin, David H. Brown ..... 146  
 Roa-Morales, Gabriela ..... 107, 114  
 Roberts, Christopher B. .... 78, 177  
 Roche, Robert T. .... 18  
 Rodrigues, André L. .... 89  
 Roosen, Philipp C. .... 166  
 Rossi, Mark ..... 22  
 Roumain, Jean-Claude..... 137, 138  
 Ruffini, Nicholas ..... 177

**S**

Salvador, Jame ..... 1  
 Sanchez, Luis ..... 166  
 Sánchez-Mendieta, Víctor..... 174  
 Sarca, Viorel D..... 99  
 Satsangi, Vibha ..... 16  
 Savelski, Mariano J..... 62  
 Savile, Christopher..... 4  
 Schulz, Brian E..... 104  
 Schulz, Michael D. .... 142  
 Schwoppe, Arthur D..... 128  
 Scott, Janet L..... 96  
 Selby, Thomas P..... 18  
 Senöz, Erman..... 14  
 Shah, Rina D..... 176  
 Shapovalov, Leonid D. .... 46  
 Sharma, Poonam ..... 10  
 Sharma, R.K..... 34, 112  
 Sheardy, Richard D. .... 32  
 Shearouse, William C. .... 178  
 Sheridan, Heather..... 75, 102  
 Shi, Chunfeng..... 81  
 Shi, Lie ..... 49  
 Shrivastav, Rohit..... 16  
 Shu, Xingtian ..... 79, 80  
 Shukla, Alka ..... 108  
 Shukla, Shyam..... 59, 66, 103, 108  
 Sidhwani, Indu Tucker..... 72, 112  
 Sidhwani, Pragya..... 72  
 Singh, Aadesh ..... 16  
 Slater, C. Stewart ..... 62  
 Sliva, Philip..... 23  
 Smith, Brandon..... 141  
 Smith, Dean..... 181  
 Smith, Milton R. .... 166  
 Solanki, Anjana ..... 16

Song, Jeff ..... 35  
 Sousa, Dora Lucia ..... 96  
 Srien, Friedrich ..... 2, 118  
 Srivastava, Anju ..... 42  
 Srivastava, Jaya ..... 16  
 Srivastava, Man Mohan..... 60  
 Srivastava, Shalini ..... 60  
 Stahl, Shannon S. .... 144  
 Ståhlberg, Tim ..... 158  
 Stanzione, Joseph F..... 134  
 Stevenson, Thomas M..... 18  
 Stewart, Kelly H. .... 77  
 Styler, Sarah ..... 7  
 Sullivan, Neil..... 73  
 Sun, Run-Cang..... 84

**T**

Tan, Siah Hong..... 15  
 Tanielyan, Setrak K..... 143, 165  
 Tate, Lauren ..... 73  
 Thiel, Indre ..... 141  
 Thompson, George R..... 92, 150  
 Tran, Anh ..... 59  
 Tucker Sidhwani, Indu..... 105  
 Turton, Clarissa L. .... 166

**V**

Van der Vorst, Geert ..... 55  
 Vanderbilt, Herbert..... 23  
 Van Langenhove, Herman ..... 55  
 Vempati, R. K. .... 137, 138  
 Vogt, Paul F. .... 36  
 Vyhmeister, Eduardo ..... 124, 175

**W**

Waddell, Daniel C..... 141  
 Wallace, Debra J..... 65  
 Wang, Wei ..... 80  
 Wang, Xieqing..... 79  
 Wang, Yan ..... 131  
 Wang, Yanan..... 116  
 Warner, John..... 160, 169  
 Warren, Timothy H..... 163  
 Watson, Jill ..... 49  
 Weiss, Richard G ..... 82, 83, 120  
 Weller, Stanley R..... 23  
 Wells, Andrew S. .... 24  
 Welton, Tom ..... 74  
 Whitmyre, Gary Keith ..... 126  
 Whitmyre, George M. .... 126  
 Wignot, Terri..... 33  
 Wilberforce, Nana ..... 152  
 Willauer, Heather D. .... 17  
 Williams, Charlotte K. .... 74  
 Williams, Frederick W..... 17  
 Wilson, Michael P. .... 38  
 Woodley, John M. .... 158  
 Woodward, Michael D. .... 18  
 Wool, Richard P. ... 14, 133, 134, 139  
 Wright, Timothy J. .... 65  
 Wu, Jun ..... 131  
 Wu, Xiaoju..... 80

**X**

Xiao, Xin ..... 119  
 Xu, Shuai..... 94

**Y**

Yang, Hee-man ..... 110  
 Yates, Matthew H..... 144  
 Ye, Xuan ..... 144  
 Yi, Kwang Bok ..... 69  
 Young, Jennifer L. .... 43

**Z**

Zhan, Mingjiang..... 139  
 Zhang, Jie ..... 94, 106  
 Zhang, Wei ..... 164  
 Zhang, Xingchen ..... 117  
 Zhao, Dishun ..... 100, 116  
 Zhu, Bin..... 79, 80, 81  
 Zhu, Ying..... 131  
 Zimmerman, Julie B..... 59, 66, 103, 108, 115



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