Welcome!

The Center for Rational Catalyst Synthesis
JR Regalbuto and Frank Gupton

State of CeRCaS

May 16-17, 2019
Richmond, VA
Thursday, May 16:

**MO:**
- Fall – IAB and student focus
- Spring – Proposal funding

<table>
<thead>
<tr>
<th>Time</th>
<th>Event Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>8:00 - 6:30 am</td>
<td>Center Director's Report: State of the CellCas (Empire Room) (Directors Jit Jagadale, Frank Gunton)</td>
</tr>
<tr>
<td>8:30 - 8:45 am</td>
<td>LIFE Review (Dr. Don Davis, NSF Evaluator)</td>
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<tr>
<td>8:45 - 10:45 am</td>
<td>Project Final Reports (LIFE forms filled out)</td>
</tr>
<tr>
<td>10:45 - 11:00 am</td>
<td>BREAK (Empire Room)</td>
</tr>
<tr>
<td>11:00 - 12:20 pm</td>
<td>Thrust 1 Proposal Presentations (LIFE forms filled out)</td>
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<tr>
<td>12:20 - 1:05 pm</td>
<td>LUNCH (Empire Room)</td>
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**Thursday, May 16:**

1:05 - 2:25 pm

**Thrust II Proposal Presentations (LIFE forms filled out):**

- **II.1** 3D Printed Catalyst: Rabin’s Year 2: Rational Investigation of How Catalyst Synthesis Affects the Nanoparticle Surface Chemistry and Activity on 3DP Monolith (Ferri, Gunton)
- **II.2** Magnetron Sputtered Supported Bimetallic Catalysts having Enhanced Activity for Cross-Coupling Reactions (Gupton, Smith, Munner, Dunn)
- **II.3** The Hydrodynamic Radius and Its Effect on Adsorption (Gupton, Regalbuto, Khanna, Ferri)
- **II.4** Thermodynamics Analysis of SEA Using Metal Adsorption Isotherm Data (Gupton, Regalbuto)

2:25 - 3:40 pm

**BREAK (Empire Room):**

2:40 - 4:00 pm

**Thrust III Proposal Presentations (LIFE forms filled out):**

- **III.1** Nanosprayed Monolithic Cu/Graphene Catalysts for Selective Electrochemical Oxidation of Alkanes (Gupton, Castano, Weisberg)
- **III.2** Computational and Experimental Analysis of Ag Catalysts with CDP or Bimetallic Materials on Direct Propylene Oxide Synthesis (Gupton, Kehrer, Munner)
- **III.3** Metal Oxide-Zeolite Core–Shell Structures for Direct CO2 Reduction (Steimetz, Guttler, Doolin, Li)
- **III.4** Bimetallic Indium-Copper Catalysts for Hydrogenation of Soybean Derived Dimethoxy Glycerol to Ethylene Glycol (Williams, Gunton, Regalbuto)

4:05 - 4:25 pm

**UCB Project Presentations (Kozar):**

- **UCB.1** Cycoaddition of CO2 and Epoxides on Hybrid Organic-Zeolite Catalysts
- **UCB.2** CO2 Sequestration on Modified Zeolite Supports

4:25 - 4:30 pm

**Review of Day 2 activities (Regalbuto):**

4:30 - 5:30 pm

**IAB Meeting (Steimetz):**
Discussion of old and new business.

5:30 - 7:00 pm

**Poster Session and Social (Flemish Room):**

- USC and VCU Postdocs and Grad Students

7:00 pm

**End of Day 1 (Dinner on your own):**
IAB Tasks and Goals of the Spring Meeting

1. Critique the six Final Project Reports (LIFE assessment)

2. Select the next set of 6 projects:
   - LIFE assessment of the fourteen proposals (today)
   - Discussion with project faculty (tomorrow morning)
   - Closed door session for selection (tomorrow)

3. IAB business (today):
   - Overall evaluation of center operation
   - New business

4. Today’s poster session:
   - Recruiting bonanza! – be on the lookout for catalyst synthesis experts

Directors’ Talk: State of CeRCaS

A. Mission
B. Highlights
C. Summary Research Output
D. Member Status and Budget
E. Renewal Proposal
F. What’s Ahead
Why CeRCaS?

1. Catalysis accounts for: (a) over 95% of all products by volume and (b) greater than 80% of the added value in the chemical industry. A full 20% of the world’s economy depends directly or indirectly on catalysis.¹

2. The majority of catalytic processes² (by volume and value) employ heterogeneous catalysts.

3. The potential cost savings of rationally synthesized catalysts may be on the order of $3–$6 billion/year, with corresponding potential savings in energy of 300 – 600 trillion Btu/year.³

→ Catalysis underpins the global economy and our standard of living

¹ Hagen, J., Economic Significance of Catalysts. In Industrial Catalysis: A Practical Approach, 2nd ed.; Hagen, J., Ed. WILEY-VCH Verlag GmbH & Co. KGaA.

But: Heterogeneous Catalyst Preparation is More Art than Science!

Goetz Veser, Pitt

Catalyst ‘Design’...

• The development of catalysts to-date still often resembles more a black art than a scientific endeavor...
• ...virtually all industrial catalysts have been found by painstaking trial-and-error procedures rather than thoughtful scientific design!

Most technical catalysts contain a large number of components (as support, active components, structural and/or mechanical stabilizers etc).

Catalyst “recipes” are among the best kept secrets in the chemical industry.
Grand Challenges for Catalysis

DOE/BES “Basic Research Needs: Catalysis Science”

→ “design and controlled synthesis of catalytic structures”

DOE/BES “Basic Research Needs: Synthesis Science”

Chemical and materials sciences have traditionally focused on understanding structure-function relationships with the goal of predicting where the atoms should be placed to achieve a targeted property or process. Much less effort has been directed toward a predictive science of synthesis—understanding how to get the atoms where they need to go to achieve the desired structure.

→ knowing and predicting how materials assemble and the consequences of the assembly for final material properties

Other DOE/BES BRN reports:

→ Rationally synthesized catalysts

BES Grand Challenges for Catalysis 2017

Design catalysts beyond the binding site

Enzymes, Nature’s catalysts, combine binding sites (localized regions that promote bond breaking/making in the reacting molecule) with precise positioning of nonreacting components that influence reaction barriers and control access to the binding site. Atomic-level, three-dimensional design of robust nonbiological catalysts that precisely positions both reacting and nonreacting components will enable fast and selective chemical transformations for energy applications under conditions currently not possible.

and control access to the binding site. Atomic-level, three-dimensional design of robust nonbiological catalysts that precisely positions both reacting and nonreacting components will enable fast and selective chemical transformations for energy applications under conditions currently not possible.

Manipulate reaction networks in complex environments to steer catalysis

Many emerging chemical feedstocks have diverse, variable compositions that impose large numbers of interconnected pathways whose contributions depend on the reaction conditions. Catalytic design that directs the chemical conversion process and breaks chemical bonds. Designing electrocatalytic systems with tailor-made interfacial environments will allow electrocatalysis with high selectivity.

Drive new catalyst discoveries by coupling data science, theory, and experiment

The complex coupling of many variables that govern catalyst reactivity and activity determine relationships between catalyst structure, composition, and activity. Identifying the important factors in such high-dimensional data, providing insights for the design of new catalysts.
The development of systematic feedback between in situ and ex situ characterization, theory and computational modeling, and experimental kinetics methods could accelerate the synthesis of catalytic materials by rational design and enable catalytic discovery extending beyond traditional empirical approaches. Nanoscale-level feedback on performance, stability, and mechanisms could expedite development of catalytic systems with improved efficacy that can perform multistep processes in complex and demanding catalytic processes.

CROSSCUTTING CHALLENGES AND OPPORTUNITIES
Multidisciplinary strategies are required to advance our current understanding of the interaction between metal centers and their surrounding environments (see Figure 4.1), ranging from redox non-innocent organic ligands in homogeneous catalysts to semiconductor or metallic surfaces with localointerfacial conditions. It is essential to correlate structure to function, including mechanistic understanding of catalyst activation by changes in the surrounding environment and passivation under reaction conditions. Operando measurements could enable direct correlation between activity and formation of key reaction intermediates, serving as feedback for theory refinement and prediction.

What’s missing?

It is essential to correlate preparation to structure...

The Focus of CeRCaS: Rational Synthesis

Rational synthesis versus rational design:

Design: what catalytic sites do we need for a particular reaction?

Synthesis: how do we actually make those sites simply, effectively, and cheaply on commercially viable materials?
CeRCaS I/UCRC:
- One of 70 in the country; 700 total industrial members
- CeRCaS is the only I/UCRC focusing on catalysis

Our vision (Phase 2):
- 15 members at $50k each
- no indirect costs; $750k → $1.2 million
- Companies pay $50k and see $1.2 million of corporate-type research

About Our Center

**THRUST 1**
Fundamentals of Metal Deposition

- Metal ammine precursors

**THRUST 2**
Thermodynamics and Kinetics of Solid-Solid Bonding

- Ir core stabilization of Ag shells

**THRUST 3**
Precision Site Synthesis for Specific Reactions

- Pd/graphene for enhanced cross-coupling
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How Members Participate

- **Active Involvement of the Industrial Advisory Board**
  - project development, selection, and mentoring
- **Regular meetings**
  - monthly updates for each project
  - spring and fall site meetings

How CeRCaS Adds Value

- **Leveraged Investment**
  - Up to 20:1 funding leverage
- **Early Access to Technology**
  - Shared intellectual property, catalyst samples
- **Interact with Customers and Suppliers**
  - Networking opportunities
- **Partner with Leaders in Catalysis Research**
  - Academia and Industry
- **Exposure to Talented Graduate Students**
  - Industrially focused
- **Access to State of the Art Instrumentation**
  - USC and VCU
Summary of CeRCAz Highlights, Years 1-4

- **Leveraged Investment**
  - $1,020,000 in IAB funding first 4 years
  - 30 publications (1 paper/$34k)
  - about $30 million in external funding of CeRCAz faculty (NSF, DOE, Gates Fdn.)

- **Early Access to Technology**
  - 1 patent awarded, three other provisional patents in the pipeline
  - catalyst samples sent to ThalesNano and BASF
  - two “Catalyzing Commercialization” feature articles in CEP

- **Interact with Customers and Suppliers**
  - BASF, ExxonMobil, UOP, INL, SRNL, Bi, Biogen, ThalesNano, Fuzionaire, GSK

- **Partner with Leaders in Catalysis Research**
  - Gupton: $25M Gates Foundation Grant (Medicines for All, 2017), ACS Award for Affordable Green Chemistry (2018)
  - Regalbuto: AIChE Fellow, 2017

- **Exposure to Talented Graduate Students**
  - two CeRCAz students have joined member companies
  - Spring meeting is great recruiting session

- **Access to State of the Art Instrumentation**
  - aberration-corrected STEM, in-situ high sensitivity XRD

Highlights: CeRCAz featured in CEP, Jan. 2018 and Apr. 2019
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**Highlight #1: Monnier election to NAE**

[Image of National Academy of Engineering website]
Highlights: Gupton Heads $25 Million M4All Center

Frank Gupton (left) and Virginia Governor Terry McAuliffe at the August kickoff of the Medicines for All Center at VCU.

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### Success Stories: CeRcAS Students to Member Companies

**Andrew Wong**

**Jayson Keels**

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### Success Stories: Projects lead to External Proposals

<table>
<thead>
<tr>
<th>CONCLUDED PROJECTS</th>
<th>Project 1</th>
<th>Project 2</th>
<th>Project 3</th>
<th>Project 4</th>
<th>Project 5</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Continuous Production of Metal Nanoparticles using Microwave Irradiation</strong> (Gupton, Carpenter, Monnier)</td>
<td><a href="#">Powerpoint</a> ➤ May 2017 Meeting Update ➤ Update Archive</td>
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<tr>
<td><strong>Enhanced stability of catalytic surfaces by bimetallic core-shell structures</strong> (Monnier, Regalbuto, Khanna)</td>
<td><a href="#">Powerpoint</a> ➤ May 2017 Meeting Update ➤ Update Archive</td>
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<td><strong>Cross coupling from a heterogeneous system based on homogeneous molecular catalysts</strong> (Vannucci, Yu)</td>
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<td><strong>Continuous catalytic oxidation in pharmaceutical processing</strong> (Awad, El-Shall, Gupton, Monnier)</td>
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New Opportunities in Catalysis with Crystalline versus Amorphous Supports

UC Berkeley as possible 3rd site
Prof. Alex Katz
Dept. of Chemical and Biomolecular Engineering

Directors’ Talk: State of CeRCaS

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# Industrial Partner Status: 2019

### Members:
- BASF
- Biogen
- Boehringer-Ingelheim
- ExxonMobil
- Fuzionaire
- GlaxoSmithKline
- Idaho National Lab
- Savannah River Nat. Lab.
- Thales Nano
- UOP

### Former Members:
- Eastman Chemical
- Afton

### Currently Recruiting:
- Albemarle
- ADM
- Aramco
- BP
- Chevron Phillips Chemical
- Clariant
- Eli Lilly
- Evonik
- Johnson Matthey
- Merck
- NIST
- Oak Ridge Natl. Lab.
- Parsons
- Pfizer
- Shell

### “Going in a Different Direction”
- DSM
- SABIC

### Industrial Partner Status

#### 2019

<table>
<thead>
<tr>
<th>VCU:</th>
<th>Members:</th>
<th>Chemical/USC</th>
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<tbody>
<tr>
<td>Biogen</td>
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<td>Boehringer-Ingelheim</td>
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<td>GSK</td>
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<td>Thales Nano</td>
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**Total: $160**

**NSF \(\rightarrow\) Good Standing (3/150)**

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<tr>
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<td>UOP</td>
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**Total: $160**

**NSF \(\rightarrow\) Good Standing**

**Phase 2 NSF \(\rightarrow\) Good Standing 4/200**
### Industrial Partner Status: 2020

#### Members:
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- Biogen
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- Clariant
- Eli Lilly
- Evonik
- Johnson Matthey
- Merck
- NIST
- Oak Ridge Natl. Lab
- Parsons
- Pfizer
- Shell

#### Not renewing to Phase 2:
- Boehringer-Ingelheim
- GlaxoSmithKline

#### Former Members:
- Eastman Chemical
- Afton

#### Pharma/VCU
- Chemical/USC
- Shepherd Chemical
- SK Biotech
- Waters
- W.L. Gore
- W.R. Grace

#### “Going in a Different Direction”
- DSM
- SABIC

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**THE CAVALRY**
**CIRCA 2020**

**W.L. GORE**
**EVONIK**
**SK BIOTEK**
**JM**
**PFIZER**
Industrial Partner Status: 2020

Members:
- BASF
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- Fuzionaire
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Membership/Budget Trends

<table>
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<th>Company</th>
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<td>1,020</td>
<td>1,340</td>
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What’s Ahead

1. Berkeley is exploring joining CeRCaS as a third site
   - Alex Katz is the champion
   - Potential companies/labs: PNNL, Berkeley Materials Solutions (SBIR), Dow, Chevron, Shell

2. NSF I/UCRC Phase 2 Renewal Proposal
   - Need signed amendments (Membership fee increase to $50/25k)
   - Need signed letters of support

3. Waiting to hear on SuNSEA
   - With M4ALL, would add another high-powered selling point to the I/UCRC

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8:45 - 10:45 am  Funded Project Final Reports (LIFE forms filled out)
                    PI1  3D Printed Catalytic Monolith (Ferry, Gupthon)
                    PI3 Hydrogenation and Suzuki Coupling Activity of Pt Particles on Modified Carbon Supports (Chea, Regebull, Gupton)
                    PI4 Mechanistic Understanding of Ethene Partial Oxidation over Bifunctional MoV-based Catalysts (Laedrmbr, Carpent)
                    PI5 Boron Nitride (BN) Supported Metal and Metal Oxide Catalysts for Selective Oxidation Reactivity (Dieo, Mornew)
                    PI6 Solid-Supported Catalyst Design for Optimized Electrocatalytic Oxidation of Alkenes to Ketones (Gastano, Gupton, Rover)
                    PI7 Ultrasmall Bimetallic Catalysts for Selective Hydrogenation of Alkenes (et-Kadri, et-Slait, Regebull)
10:45 - 11:00 am  BREAK (Caynly Room)
11:00 - 12:00 pm  Thrust 1 Proposal Presentations (LIFE forms filled out)
                    I.1 Development of Highly Dispersed Bimetallic Catalysts using the Method of Galvanic Displacement (Dats, Nemer)
                    I.2 Synthesis, Structure and Catalytic Studies of Silica-Graphite Composite-Supported Catalysts for Selective Hydrogenation Reactions (Gupthon, Regebull, Herban)
                    I.3 The Effect of Nitrogen Doping on Carbon Supported Pt (et-Kader, Khunna, Regebull, Nemer)
                    I.4 Precision Tuning of Supported Nanoparticle Size (Mannher, Regebull)
12:20 - 1:05 pm  LUNCH (Empire Room)
The Potential to Improve Catalyst Preparation

Catalysis underpins the world economy and standard of living
Most heterogeneous catalysts are prepared by incipient wetness impregnation
IWI typically results in poor metal utilization and control of particle size
IWI can be improved by studying the chemical fundamentals of metal deposition, nanoparticle genesis and stability.
The Center for Rational Catalyst Synthesis

**Mission:** To transform the art of supported metal catalyst preparation into a science.

- Regalbuto (strong electrostatic adsorption), **Monnier** and Diao (electroless deposition), Williams and Alexeev (dendrimers), Lauterbach (controlled nanoparticle shape), Sasmaz (combustion synthesis), Chen (nanoparticles on planar substrates), Adams (organometallic clusters), Popov and Mustain (electrocatalysts), Vannucci (single site) and Heyden (computational nanoparticle stability)

- **Gupton** (microwave synthesis), El-Shall (graphene supports), Carpenter (nanoparticle synthesis), El-Kaderi (organometallic clusters), Khanna (metal clusters), Ellis (organic synthesis), Tang (organic synthesis), Castano (tailored surface properties), Ferri (dispersed fluids)