The Center for Rational Catalyst Synthesis

JR Regalbuto and Frank Gupton

State of the CeRCaS

May 18-19, 2017
Richmond, VA
<table>
<thead>
<tr>
<th>Time</th>
<th>Event</th>
</tr>
</thead>
</table>
| 8:15 - 8:45 am | **Center Director Report: State of the CeRCaS**  
Director's JR Regalbuto, Frank Gupton |
| 8:45 - 9:00 am | **LIFE Review** (Dr. Don Davis, NSF Evaluator)                                             |
| 9:00 - 10:15 am | **Funded Project Updates (LIFE forms filled out)**  
F.I.1 Continuous Production of Metal Nanoparticles using Microwave Irradiation (Carpenter)  
F.II.1 Enhanced Stability of Catalytic Surfaces by Bimetallic Core-Shell structures (Monnier)  
F.III.1 Evaluation of Palladium/Graphene Surface Properties for Cross-Coupling and C-H activation (Ellis) |
| 10:15 - 10:30 am | **BREAK** (Atrium Balcony)                                                                 |
| 10:30 - 12:10 pm | **Funded Project Updates (LIFE forms filled out)**  
F.I.2 “Real-world” Nanoparticle Synthesis on Model Supports (Chen)  
F.II.2 Cross-Coupling from a Heterogeneous System Based on a Homogeneous Molecular Catalyst (Vannucci)  
F.III.2 Continuous Catalytic Oxidation in Pharmaceutical Processing (El-Shell)  
F.I.3 Statistical Design for Guided Nanoparticle Synthesis (Lauterbach) |
| 12:10 - 1:10 pm | **LUNCH** (Atrium Balcony)                                                                   |
| 1:10 - 2:00 pm | **Thrust I Proposal Presentations (LIFE forms filled out)**  
I.1 Continuous Production of Copper and Copper/Ceria Nanoparticles (Carpenter)  
I.2 Preparation of Bimetallic Catalysts Using Continuous Processing Methods (Monnier) |
| 2:00 - 2:50 pm | **Thrust I/II Proposal Presentations (LIFE forms filled out)**  
I.3 Novel Approach for Continuous Synthesis of Supported Transition Metals Through X-ray Radiolysis (Castano)  
II.1 Catalytic Upgrading of Hydrocarbons by Selective Oxidation (Williams) |
| 2:50 - 3:10 pm | **BREAK** (Atrium Balcony)                                                                   |
| 3:10 - 4:00 pm | **Thrust II/III Proposal Presentations (LIFE forms filled out)**  
II.1 In-Situ XRD to Study Monometallic and Bimetallic Catalysts (Monnier)  
III.1 Atomic Layer Deposition of Single-Atom Catalysts for Selective Hydrogenation of Alkenes (El-Kaderi) |
| 4:00 - 5:25 pm | **IAB Meeting** (Steinmetz)  
Discussion of i) funding cycle and budget, ii) feedback on pre-LIFE, iii) evaluative focus, iv) potential ERC proposal, etc. |
| 5:25 - 5:30 pm | **Review of Day 2 activities** (Regalbuto)                                                   |
| 5:30 - 7:00 pm | **Poster Session and Social** (Potomac Room)  
*(USC and VCU Grad Students)*                                                             |
| 7:00 pm       | **End of Day 1 (Dinner on your own)**                                                        |
Welcome!

Fuzionaire

THALESNano

UOP

ExxonMobil

A Honeywell Company

Biogen

Afton

Boehringer Ingelheim

EASTMAN

INL

Idaho National Laboratory

BASF

We create chemistry
Goals of the Fall Meeting

1. Evaluate and critique six current research project updates (LIFE assessment)

2. Evaluate and critique six research proposals (LIFE assessment)

3. Rank order top 3 proposals

4. IAB Business - input needed on:
   a) Possible change of funding cycle
   b) Pre-LIFE assessment
   c) Proper weight on catalyst evaluation
   d) Project 5 mentor (dual mentors?)
   e) Potential ERC proposal
Directors’ Talk: State of the CeRCaS

A. Mission

B. Highlights

C. Summary Research Output

D. Pre-LIFE Assessment

E. Inside View of the CeRCaS

F. Reaction to IAB Input:
   1. Project reports
   2. Pre-LIFE assessment
   3. Catalyst evaluation

G. Member Status and Budget

H. Potential affiliation with ERC proposal
Grand Challenges for Catalysis

DOE/BES “Basic Energy Needs: Catalysis for Energy” report:
→ one of the two grand challenges is the “design and controlled synthesis of catalytic structures”.

NSF report: Inorganic catalysis the key to “Breaking the Chemical and Engineering Barriers to Lignocellulosic Biofuels: Next Generation Hydrocarbon Biofuels”

→ the cost savings of rationally designed catalysts is on the order of $3 – 6 billion/year, with corresponding energy savings of 300 – 600 trillion BTU/year
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** (electroless deposition), Williams and Alexeev (dendrimers), Lauterbach (controlled nanoparticle shape), Hattrick-Simpers (thin film deposition), Chen (nanoparticles on planar substrates), Adams (organometallic clusters), Zhou (controlled-shape nanoparticles), Popov (electrocatalysts), Vannucci (single site) and Heyden (computational nanoparticle stability)

**Gupton** (microwave synthesis), El-Shell (graphene supports), Carpenter (nanoparticle synthesis), El-Kaderi (organometallic clusters), Khanna (metal clusters), Bertino (nanoparticles on porous monoliths), Ellis (organic synthesis), Tang (organic synthesis), Castano (tailored surface properties)
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 Research Thrusts

1. Fundamentals of metal deposition and nanoparticle formation
   a) In-situ spectroscopic or EM studies of metal adsorption
   b) Genesis of nanoparticles from adsorbed precursors
   c) Continuous nanoparticle synthesis

2. Thermodynamics and kinetics of solid-solid bonding in supported nanoparticles – “Better nanoparticles through computation”
   a) Sintering and wetting of metals and metal oxides
   b) Prediction of size and shape of supported nanoparticles as function of environment
   c) Prediction of surface composition in bimetallic nanoparticles

3. Precision catalyst site synthesis for specific reactions
   a) Pharma-related
   b) Commodity and specialty chemical applications
   c) Alternate energy and methane utilization
Mission: To transform the art of supported metal catalyst preparation into a science.

**THRUST 1**  
Fundamentals of Metal Deposition  
Metal ammine precursors  
H₂, Δ  
1.0 nm bimetallic nanoparticles

**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

http://www.che.sc.edu/centers/cercas/
<table>
<thead>
<tr>
<th>Update Links</th>
<th>Project</th>
<th>Principal Investigators</th>
<th>Industrial Mentor</th>
<th>Reports</th>
<th>Call In*</th>
<th>Next Date**</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Continuous Production of Metal Nanoparticles using Microwave Irradiation</td>
<td>Carpenter Gupton (VCU) Monnier (USC)</td>
<td>Devlin (Afton)</td>
<td>First Tuesday (Morning)</td>
<td>1 408 638-0968 US TOLL</td>
<td>05/18-19 CeRCaS Mtg.</td>
</tr>
<tr>
<td></td>
<td>Enhanced Stability of Catalytic Surfaces by Bimetallic Core-shell Structures</td>
<td>Monnier Regalbuto (USC) Khanna (VCU)</td>
<td>Liu/McMillan (Eastman)</td>
<td>Second Tuesday (Morning)</td>
<td>1 800 753-1965</td>
<td>05/18-19 CeRCaS Mtg.</td>
</tr>
<tr>
<td></td>
<td>Evaluation of Palladium/Graphene Surface Properties for Cross Coupling and C-H activation</td>
<td>Ellis Gupton (VCU) Williams (USC)</td>
<td>TBD (Biogen)</td>
<td>Third Tuesday (Morning)</td>
<td>1 408 638-0968 US TOLL</td>
<td>05/18-19 CeRCaS Mtg.</td>
</tr>
<tr>
<td></td>
<td>&quot;Real World&quot; Nanoparticle Synthesis on Model Supports</td>
<td>Chen Regalbuto (USC)</td>
<td>Soled (ExxonMobil)</td>
<td>Fourth Tuesday (Morning)</td>
<td>1 800 753-1965</td>
<td>05/18-19 CeRCaS Mtg.</td>
</tr>
<tr>
<td></td>
<td>Continuous Catalytic Oxidation in Pharmaceutical Processing</td>
<td>Awad El-Shell Gupton (VCU) Monnier (USC)</td>
<td>TBD</td>
<td>First Tuesday (Afternoon)</td>
<td>1 408 638-0968 US TOLL</td>
<td>05/18-19 CeRCaS Mtg.</td>
</tr>
<tr>
<td></td>
<td>Cross Coupling from a Heterogeneous System based on Homogeneous Molecular Catalyst</td>
<td>Vannucci Yu (USC)</td>
<td>Senanayake (BI)</td>
<td>Second Tuesday (Afternoon)</td>
<td>1 800 753-1965</td>
<td>05/18-19 CeRCaS Mtg.</td>
</tr>
<tr>
<td></td>
<td>Statistical design for guided nanoparticle synthesis</td>
<td>Lauterbach Hattrick-Simpers Wen (USC)</td>
<td>Deutsch (BASF)</td>
<td>Third Tuesday (Afternoon)</td>
<td>1 800 753-1965</td>
<td>05/18-19 CeRCaS Mtg.</td>
</tr>
</tbody>
</table>
Directors’ Talk Outline

A. Mission

B. Highlights

C. Summary Research Output

D. Pre-LIFE Assessment

E. Inside View of the CeRCaS

F. Reaction to IAB Input:
   1. Project reports
   2. Pre-LIFE assessment
   3. Catalyst evaluation

G. Member Status and Budget

H. Potential affiliation with ERC proposal
Dr. John R. Monnier

<table>
<thead>
<tr>
<th>Title</th>
<th>Research Professor</th>
</tr>
</thead>
<tbody>
<tr>
<td>Organization</td>
<td>University of South Carolina</td>
</tr>
<tr>
<td>Election Year</td>
<td>2017</td>
</tr>
<tr>
<td>Primary Section</td>
<td>03. Chemical Engineering</td>
</tr>
<tr>
<td>Member Type</td>
<td>Member</td>
</tr>
</tbody>
</table>

For the discovery and development of the silver-catalyzed epoxidation of non-allylic olefins to produce 3, 4-epoxy-1-butene and other non-allylic olefin epoxides.
Graphene Support Engineering

- **Traditional Tube Furnace Reduction**
  - High metal dispersion
  - Nanoparticles on surface of support

- **Microwave Reduction**
  - Solventless
  - Simultaneous formation of nanoparticles and defect sites
1. Pd deposition onto graphene via “Strong Electrostatic Adsorption” with microwave reduction (SEA-MW)

2. Computations suggest Pd clusters stabilized at graphene defects

3. Activity far superior to commercial catalysts

Applications:
- Anticancer drugs (Crizotinig, Lapatinib)
- Antibiotic (Garenoxacin)
- Hypertension (Nebivolol)

Prof. Suzuki shared 2010 Nobel for this reaction

Pd/graphene for dramatically enhanced Suzuki cross-coupling reactivity

[Link to Center for Rational Catalyst Synthesis](http://www.che.sc.edu/centers/cercas/)
Charge-Enhanced Dry Impregnation (CEDI)

- DI with basic solution to create surface charge

\[ \text{Pt(NH}_3\text{)}_4\text{Cl}_2 \]

- Eliminating chloride counterion in synthesis or by washing reduces particle size
- Pt, Pd, Co, Ni
Simultaneous SEA (co-SEA)

- resulting close packed monolayer of ionic complex (retaining hydration sheaths) with strong interaction with support

- resulting smaller catalyst particles and close intimacy between two metal particles

<table>
<thead>
<tr>
<th></th>
<th>Co</th>
<th>Ni</th>
<th>Cu</th>
<th>Pt</th>
<th>Pd</th>
</tr>
</thead>
<tbody>
<tr>
<td>Co</td>
<td>0.86Co</td>
<td>0.94Ni/0.97Co</td>
<td>0.70Cu/0.66Co</td>
<td>3.2Pt/0.8Co</td>
<td>0.7Co/1.3Pd</td>
</tr>
<tr>
<td>Ni</td>
<td>1.84Ni</td>
<td>0.89Cu/0.63Ni</td>
<td>2.6Pt/0.79Ni</td>
<td>0.52Ni/1.2Pd</td>
<td></td>
</tr>
<tr>
<td>Cu</td>
<td></td>
<td>2.25Cu</td>
<td>2.2Pt/0.94Cu</td>
<td>1.0Cu/2.1Pd</td>
<td></td>
</tr>
<tr>
<td>Pt</td>
<td></td>
<td>0.95Pt</td>
<td>1.31Pt/0.7Pd</td>
<td>1.27Pd</td>
<td></td>
</tr>
<tr>
<td>Pd</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Nominal loading: 1:1 atomic ratios
co-SEA Characterization

XEDS Scans (SEA)

<table>
<thead>
<tr>
<th>#</th>
<th>Cu wt%</th>
<th>Pd wt%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nom</td>
<td>32</td>
<td>68</td>
</tr>
<tr>
<td>1</td>
<td>20.7</td>
<td>79.3</td>
</tr>
<tr>
<td>2</td>
<td>14.9</td>
<td>85.1</td>
</tr>
<tr>
<td>3</td>
<td>31.6</td>
<td>68.4</td>
</tr>
<tr>
<td>4</td>
<td>31.0</td>
<td>69.0</td>
</tr>
<tr>
<td>5</td>
<td>31.4</td>
<td>68.6</td>
</tr>
<tr>
<td>6</td>
<td>19.8</td>
<td>80.2</td>
</tr>
<tr>
<td>7</td>
<td>33.4</td>
<td>66.6</td>
</tr>
</tbody>
</table>

- **co-SEA:** Average size 1.0 nm, spot analy shows well alloyed
- **DI:** larger, inhomog’ly alloyed
High Resolution Z-contrast Imaging

- Speckling confirms nanoparticle heterogeneity
Directors’ Talk Outline

A. Mission

B. Highlights

C. Summary Research Output

D. Pre-LIFE Assessment

E. Inside View of the CeRCaS

F. Reaction to IAB Input:
   1. Project reports
   2. Pre-LIFE assessment
   3. Catalyst evaluation

G. Member Status and Budget

H. Potential affiliation with ERC proposal
CeRCaS Research Results

1. Direct project papers: 2
2. Related papers: 4
3. Papers in preparation: 9
4. Presentations: 9

CeRCaS Papers and Presentations to Date, May 2017

Project 1
Continuous Production of Metal Nanoparticles using Microwave Irradiation

Related Papers:


Project 2
Enhanced stability of catalytic surfaces by bimetallic core-shell structures

Related Papers:

Papers in Preparation:
CeRCaS Research Products

1. Direct project papers
   • Direct result of CeRCaS funding
   • I/P agreement: 60 day IAB review before publication
   • Two such papers have been published without IAB review…

2. Related papers
   • Related in content, minimal or no funding from CeRCaS
   • To this point, no IAB review assumed

3. Papers in preparation
   • Direct and related papers

4. Presentations
   • Direct and related papers
Directors’ Talk Outline

A. Mission

B. Highlights

C. Summary Research Output

D. Pre-LIFE Assessment

E. Inside View of the CeRCaS

F. Reaction to IAB Input:
   1. Project reports
   2. Pre-LIFE assessment
   3. Catalyst evaluation

G. Member Status and Budget

H. Potential affiliation with ERC proposal
Typical NSF grant:
100k/y, 1 student, one mo. summer salary

Direct cost of one student: $71,000

CeRCaS award: $54,000 ($60k less 10% director tax)

CeRCaS projects involve 2 PIs; budget is split between them

PIs receive $27k (<$71k)

Almost no PI can support a student with a single CeRCaS project

Most PIs have other funds to tap; CeRCaS funding augments those
How CeRCaS Can Add Value

- **Leveraged Investment**
  - High funding leverage
- **Early Access to Technology**
  - Shared intellectual property
- **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
How CeRCaS Can Add Value to PIs

- Partial student funding always helps
- Access to Instrumentation
- Pipeline for IP
- Pipeline for Talented Graduate Students
- Synergize with Leaders in Catalysis Research
  - Ideas for additional single/dual PI grants
  - Potential center grants
Directors’ Talk Outline

A. Mission

B. Highlights

C. Summary Research Output

D. Pre-LIFE Assessment

E. Inside View of the CeRCaS

F. Reaction to IAB Input:
   1. Project reports
   2. Pre-LIFE assessment
   3. Catalyst evaluation

G. Member Status and Budget

H. Potential affiliation with ERC proposal
Budget for Small Project Proposals
G. Steinmetz email to IAB, Sunday, April 23, 2017

Motivation:

1) projects may not have it in their initial scope to evaluate … materials. A proposal to develop a series of test reactions that will be used to evaluate novel compounds may be both useful and cost effective.

2) If there is a need to leverage … equipment to make or evaluate catalysts, a funding protocol to use that equipment would be beneficial.

3) Often project proposals would be stronger if they had preliminary data… Funding of these “seed” projects may enable CeRCA to be more proactive in generating ideas.
Budget for Small Project Proposals
G. Steinmetz email to IAB, Sunday, April 23, 2017

CeRCaS ExCo Response:

1) It would be difficult to accomplish much with $2-10K.
2) Many professors already leverage other funds to do scoping experiments without writing a new proposal.
3) Any dollars used to create the small project budgets would take away money from funding larger projects.
4) With respect to setting up test protocols to evaluate new catalysts, … place testing protocols in … proposals versus a separate but smaller proposal.
For continued discussion:

1) …there would be value to funding a limited number of small projects at request. Such efforts could be used to generate a data set which strengthens the case for a full project proposal or to supplement an existing program to deliver more impact.

2) One such small project example… is to use a high throughput plate from the Lauterbach lab to test catalysts from Projects 1 & 2. This proposal is highly focused (much too small to be a project) and would be valuable…

Path Forward:

1) (CeRCA2S) is going to create a list of equipment capabilities at both USC and VCU such that this subject can be discussed later with a better understanding of CeRCA2S testing abilities.
CENTER FOR RATIONAL CATALYST SYNTHESIS: FACILITIES

Atomic Force, Scanning Tunneling and Aberration Corrected Analytical Electron Microscopies (USC and VCU)
Imaging and elemental mapping of metal nanoparticles

X-ray Photoelectron Spectroscopy/Secondary Ion Mass Spectroscopy (USC and VCU)
Surface composition of catalysts

Reactivity Testing (USC and VCU)
Catalytic activity and selectivity over wide ranges of pressure, temperature, and concentration

High Throughput Testing (USC)
For catalyst screening and nanoparticle synthesis

Links
- Members/Attendees
- Benefits to Industrial Partners
- Cost and IP/Member Agreement
- Our Researchers
- Research Thrusts
- Specific Projects
- Publications and Presentations
- Facilities
- Home

Contacts
- J.R. Regalbuto, Director
  Professor of Chemical Engineering
  SmartState Chair of Catalysis for Renewable Fuels
  Phone: 803-777-5501
  jregalbu@cec.sc.edu

- Frank Gorton, Co-Director and VCU Site Director
  Research Professor and Interim Chair
  Department of Chemical and Life Science Engineering
  Phone: 804-828-4759
  bgorton@vcu.edu
CeRCaS Research Thrusts

1. Fundamentals of metal deposition and nanoparticle formation
   a) In-situ spectroscopic or EM studies of metal adsorption
   b) Genesis of nanoparticles from adsorbed precursors
   c) Continuous nanoparticle synthesis

2. Thermodynamics and kinetics of solid-solid bonding in supported nanoparticles – “Better nanoparticles through computation”
   a) Sintering and wetting of metals and metal oxides
   b) Prediction of size and shape of supported nanoparticles as function of environment
   c) Prediction of surface composition in bimetallic nanoparticles

3. Precision catalyst site synthesis for specific reactions
   a) Pharma-related
   b) Commodity and specialty chemical applications
   c) Alternate energy and methane utilization
### CERCAS RESEARCH THRUSTS

<table>
<thead>
<tr>
<th>THRUST 1</th>
<th>THRUST 2</th>
<th>THRUST 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fundamentals of Metal Deposition</td>
<td>Thermodynamics and Kinetics of Solid-Solid Bonding</td>
<td>Precision site synthesis for specific reactions</td>
</tr>
</tbody>
</table>

### CURRENT PROJECTS

<table>
<thead>
<tr>
<th>Project 1</th>
<th>Project 2</th>
<th>Project 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Continuous Production of Metal Nanoparticles using Microwave Irradiation (Gupton, Carpenter, Monnier) Powerpoint</td>
<td>Enhanced stability of catalytic surfaces by bimetallic core-shell structures (Monnier, Regalbuto, Khanna) Powerpoint</td>
<td>Evaluation of Palladium/Graphene Surface Properties for Cross-Coupling and C-H activation (Gupton, El-Shall, Ellis, Williams) Powerpoint</td>
</tr>
<tr>
<td>← Latest Update (11-01-2016)</td>
<td>← Latest Update (11-08-2016)</td>
<td>← Latest Update (11-15-2016)</td>
</tr>
<tr>
<td>← Update Archive</td>
<td>← Update Archive</td>
<td>← Update Archive</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Project 4</th>
<th>Project 5</th>
<th>Project 6</th>
</tr>
</thead>
<tbody>
<tr>
<td>&quot;Real World&quot; Nanoparticle Synthesis on Model Supports (Chen, Regalbuto) Powerpoint</td>
<td>Continuous catalytic oxidation in pharmaceutical processing (Awad, El-Shall, Gupton, Monnier) Presentation</td>
<td>Cross coupling from a heterogeneous system based on homogeneous molecular catalyst (Yannucio, Yu) Presentation</td>
</tr>
<tr>
<td>← Latest Update (11-22-2016)</td>
<td>← Latest Update (11-01-2016)</td>
<td>← Latest Update (11-08-2016)</td>
</tr>
<tr>
<td>← Update Archive</td>
<td>← Update Archive</td>
<td>← Update Archive</td>
</tr>
</tbody>
</table>

### POTENTIAL PROJECTS

1. Continuous Production of Copper and Copper/Ceria nanoparticles (Carpenter, Monnier, Gupton)
2. Catalytic Upgrading of Hydrocarbons by Selective Oxidation (Williams, Adams, Khanna)
4. Statistical design for guided nanoparticle synthesis (Lauterbach, Hattrick-Simpers, Wen, Kusne)
5. Predicting nanoparticle size and shape (Regalbuto, Chen, Hayden, Khanna)
6. Preparation of bimetallic catalysts using continuous processing methods (Monnier, Akkarat, Blom)
Directors’ Talk Outline

A. Mission

B. Highlights

C. Summary Research Output

D. Pre-LIFE Assessment

E. Inside View of the CeRCaS

F. Reaction to IAB Input:
   1. Project reports: Report Booklet with NSF Annual Report
   2. Pre-LIFE assessment
   3. Catalyst evaluation

G. Member Status and Budget

H. Potential affiliation with ERC proposal
<table>
<thead>
<tr>
<th>Title</th>
<th>VI</th>
<th>I</th>
<th>I/C</th>
<th>NI</th>
<th>A</th>
<th>Σ</th>
<th>Rank</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) T1.1-Continuous Production of Copper an ...</td>
<td>3</td>
<td>4</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>18</td>
<td>1</td>
</tr>
<tr>
<td>- Carpenter, Monnier, Gupton</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(2) T1.2-Preparation of bimetallic catalyst ...</td>
<td>3</td>
<td>2</td>
<td>2</td>
<td>0</td>
<td>0</td>
<td>15</td>
<td>2</td>
</tr>
<tr>
<td>- Monnier, Akkarat, Blom</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(3) T1.3-Exploring Solid-Liquid Interfacial ...</td>
<td>2</td>
<td>1</td>
<td>1</td>
<td>3</td>
<td>1</td>
<td>9</td>
<td>3</td>
</tr>
<tr>
<td>- Williams, Regalbuto, Monnier</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(4) T1.4-Determination of degree of hydrat ...</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>5</td>
<td>1</td>
<td>5</td>
<td>3</td>
</tr>
<tr>
<td>- Regalbuto, Khanna</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(5) T1.5-Novel approach for continuous synt ...</td>
<td>2</td>
<td>4</td>
<td>0</td>
<td>2</td>
<td>1</td>
<td>14</td>
<td>3</td>
</tr>
<tr>
<td>- Castano, Rojas, Gupton</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(6) T2.1-Catalytic Upgrading of Hydrocarbon ...</td>
<td>2</td>
<td>3</td>
<td>0</td>
<td>4</td>
<td>0</td>
<td>12</td>
<td>5</td>
</tr>
<tr>
<td>- Williams, Adams, Khanna</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(7) T2.2-Predicting nanoparticle size and s ...</td>
<td>1</td>
<td>3</td>
<td>1</td>
<td>2</td>
<td>1</td>
<td>10</td>
<td>6</td>
</tr>
<tr>
<td>- Regalbuto, Chen, Heyden, Khanna</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(8) T2.3-In situ XRD to study the effects o ...</td>
<td>2</td>
<td>2</td>
<td>1</td>
<td>2</td>
<td>2</td>
<td>11</td>
<td>7</td>
</tr>
<tr>
<td>- Monnier, Carpenter</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(9) T2.4-The Influence of Crystallographic ...</td>
<td>0</td>
<td>1</td>
<td>2</td>
<td>4</td>
<td>1</td>
<td>4</td>
<td>7</td>
</tr>
<tr>
<td>- Lauterbach, Hattrick-Simpers</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(10) T2.5-Engineered defects in graphitic c ...</td>
<td>0</td>
<td>3</td>
<td>1</td>
<td>3</td>
<td>1</td>
<td>7</td>
<td>8</td>
</tr>
<tr>
<td>- Chandrashekhar, Williams, Weidner, Gupton</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(11) T3.1-Evaluation of Iron-based/Graphene ...</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>6</td>
<td>0</td>
<td>5</td>
<td>9</td>
</tr>
<tr>
<td>- El-Shall, Lauterbach</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(12) T3.2-Evaluation of Heterogeneous Asymm ...</td>
<td>2</td>
<td>1</td>
<td>0</td>
<td>4</td>
<td>2</td>
<td>8</td>
<td>10</td>
</tr>
<tr>
<td>- Gupton, Monnier, Carpenter</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(13) T3.3-Simple Synthesis of Highly-Active ...</td>
<td>1</td>
<td>3</td>
<td>0</td>
<td>3</td>
<td>1</td>
<td>9</td>
<td>11</td>
</tr>
<tr>
<td>- El-Kaderi, Regalbuto, Weidner</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(14) T3.4-Understanding Active Sites in Bim ...</td>
<td>0</td>
<td>2</td>
<td>0</td>
<td>5</td>
<td>1</td>
<td>4</td>
<td>12</td>
</tr>
<tr>
<td>- Chen, Heyden, Monnier</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(15) T3.5-Controlled shape electrocatalysts ...</td>
<td>1</td>
<td>2</td>
<td>1</td>
<td>5</td>
<td>0</td>
<td>8</td>
<td>13</td>
</tr>
<tr>
<td>- Zhang, Weidner, Chen</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(16) T3.6-Atomic Layer Deposition of Single ...</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>1</td>
<td>12</td>
<td>14</td>
</tr>
<tr>
<td>- El-Kaderi, El-Shall, Regalbuto</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Directors’ Talk: State of the CeRCaS

A. Mission
B. Highlights
C. Summary Research Output
D. Pre-LIFE Assessment
E. Inside View of the CeRCaS
F. Reaction to IAB Input:
   1. Project reports
   2. Pre-LIFE assessment
   3. Catalyst evaluation
G. Member Status and Budget
H. Potential affiliation with ERC proposal
Industrial Partner Status: 12/16

Currently Recruiting

Oak Ridge Natl. Lab
Parsons
Pfizer
Shell
Waters
W.R. Grace

Members:

Afton
BASF
Biogen
Boehringer-Ingelheim
Eastman Chemical
ExxonMobil
Thales Nano
UOP

Currently Recruiting

Albemarle
ADM
Aramco
BP
Chevron Phillips Chemical
Clariant
Eli Lilly
Evonik
GlaxoSmithKline
Johnson Matthey
Merck
NIST

Guests:

Idaho National Lab
Savannah River Nat. Lab.

“Going a Different Direction”

DSM
SABIC
Members:

- Afton
- BASF
- Biogen
- Boehringer-Ingelheim
- Eastman Chemical
- ExxonMobil
- Fuzionaire
- Idaho National Lab
- Thales Nano
- UOP

Currently Recruiting:

- Albemarle
- ADM
- Aramco
- BP
- Chevron Phillips Chemical
- Clariant
- Eli Lilly
- Evonik
- GlaxoSmithKline
- Johnson Matthey
- Merck
- NIST
- Savannah River Nat. Lab.

"Going a Different Direction"

- Oak Ridge Natl. Lab
- Parsons
- Pfizer
- Shell
- Waters
- W.R. Grace
- DSM
- SABIC
## Industrial Partner Status

<table>
<thead>
<tr>
<th>VCU:</th>
<th>Pharma/VCU</th>
</tr>
</thead>
<tbody>
<tr>
<td>Afton</td>
<td>$40k</td>
</tr>
<tr>
<td>Biogen</td>
<td>$40</td>
</tr>
<tr>
<td>Boehringer-Ingeheim</td>
<td>$40</td>
</tr>
<tr>
<td>Fuzionaire</td>
<td>$20</td>
</tr>
<tr>
<td>Thales Nano</td>
<td>$20</td>
</tr>
<tr>
<td><strong>Total:</strong></td>
<td><strong>$160</strong></td>
</tr>
</tbody>
</table>

**NSF → Good Standing (3/150)**

<table>
<thead>
<tr>
<th>USC:</th>
<th>Chemical/USC</th>
</tr>
</thead>
<tbody>
<tr>
<td>BASF</td>
<td>$40k</td>
</tr>
<tr>
<td>Eastman Chemical</td>
<td>$40</td>
</tr>
<tr>
<td>Fuzionaire</td>
<td>$40</td>
</tr>
<tr>
<td>Idaho National Lab</td>
<td>$20</td>
</tr>
<tr>
<td>Thales Nano</td>
<td>$40</td>
</tr>
<tr>
<td><strong>Total:</strong></td>
<td><strong>$180</strong></td>
</tr>
</tbody>
</table>

**NSF → Good Standing (3/150)
# Running Income and Expenditures

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>P1</td>
<td>50</td>
<td>60</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>P2</td>
<td>50</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>P3</td>
<td></td>
<td></td>
<td></td>
<td>30</td>
<td>60</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>P4</td>
<td></td>
<td>60</td>
<td>30</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>P5</td>
<td></td>
<td></td>
<td>60</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>P6</td>
<td></td>
<td></td>
<td></td>
<td>60</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>P7</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>60</td>
</tr>
<tr>
<td>P8</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>60</td>
<td></td>
<td></td>
</tr>
<tr>
<td>P9</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>60</td>
<td></td>
<td></td>
</tr>
<tr>
<td>P10</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>60</td>
</tr>
<tr>
<td>P11</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>P12</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>P13</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>P14</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>P15</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>P16</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Rec'd</th>
<th>$</th>
<th>100</th>
<th>220</th>
<th>340</th>
<th>360</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>cum $</td>
<td>100</td>
<td>320</td>
<td>660</td>
<td>1,020</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Awd'd</th>
<th>$</th>
<th>100</th>
<th>120</th>
<th>240</th>
<th>120</th>
<th>180</th>
<th>360</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>cum $</td>
<td>100</td>
<td>220</td>
<td>460</td>
<td>580</td>
<td>760</td>
<td>1,120</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(140)</td>
<td>(100)</td>
<td>(100)</td>
<td>(100)</td>
<td>(100)</td>
<td>(100)</td>
<td>(100)</td>
</tr>
</tbody>
</table>
Directors’ Talk: State of the CeRCaS

A. Mission

B. Highlights

C. Summary Research Output

D. Pre-LIFE Assessment

E. Inside View of the CeRCaS

F. Reaction to IAB Input:
   1. Project reports
   2. Pre-LIFE assessment
   3. Catalyst evaluation

G. Member Status and Budget

H. Potential affiliation with ERC proposal
The Process Intensification Engineering Research Center (PIERCe)

Major Thrust Areas

<table>
<thead>
<tr>
<th>Continuous reactor systems</th>
<th>Implementation &amp; Knowledge Dissemination</th>
</tr>
</thead>
<tbody>
<tr>
<td>Student exchanges / faculty sabbaticals (Industrial &amp; Academic)</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Real-time analytics, feedback, and control</th>
<th>Remote laboratories</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Ultra-efficient, recyclable catalytic systems</th>
<th>Foundation support for global health</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Modeling, simulation, and automation</th>
<th>Industrial partnerships</th>
</tr>
</thead>
</table>
PIERCe Innovation Ecosystem
8:15 – 8:45 am  Center Director Report: State of the CeRCaS
(Shenandoah Room)
(Directors JR Regalbuto, Frank Gupton)

8:45 – 9:00 am  LIFE Review (Dr. Don Davis, NSF Evaluator)

9:00 - 10:15 am  Funded Project Updates (LIFE forms filled out)
F.I.1 Continuous Production of Metal Nanoparticles using
Microwave Irradiation (Carpenter)
F.II.1 Enhanced Stability of Catalytic Surfaces by Bimetallic
Core-Shell structures (Monnier)
F.III.1 Evaluation of Palladium/Graphene Surface Properties for Cross-Coupling
and C-H activation (Ellis)

10:15 - 10:30 am  BREAK (Atrium Balcony)

10:30 - 12:10 pm  Funded Project Updates (LIFE forms filled out)
F.I.2 “Real-world” Nanoparticle Synthesis on Model Supports (Chen)
F.II.2 Cross-Coupling from a Heterogeneous System Based on a Homogeneous
Molecular Catalyst (Vannucci)
F.III.2 Continuous Catalytic Oxidation in Pharmaceutical Processing (El-Shell)
F.I.III.3 Statistical Design for Guided Nanoparticle Synthesis (Lauterbach)

12:10 - 1:10 pm  LUNCH (Atrium Balcony)

1:10 – 2:00 pm  Thrust I Proposal Presentations (LIFE forms filled out)
I.1 Continuous Production of Copper and Copper/Ceria Nanoparticles
(Carpenter)
I.2 Preparation of Bimetallic Catalysts Using Continuous Processing Methods
(Monnier)

2:00 - 2:50 pm  Thrust I/II Proposal Presentations (LIFE forms filled out)
I.3 Novel Approach for Continuous Synthesis of Supported Transition Metals
Through X-ray Radiolysis (Castano)
II.1 Catalytic Upgrading of Hydrocarbons by Selective Oxidation (Williams)

2:50 - 3:10 pm  BREAK (Atrium Balcony)

3:10 – 4:00 pm  Thrust II/III Proposal Presentations (LIFE forms filled out)
II.1 In-Situ XRD to Study Monometallic and Bimetallic Catalysts
(Monnier)
III.1 Atomic Layer Deposition of Single-Atom Catalysts for Selective
Hydrogenation of Alkenes (El-Kaderi)

4:00 - 5:25 pm  IAB Meeting (Steinmetz)
Discussion of i) funding cycle and budget, ii) feedback on pre-LIFE, iii) evaluation
focus, iv) potential ERC proposal, etc.

5:25 – 5:30 pm  Review of Day 2 activities (Regalbuto)

5:30 - 7:00 pm  Poster Session and Social (Potomac Room)
(USC and VCU Grad Students)

7:00 pm  End of Day 1 (Dinner on your own)
**Friday, May 19:**

<table>
<thead>
<tr>
<th>Time</th>
<th>Event</th>
<th>Location</th>
</tr>
</thead>
<tbody>
<tr>
<td>7:30 - 8:00 am</td>
<td><strong>Breakfast</strong> (Shenandoah Room)</td>
<td></td>
</tr>
<tr>
<td>8:00 – 9:45 am</td>
<td><strong>LIFE Form Review and Discussion</strong> (Shenandoah Room)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>NSF Moderator (Davis)</td>
<td></td>
</tr>
<tr>
<td>9:45 - 10:00 am</td>
<td><strong>BREAK</strong> (Shenandoah Room)</td>
<td></td>
</tr>
<tr>
<td>10:00 - 11:30 am</td>
<td><strong>IAB Meeting (IAB Members and NSF)</strong></td>
<td>Projects: Discussion of proposed projects, voting and discussion of results, formulation of funding recommendation to center leadership.</td>
</tr>
<tr>
<td>11:30 - 12:15 am</td>
<td><strong>IAB Report Out, Discussion</strong> (IAB, Center directors, NSF)</td>
<td></td>
</tr>
<tr>
<td>12:15 - 12:25 am</td>
<td><strong>Action Items and Plans for Next Semiannual Meeting</strong></td>
<td>(IAB, Center Directors and NSF)</td>
</tr>
<tr>
<td>12:25 – 12:30</td>
<td><strong>Summary and Closing Remarks</strong></td>
<td></td>
</tr>
<tr>
<td>12:30 pm</td>
<td><strong>ADJOURN (Box lunches)</strong> (Shenandoah Room)</td>
<td></td>
</tr>
<tr>
<td>1:00 – 2:00 pm</td>
<td><strong>USC and VCU faculty debriefing</strong> (Shenandoah Room)</td>
<td></td>
</tr>
</tbody>
</table>