8:30 – 9:00 am  Center Director Report: CeRcAS Vision, Capabilities, and Current Status (Empire Room) (Directors JR Regalbuto, Frank Gupton)

9:00 – 9:15 am  LIFE Intro (Dr. Donald Davis, Old Dominion U., NSF Evaluator)

9:15 - 10:05 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)

10:05 - 10:20 am  BREAK (Mezzanine)

10:20 - 11:10 pm  Funded Project Updates (LIFE forms filled out)
   F.III.1 Evaluation of Palladium/Graphene Surface Properties for Cross-Coupling and C-H activation (Ellis)
   F.I.2 “Real-world” Nanoparticle Synthesis on Model Supports (Chen)

11:10 – 12:00 pm  Thrust I Proposal Presentations (LIFE forms filled out)
   I.1 Exploring Solid-Liquid Interfacial Chemistry During Catalyst Synthesis (Williams)
   I.2 Statistical design for guided nanoparticle synthesis (Lauterbach)

12:00 - 1:30 pm  LUNCH (Nanocenter Atrium, with tours)

1:30 - 2:20 pm  Thrust II Proposal Presentations (LIFE forms filled out)
   II.1 Cross Coupling from a Heterogeneous System Based on a Homogeneous Molecular Catalyst (Vannucci)
   II.2 Catalytic Upgrading of Hydrocarbons by Selective Oxidation over RuAu Bimetallic Catalysts (Williams)

2:20 - 2:35 pm  BREAK (Mezzanine)

2:35 - 3:50 pm  Thrust III Proposal Presentations (LIFE forms filled out)
   III.1 Continuous Catalytic Oxidation in Pharmaceutical Processing (El-Shall)
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   III.3 Highly-Active and Stable Hybrid Cathode Catalyst for PEM Fuel Cells for Automotive Application (Regalbuto)

3:50 - 4:20 pm  IAB Meeting (Steinmetz)
   Election of Chair and Chair-Elect

4:20 - 4:30 pm  Review of Day 2 activities (Regalbuto)

4:30 - 6:00 pm  Poster Session and Social (Flemish Room)
   (USC and VCU Grad Students)

6:00 pm  End of Day 1 (Dinner on your own)
The Center for Rational Catalyst Synthesis

JR Regalbuto and Frank Gupton

CeRCaS Spring Meeting

May 19-20, 2016

Virginia Commonwealth University
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
**Typical catalyst ordering specifications:**

- Metal
- Support
- Wt% metal

“Supplier: Here’s what we have.”

**Alfa Aesar:** 5 wt% Ru/Alumina

→ Average size 4.8 ± 2.2 nm

**Industry:** Pd/Carbon, 30 wt% Pd

→ Average size 4.7 ± 1.7 nm
EM image comparison, USC and Industrial catalyst

STEM micrographs of alumina supported samples: (a) 2.0RuAl-SEA, (b) 2.0RuAl-DI, (c) 5.0RuAl-com.
EM image comparison, USC and Industrial catalyst

USC: Pt/Carbon, SEA (20 wt% Pt)  
Premetek 20% Pt/VXC72 Carbon

→ Average size 2.3 ± 0.6 nm  
→ Average size > 5 nm
Partial and Multilayer Shell Synthesis with ED:

Ru shells on Pt cores on carbon

Pt shells on Ru cores on carbon

Pt shells on Pd on carbon

Pt on Co on carbon
Controlled Shapes of Nanoparticles

Rods vs. spheres

DOE for CO oxidation catalysts

Co nanorods

Co nanoparticles

Temperature (°C)

Max Temp (deg C)

Particle size (nm)

Intensity (Counts)

89-7099 > CoO - Cobalt Oxide (100.0%)
Continuous Nanoparticle Production

- DLS Size (d.nm): 5.337 (99.7%), 70.63 (0.3%)
Better Nanoparticles via Computations

Energetics of Model 50-50 Ag-Ir Nanoparticles

Ag-Shell
Ir-Core
Most Stable

ΔE = 0.00 eV
A.E./Atom = 4.11 eV

α-Al$_2$O$_3$
Alloyed

Ir-Shell
Ag-Core

ΔE = +0.29 eV

Ag-Shell
Ir-Core
Most Stable

ΔE = 0.00 eV
A.E./Atom = 4.38 eV

γ-Al$_2$O$_3$
Alloyed

Ir-Shell
Ag-Core

ΔE = +1.44 eV

ΔE = +0.91 eV

ΔE = +0.17 eV
- Metal
- Support
- Wt% metal

- Average particle size
  _ 1 nm _ 2 nm _ 3 nm _ 4 nm _ 5 nm _ other (specify)

- Desired particle size distribution (% of average size)
  _ 10% _ 25% _ 50% _ 100% _ 200% _ other (specify)

- Stability to what temperature in (__________ specify gas/liquid):
  _ 100ºC _ 200ºC _ 400ºC _ 600ºC _ 800ºC _ other (specify)

_Pt on: silica_ _ alumina_ _ carbon_ _ titania_
Future bimetallic ordering specifications:

- Metal 1
- Metal 2
- Support
- Wt% metal 1, 2

- Average particle size
  __ 1 nm  __ 2 nm  __ 3 nm  __ 4 nm  __ 5 nm  __ other (specify)

- Desired particle size distribution (% of average size)
  __ 1 nm  __ 2 nm  __ 3 nm  __ 4 nm  __ 5 nm  __ other (specify)

- Desired particle morphology
  __ homogeneous alloy  __ core metal 1, shell metal 2  __ core metal 2, shell metal 1  __ other (specify)
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 (reverse micelles), 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-Shall (graphene supports), Carpenter (magnetic bimetals), El-Kaderi (organometallic clusters), Khanna (metal clusters), Bertino (nanoparticles on porous monoliths), Ellis (organic synthesis), Tang (organic synthesis)
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 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
# CENTER FOR RATIONAL CATALYST SYNTHESIS: SPECIFIC PROJECTS

FOR MORE INFORMATION REGARDING THESE PROJECTS
CONTACT: JR REGALBUTO

## CERCAS RESEARCH THRUSTS

<table>
<thead>
<tr>
<th>THRUST 1</th>
<th>THRUST 2</th>
<th>THRUST 3</th>
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</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>
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</tbody>
</table>

## CURRENT PROJECTS

1. **Continuous Production of Metal Nanoparticles using Microwave Irradiation**
   - Gupton, Carpenter, Monnier/Presentation
   - Latest Update (05-03-2015)
   - Post Updates

2. **Continuous Stability of Catalyst Surfaces by Heterogeneous Core-Shell Structures**
   - Monnier, Khan/Work
   - Latest Update (05-10-2015)
   - Post Updates

3. **Evaluation of Palladium/Graphene Surface Properties for Cross-Coupling and C-H Activation**
   - Gupton, El-Shall, Ellis/Work
   - Latest Update (04-19-2016)
   - Post Updates

4. **Real World** Nanoparticle Synthesis on Model Supports
   - Chen, Regalbuto/Presentation
   - Latest Update (04-26-2015)
   - Post Updates

## SUGGESTED (PRESENTED) PROJECTS

1. **Exploring Solid-Liquid Interfacial Chemistry During Catalytic Synthesis**
   - Williams, Regalbuto, Monnier/Presentation

2. **Understanding Catalytic Coking and Stability during Hydrocracking**
   - Prosser, Heyden, Lauterbach/Presentation

2. **Nanoparticle stabilization via scalable ALD/MOCVD coating**
   - Gupton, Regalbuto/Presentation

2. **Evaluation of Heterogeneous Acetylene Hydrogenation Catalyst**
   - Monnier, Heyden, Williams/Presentation

## OTHER PROJECTS

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**Links**

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

**Contacts**

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

Frank Gupton, Co-Director and VCU Site Director
Research Professor and Interim Chair
Department of Chemical and Life Science Engineering
Phone: 804-828-4706
bgupton@vcu.edu

CeRCaS homepage: www.che.sc.edu/centers/cercas
Industrial Partner Status

Members:
BASF
Biogen
Boehringer-Ingelheim
Eastman Chemical
ExxonMobil
Thales Nano
Afton

Currently Recruiting
Albemarle
ADM
Aramco
BP
Chevron Phillips Chemical
Clariant
Eli Lilly
GlaxoSmithKline
Johnson Matthey
Merck
NIST
Oak Ridge Natl. Lab
Parsons
Pfizer
Shell
Waters
W.R. Grace

“Just Not This Year”
Evonik
UOP

“Going a Different Direction”
DSM
SABIC
Savannah River Nat. Lab.

Guests:
Idaho National Lab
# Industrial Partner Status

## Pharma/VCU

**Members:**
- BASF
- Biogen
- Boehringer-Ingelheim
- Eastman Chemical
- ExxonMobil
- Thales Nano
- Afton

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**Total:** $150

**VCU:** Good Standing → $150k NSF match

## Chemical/USC

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<tr>
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**Total:** $120

**USC:** NSF Match → $85k until good standing is achieved
## Current Budget

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<th>Date Joined</th>
<th>2015</th>
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**Yearly total**
- 2015: 80,000
- 2016: 230,000
- 2017: 270,000

**Cumulative**
- 2015: 80,000
- 2016: 310,000
- 2017: 580,000

**Funded to date:**
- 210,000

**Funding dollars:**
- 100,000
- 270,000

This Year: Fund two projects at $50/60k

Next Year: Fund four at once, or fund continuously? (IAB preference)
Goals of the Fall Meeting

1. Evaluate and critique four current research projects

2. Choose two new projects

3. IAB Business:
   a) Choose IAB Chair and Chair-elect
   b) Discuss in-kind contribution, membership of INL
   c) Future meeting format:
      1) Consecutive meetings for project selection and project review
      2) Project selection and review in every meeting
8:30 – 9:00 am  Center Director Report: CeRCaS Vision, Capabilities, and Current Status (Empire Room) (Directors JR Regalbuto, Frank Gupton)

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4:30 - 6:00 pm  Poster Session and Social (Flemish Room) (USC and VCU Grad Students)

6:00 pm  End of Day 1 (Dinner on your own)
Friday, May 20:

8:00 - 8:30 am  Breakfast (Empire Room)

8:30 - 10:00 am  LIFE Form Review and Discussion (Empire Room)
NSF Moderator (Davis)

10:00 - 10:15 am  BREAK (Mezzanine)

10:15 - 11:00 am  IAB Meeting (IAB Members and NSF)
Projects: Discussion of proposed projects, voting and discussion of results, formulation of funding recommendation to center leadership.

11:00 - 11:30 am  IAB Report Out, Discussion (IAB, Center directors, NSF)

11:30 - 11:50 am  Action Items and Plans for Next Semiannual Meeting
(IAB, Center Directors & NSF)

11:50 – 12:00  Summary and Closing Remarks

12:00 pm  ADJOURN (Box lunches) (Mezzanine)

12:15 – 1:00 pm  USC and VCU faculty debriefing (Empire Room)
The Center for Rational Catalyst Synthesis

2016-17 Meeting Dates

Proposed:

December, 2016
University of South Carolina

May, 2017
Virginia Commonwealth University
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