The Center for Rational Catalyst Synthesis (CeRCaS)

Kickoff Meeting Agenda

Thursday, May 21:

7:30 am  
Participant Registration  (Horizon Building, 2nd floor conference room)

7:30 - 8:15 am  
Breakfast and Networking Time

8:15 - 8:30 am  
Welcome Remarks  (USC, VCU Administration)

8:30 - 9:15 am  
Kickoff Meeting Goals, Vision and Capabilities of the Center  
(Directors JR Regalbuto, Frank Gupton)

9:15 - 10:00 am  
NSF I/UCRC Presentation  (Dr. Raffaella Montelli, NSF I/UCRC Program Director and Dr. Donald Davis, Old Dominion U., NSF Evaluator)

10:00 - 10:15 am  
BREAK

10:15 - 12:15 pm  
Project Proposal Presentations (LIFE forms filled out)  
1.1 Continuous Production of Metal Nanoparticles using Microwave Irradiation  (Carpenter)  
1.2 Exploring Solid-Liquid Interfacial Chemistry During Catalyst Synthesis  (Williams)  
1.3 Statistical design for guided nanoparticle synthesis  (Lauterbach)  
1.4 Synthesis of Ultrasmall Noble Metal Particles on Graphene  (Regalbuto)  
1.5 Understanding supported metal oxide wetting and sintering  (Regalbuto)

12:15 - 1:15 pm  
LUNCH

1:15 - 3:15 pm  
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II.2 Nanoparticle stabilization via scalable ALD/MLD coating  (Yu)  
II.3 Enhanced stability of catalytic surfaces by bimetallic core-shell structures  (Monnier)  
II.1 Evaluation of Palladium/Graphene Surface Properties for Cross-Coupling and C-H activation  (Ellis)  
II.2 Continuous catalytic oxidation in pharmaceutical processing  (Gupton)  
II.3 Evaluation of Heterogeneous Asymmetric Hydrogenation Catalysts  (Gupton)

3:15 - 3:30 pm  
BREAK

3:30 - 3:45 pm  
Review of evening and Day 2 activities  (JR Regalbuto)

3:45 - 5:00 pm  
IAB Organizational Meeting and Formative Discussion  (IAB Members and NSF only)  
Impressions of Day 1  
Day 2 voting process  
Project management and mentoring framework for selected projects  
Election of IAB Chair, Chair-Elect (secretary), and Bylaws Committee

5:00 – 6:00 pm  
Poster Session and Social  (USC and VCU Grad Students, Horizon Foyer)
The Center for Rational Catalyst Synthesis

JR Regalbuto and Frank Gupton

CeRCaS Kickoff

May 21-22, 2015

University of South Carolina
Introductions
Goals of the Kickoff Meeting

A. Review and marvel at CeRCA's vision and capabilities

B. Evaluate and shape research projects

C. Choose the initial set of projects

D. Begin working on bylaws
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Outline

A. Vision

B. Research Thrusts

C. Capabilities

D. Member Status
Catalysis: The Hidden But Crucial Science

Catalysis underpins our standard of living and world economy:
- 95% (by volume) of all products, 80% of added value in the chemical industry
- 20 – 35% of world’s GDP depends directly or indirectly on catalysis
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

Industry: Pd/Carbon, 30 wt% Pd

→ Average size 4.8 ± 2.2 nm

→ Average size 4.7 ± 1.7 nm
**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)

- Average size $2.3 \pm 0.6$ nm

Premetek 20% Pt/VXC72 Carbon

- Average size $> 5$ nm
**Why CeRCaS?**

- Catalyst synthesis/development is still relatively empirical

- The most common method, impregnation, often yields poorly dispersed, poorly distributed supported nanoparticles

- Many “rational syntheses” are complex, expensive → not scalable

- Ideal synthesis of supported nanoparticles: cheap, simple process to give metal nanoparticles high dispersion, tight size distribution, and uniform particle distribution on high surface area supports

<table>
<thead>
<tr>
<th>Pt on: silica</th>
<th>alumina</th>
<th>carbon</th>
<th>titania</th>
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<tr>
<td><img src="511x637.png" alt="Image" /></td>
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<th>5 nm</th>
<th>4 nm</th>
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<td>1.0 nm</td>
<td>1.3 nm</td>
<td>1.4 nm</td>
<td>1.2 nm</td>
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Future ordering specifications:

- 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

5 nm * 1.0 nm
4 nm * 1.3 nm
7 nm * 1.4 nm
7 nm * 1.2 nm
Particle size control, starting with the smallest:

**Hard chemistry (heat and moisture)**

**Soft chemistry (salts)**

- Pt/SiO₂ with chloride
- Au/C with ammonia

**Ru/SBA-15**

- 4.5 nm
- 3.8 nm
- 3 nm
- 1.4 nm

**Pt/SBA-15**

- 3.6 nm
- 2.8 nm
- 2.0 nm
- 1.0 nm
Controlled Shapes of Nanoparticles

**Rods vs. spheres**

- **CO$_2$ conversion**
- **CO selectivity**
- **C1-C5 selectivity**
- **C1-C5 yield**

**DOE for CO oxidation catalysts**

- **Particle size (nm)**
- **Max Temp (deg C)**

---

Co nanorods

Co nanoparticles

---

(220)

5 nm

(111)

(200)

(220)

(311)

(222)

---

Intensity (Counts) x 10$^3$

Intensity (Counts)

---

CoO - Cobalt Oxide (100.0%)
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)
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
Rational Synthesis Roadmap - Bimetals

Pt/Pd nanoparticles

- Co-DI: poor dispersion & alloying
- Co-SEA: homogeneous alloys
- Seq-SEA: partial shells
- SEA-ED: full shells
How Can We Produce Catalyst Bistros?

- The chemical fundamentals of supported nanoparticle synthesis must be studied with complex and interdisciplinary methods.
- Good thing we have a center!

CeRCaS Mission

- CeRCaS will conduct the watershed research in the history of catalysis which transforms the art of supported nanoparticle synthesis into a science.
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 metal 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 bimetallics), El-Kaderi (organometallic clusters), Khanna (metal clusters), Bertino (nanoparticles on porous monoliths), Ellis (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 electroless deposition

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
Attenuated Total Reflection FTIR and Raman Spectroscopy

- Allows investigation of real catalysts and supports:
  - powders of oxides, oxide-supported metals, also thin metal films
- Conduct techniques under catalyst synthesis conditions
  - Liquid phase, various precursor concentrations, T and P
  - Detect surface adsorbed precursors, reducing agents and fragments
  - Explore addition of surface probe molecules such as CO
Some Open Challenges for ED (cont.)

- Enhanced Control over Electroless Deposition Process?
  - Tuning of catalytic vs. autocatalytic deposition pathways
  - Directing the surface location of the second metal catalytic deposition

- Probing surface chemistry during the ED process is the key to understanding and controlling these phenomena
  - Reducing agent fragments on surface acting as a poison for further deposition? Use of CO as a directing agent?

Fig. 4. Transmission FTIR spectra of CO adsorption on Ag/SiO₂, Pd/SiO₂ and Ag-Pd/SiO₂ catalysts. Arrows highlight peak intensity losses (∆) as Ag wt.% increases.
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Computations and experiment on metal oxide wetting

The decrease in Pt dispersion and the increase in Ag dispersion with increasing calcinations temperature.

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<th>Surface free energies of various oxides</th>
<th>( \gamma_{\text{surf}} ) (J/m(^2))</th>
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<tbody>
<tr>
<td>T = 300 K, ( P_{O2} = 1 \text{ atm} )</td>
<td></td>
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<tr>
<td>TiO(_2) (110)</td>
<td>0.38</td>
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<tr>
<td>RuO(_2) (110)</td>
<td>1.07</td>
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<tr>
<td>RhO(_2) (110)</td>
<td>1.12</td>
</tr>
<tr>
<td>Rh(_2)O(_3)(0001)-O-terminated</td>
<td>0.09</td>
</tr>
<tr>
<td>PdO(100)-PdO-terminated</td>
<td>0.10</td>
</tr>
<tr>
<td>Ag(_2)O(100)-O-terminated</td>
<td>0.78</td>
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Thermodynamics suggests that if the interface free energy, \( \gamma_{ox/TiO2} \), is larger than the difference of the surface free energy of titania, \( \gamma_{v/TiO2} \), and the oxide, \( \gamma_{v/ox} \), then the oxide does not wet the titania/vacuum interface (\( \gamma_{ox/TiO2} > \gamma_{v/TiO2} - \gamma_{v/ox} \)).
Computations and experiment to predict particle size as a function of facet

**Figure 3.** Multiscale facets of titania support forms; a. STM image of TiO$_2$ (110) from Chen lab, b. macro-faceted metal sphere from [23], c. meso-faceted titania polyhedral from [24], d. TEM image of commercially available Degussa P25 titania.

**Figure 5.** a) SEA deposition of adsorbed metal coordination complexes [42] and b) STM image of Pt nanoparticles synthesized from PTA over TiO$_2$ (110) and c) STEM image of Pt over high surface area TiO$_2$. 
Theoretical Determination of Optimal Core Metals

- Metals with High Surface Energy will prefer core.
- Ideal Core Metal will bind strongly to support.
- Co, Ru, Ir chosen as Core metals for preliminary study.
Enhanced Stability in Model Core-Shell Clusters

Pt\textsubscript{7}, Pd\textsubscript{7} serve as model for small Core-shell Cluster.

Replacing core Atom Increases Binding Energy.

Pt: Metal Shell

Ru: Core Metal

α-Al\textsubscript{2}O\textsubscript{3}

Co: Core Metal

α-Al\textsubscript{2}O\textsubscript{3}
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Electroless Deposition (ED)

(Monnier)

Electroless deposition steps
A: ED bath at time = 0
B: Activation of reducing agent
C: Reduction and deposition of $M_2^{y+}$
D: Catalytic deposition
E: Autocatalytic deposition

Glycerol oxidation over Au-Pd catalysts

**Reaction conditions:** 0.1M Glycerol, 1M OH⁻, 60 °C, 150 psig O₂, 30-150 mg catalyst.

**Transition state**

\[
\text{HOCH}_2\text{CH}_2\text{CH}_2\text{O} \quad \rightarrow \quad \text{HOCH}_2\text{CH}_2\text{C} = \text{H} + \text{H} \quad \text{Pd}
\]

## Current Capabilities

### Catalyst Synthesis
- Organometallics
- Strong electrostatic adsorption
- Vapor deposition
- Electroless deposition
- Atomic and molecular layer deposition
- Dendrimer encapsulation
- Multiple metal sputtering
- Micelles
- Continuous nanoparticle manufacture
- Computational methods

### Catalyst characterization
- Chemisorption (2)
- BET surface area
- Temp prog methods (3)
- FTIR of adsorbates (2)
- ATR-IR
- XPS w/ SIMS
- UHV surface analysis
- XRD (2)
- Aberration-corrected STEM-EDS
- GC/MS
- Mass specs (5)
- Electrochemical tools

### Catalyst evaluation
- Flow reactors, 1-30 bar (9)
- HP batch reactors (5)
- HP CSTR flow reactors (2)
- Recirculation loop reactor
- HT -16 small ID flow reactors
- HT - 8 larger ID flow reactors
- Liq. feed, gas phase reactors (2)
- On-line GC’s (9)
- GC/autosamplers (3)
- HPLC (1)
How CeRCaS Can Add Value

- **Leveraged Investment**
  - Up to 20:1 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
We seek direct participation

- IAB should determine one mentor for each selected project

- Industrial members can/should participate in bi-monthly meetings with research team

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<th>Title</th>
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<th>Spons2</th>
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Industrial Partner Status

Letters received from:
- BASF
- Eastman Chemical
- Thales Nano
- UOP

Companies attending as guests:
- Albemarle
- Boehringer-Ingelheim
- Evonik

Letters pending from:
- Afton
- DSM
- SABIC
- Savannah River Natl. Lab. (X)

Companies needing bylaws passed with their articles:
- Aramco (export control)
- ExxonMobil (antitrust, confidentiality)

Companies needing MOU/Side Letter:
- Merck (felon clause)

Currently Recruiting
- Biogen
- BP
- Chevron Phillips Chemical
- Clariant
- Eli Lilly
- GlaxoSmithKline
- Idaho National Lab
- Johnson Matthey
- Oak Ridge Natl. Lab
- Parsons
- Pfizer
- Shell
- Waters
- W.R. Grace
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 Homework:
Look at draft of bylaws; passage gains us two companies.
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Election of IAB Chair, Chair-Elect (secretary), and Bylaws Committee

5:00 - 6:00 pm  
Poster Session and Social (USC and VCU Grad Students, Horizon Foyer)
Friday, May 21:

7:30 - 8:00 am  **Arrival and Breakfast**  (Horizon Building, 2nd floor conference room)

8:00 - 9:30 am  **LIFE FORM review and Discussion** - NSF Moderator (Dr. Davis)
All participants - at IAB discretion.

9:30 - 10:45 am  **IAB Meeting (IAB Members and NSF)**
Projects: Discussion of proposed projects, voting and discussion of results, formulation of funding recommendation to center leadership. Finalize discussion of topics started at the day 1 formative IAB meeting.

10:45 - 11:00 am  **BREAK**

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)