CeRCaS News Blast 11/8/16

Ring 1: Your input needed in our preliminary LIFE analysis.
Member companies will now be directly involved in selecting the potential projects presented at the semiannual meetings. You will shortly receive instructions from our evaluator, Dr. Don Davis, on filling out a preliminary Level of Interest Feedback Evaluation from our list of Potential Projects (see www.che.sc.edu/centers/cercas/projects.html, and below). Six of the fifteen potential projects will be selected for presentation at the fall meeting. Stay on the lookout for the detailed instructions.

CERCAS RESEARCH THRUSTS

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<th>THRUST 1</th>
<th>THRUST 2</th>
<th>THRUST 3</th>
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<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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CURRENT PROJECTS

Project 1
Continuous Production of Metal Nanoparticles using Microwave Irradiation (Gupton, Carpenter, Monnier) Powerpoint
 ⇨ Latest Update (11-01-2016)
 ⇨ Update Archive

Project 2
Enhanced stability of catalytic surfaces by bimetallic core-shell structures (Monnier, Regalbuto, Khanna) Powerpoint
 ⇨ Latest Update (10-11-2016)
 ⇨ Update Archive

Project 3
Evaluation of Palladium/Graphene Surface Properties for Cross-Coupling and C-H activation (Gupton, El-Shall, Ellis, Williams) Powerpoint
 ⇨ Latest Update (10-18-2016)
 ⇨ Update Archive

Project 4
"Real World" Nanoparticle Synthesis on Model Supports (Chen, Regalbuto) Powerpoint
 ⇨ Latest Update (10-25-2016)
 ⇨ Update Archive

Project 5
Continuous catalytic oxidation in pharmaceutical processing (Awad, El-Shall, Gupton, Monnier) Powerpoint
 ⇨ Latest Update (11-01-2016)
 ⇨ Update Archive

Project 6
Cross coupling from a heterogeneous system based on homogeneous molecular catalyst (Vannucci, Yu) Presentation
 ⇨ Latest Update (10-11-2016)
 ⇨ Update Archive

POTENTIAL PROJECTS

1. Continuous Production of
2. Catalytic Upgrading of Hydrocarbons by
3. Simple Synthesis of Highly-Active and
Copper and Copper/Ceria nanoparticles (Carpenter, Monnier, Gupton) May 2016 Presentation

Selective Oxidation (Williams, Adams, Khanna) May 2016 Presentation

Stable PtCo/Carbon Oxygen Reduction Reaction Catalyst (El-Kaderi, Regalbuto, Weidner)

2. Exploring Solid-Liquid Interfacial Chemistry During Catalyst Synthesis (Williams, Regalbuto, Monnier) May 2016 Presentation

2. In situ XRD to study the effects of temperature and gas phase on the structure of bimetallic catalysts (Monnier, Carpenter) May 2016 Presentation

2. Evaluation of Heterogeneous Asymmetric Hydrogenation Catalysts (Gupton, Monnier, Carpenter) May 2016 Presentation

3. Statistical design for guided nanoparticle synthesis (Lauterbach, Hattrick-Simpers, Wen, Kusne) May 2016 Presentation

3. The Influence of Crystallographic Faceting on Self-Reducing Metallic Catalysts in Oxidative Environments (Lauterbach, Hattrick-Simpers)

3. Understanding Active Sites in Bimetallic Catalysts for Hydrodeoxygenation (Chen, Heyden, Monnier)

4. Preparation of bimetallic catalysts using continuous processing methods (Monnier, Akkartat, Blom)

4. Engineered defects in graphitic carbon/graphene (Chandrashekhar, Williams, Weidner, Gupton, El-Shall)


5. Determination of degree of hydration as electrostatic adsorption uptake limit (Regalbuto, Khanna)

5. Predicting nanoparticle size and shape (Regalbuto, Chen, Heyden, Khanna)

5. Controlled shape electrocatalysts for conversion of CO2 to liquid fuels (Zhang, Weidner, Chen)

**Ring 2: Save the Date! Fall CeRCaS Meeting (Dec. 15-16, 2016) in Columbia at the Courtyard Marriott.**

The Fall CeRCaS meeting will be held at the Courtyard Columbia Downtown at USC (630 Assembly Street, Columbia SC, 29201, phone 803-799-7800) on the west side of campus. The group rate is $134; mention that you will be attending the “CeRCaS Meeting” in order to join the block. This discount is available until 11/24/16. A full agenda will circulate soon; plan on arriving Wednesday evening (Dec. 14th). The meeting will end with lunch, Friday Dec. 16th.
Ring 3: Recent Results Achieved for

Project 1. Continuous Production of Metal Nanoparticles

Everett Carpenter and his team at VCU and USC have demonstrated the synthesis of ultrasmall (<2 nm) Pt nanoparticles in solution and are now focusing on synthesizing them in formed catalyst supports.

Project 2: Enhanced stability of catalytic surfaces by bimetallic core-shells

John Monnier with his USC and VCU team have identified unusual chemisorption uptake of the Ag and Au shells in Ir core-shell particles; computations at VCU are progressing to explain this unusual finding.
Project 3: Evaluation of Pd/graphene surface properties for cross-coupling and C-H activation

Keith Ellis and his team at VCU and USC have developed methods to deposit sub-2 nm Pd particles on graphene oxide, some of which exhibit remarkably high catalytic activity. Samples are being sent to member companies for further testing.

Project 4: “Real world” nanoparticle synthesis on model supports

Donna Chen and her team at USC have discovered a previously unreported oxidation of Pt(II) complexes when they adsorb on both model and high surface area graphite surfaces.
**Project 5: Continuous Catalytic Oxidation in Pharmaceutical Processing**

Frank Gupton and his team at VCU and USC are synthesizing several series of bimetallic catalysts with enhanced performance for benzyl alcohol oxidation.

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**Electroless Deposition of Au on Pd**

<table>
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<tr>
<th>Electroless Developer Bath</th>
<th>(based on prior work by Rodriguez et al.)</th>
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<tbody>
<tr>
<td>Au precursor: [Au(CN)₄]⁻</td>
<td>from KAu(CN)₆</td>
</tr>
<tr>
<td>Reducing Agent: Hydrazine (N₂H₄)</td>
<td>N₂H₄/Au = 5:1</td>
</tr>
<tr>
<td>Catalyst/Volume = 0.50 g/250 mL</td>
<td>Bath pH: 10</td>
</tr>
<tr>
<td>Temperature: (Room Temp)</td>
<td>Fresh N₂H₄ (of same initial amount) added every 30 min</td>
</tr>
</tbody>
</table>

- Varying theoretical monodisperse coverage of Au deposited.
- Amount of Au controlled by initial concentration.
- Complete deposition after 60 min.
- Filtered and washed copiously with de-ionized water.

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**Project 6: Cross Coupling from a Heterogeneous System based on Homogeneous Molecular Catalyst**

Aaron Vannucci and his team at USC have demonstrated relatively high yields, turnover numbers and turnover frequencies in anchoring molecular Ni based catalysts on carbon supported oxide nanoparticles.

⇒ Members can access current and past updates at: www.che.sc.edu/centers/cercas/projects.html

For more information:
http://www.che.sc.edu/centers/cercas/