CERCAS

The Center for Rational Catalyst Synthesis

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

THRUST 1	THRUST 2	THRUST 3
Fundamentals of Metal Deposition	**Thermodynamics and Kinetics of Solid-Solid Bonding**	**Precision site synthesis for specific reactions**

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

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

POTENTIAL PROJECTS

1. Continuous Production of

1. Catalytic Upgrading of Hydrocarbons by

1.Simple Synthesis of Highly-Active and

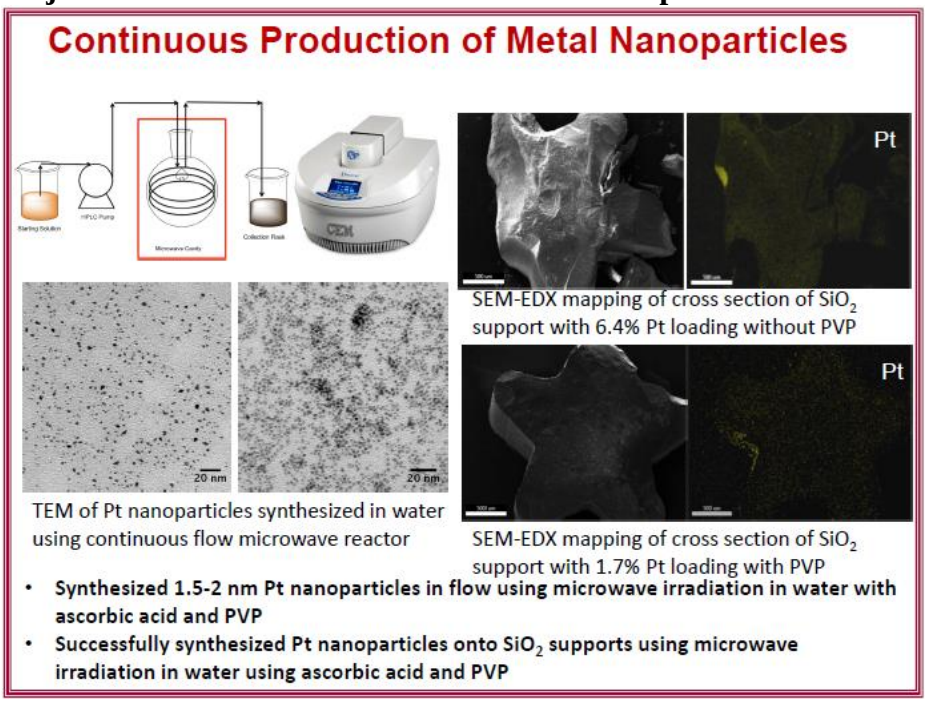
Copper and Copper/Ceria nanoparticles*(Carpenter, Monnier, Gupton)* May 2016 Presentation	Selective Oxidation *(Williams, Adams, Khanna)* May 2016 Presentation	Stable Pt_3Co/Carbon Oxygen Reduction Reaction Catalyst *(El-Kaderi, Regalbuto, Weidner)*
2. Exploring Solid-Liquid Interfacial Chemistry During 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)*	2.Evaluation of Heterogeneous Asymmetric Hyrdogenation 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, Akkarat, Blom)*	4. Engineered defects in graphitic carbon/graphene *(Chandrashekhar, Williams, Weidner, Gupton, El-Shall)*	4.Evaluation of Iron-based/Graphene Catalysts for Fischer-Tropsch Synthesis of Zero-Sulfur Transportation Fuels *(El-Shall, Lauterbach)*
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.

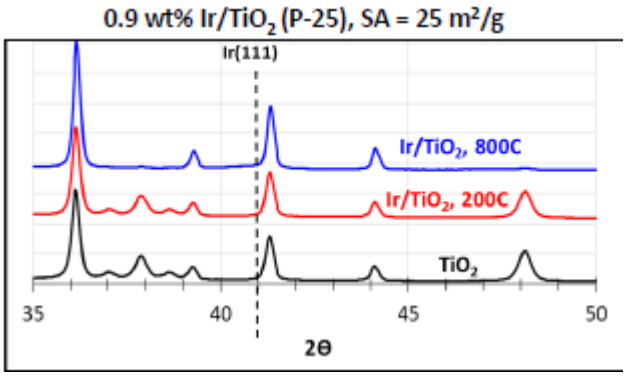
Ring 3: Recent Results Achieved for

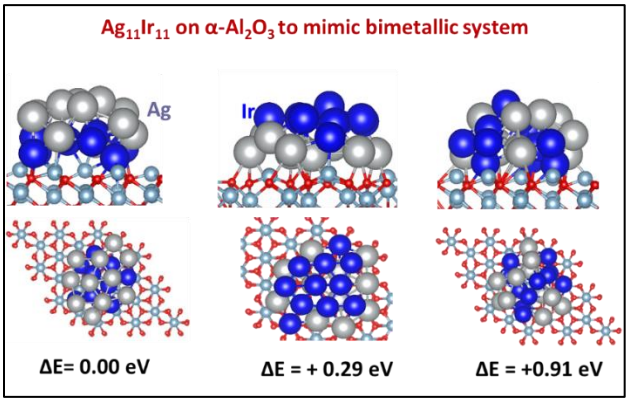
Project 1. Continuous Production of Metal Nanoparticles

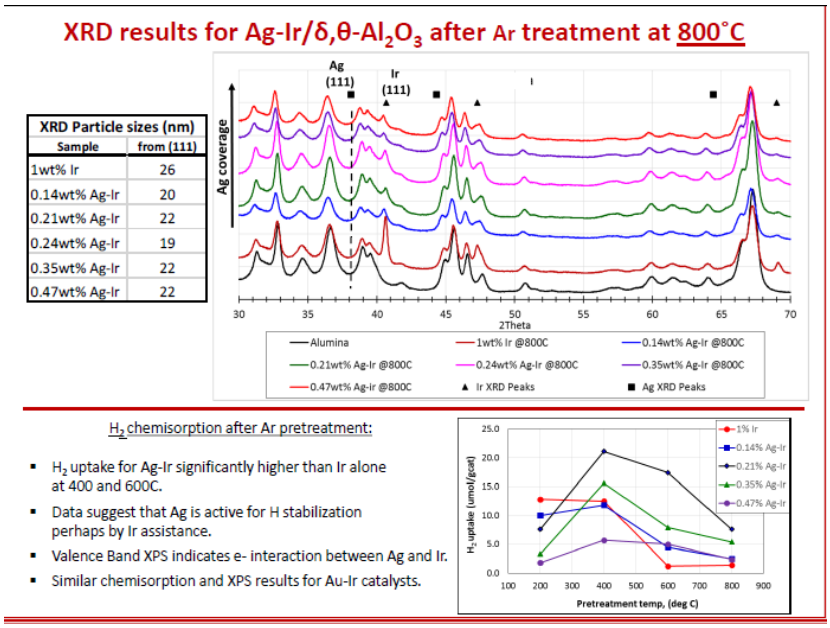


Everett Carpenter and his team at VCU and USC have demonstrated the synthesis of ultrasmall (<2 nm) Pt nanoparticles in solution and are now focusing on synthesizing them in formed catalyst supports.

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

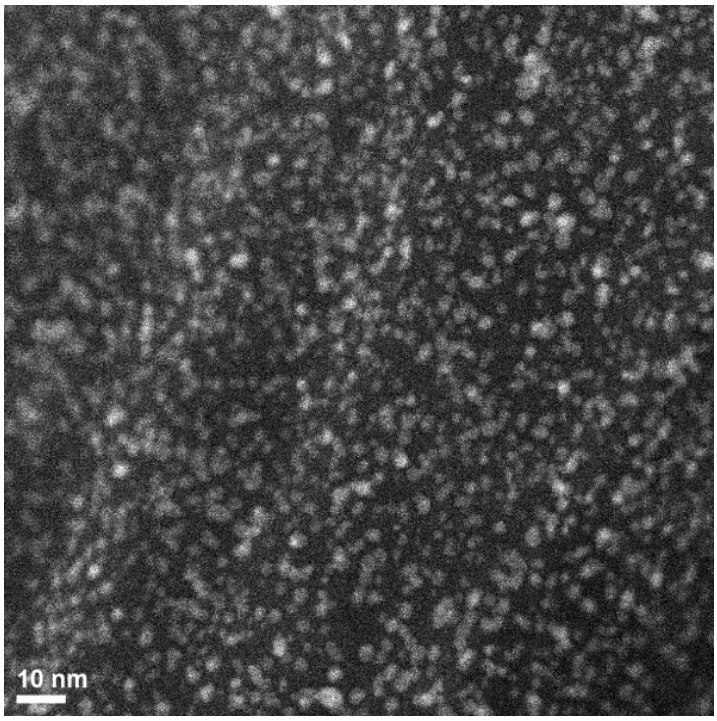




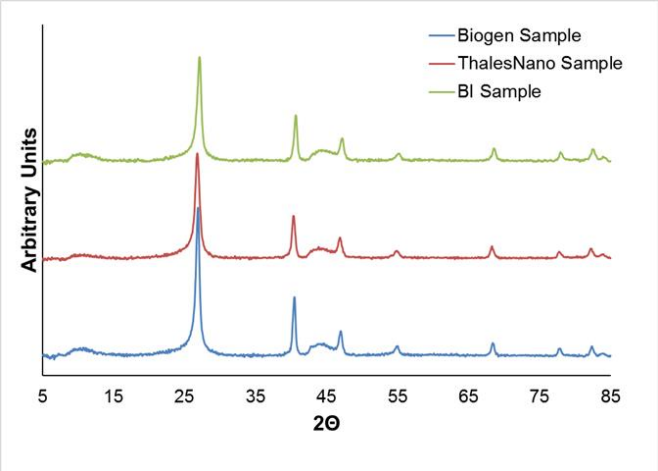


John Monnier with his USC and VCU team have identified unusual chemisorption uptake of the Ag and Au shells in Ir core-shell particles; computations at VCU are progressing to explain this unusual finding.

Project 3: Evaluation of Pd/graphene surface properties for cross-coupling and C-H activation

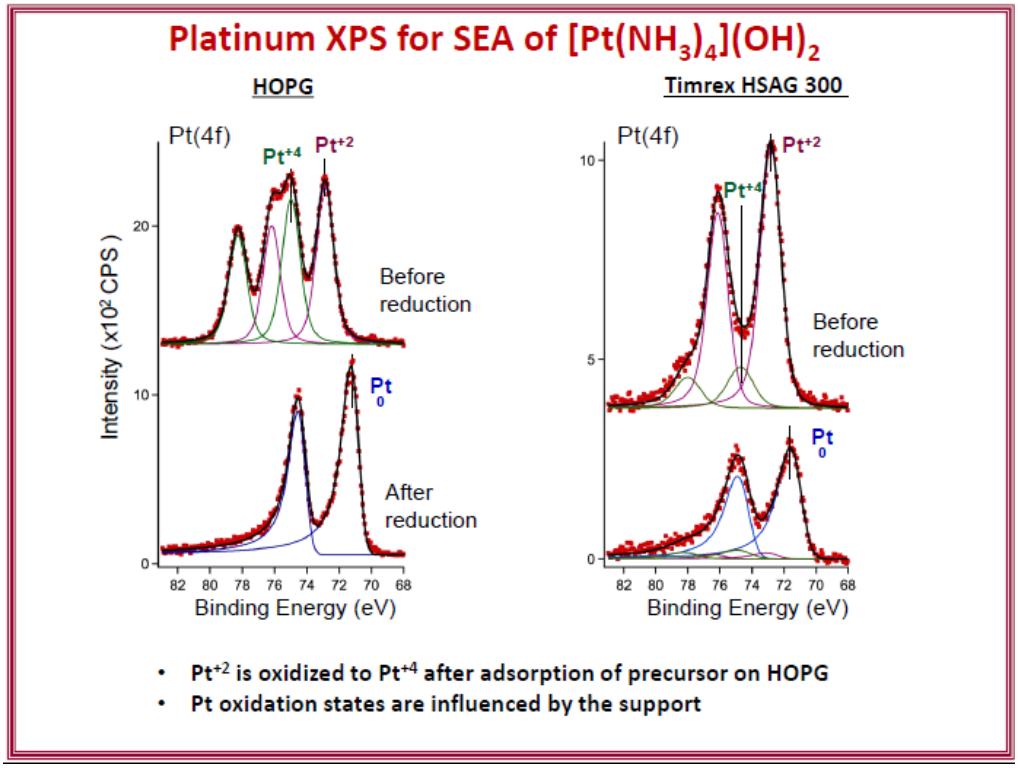


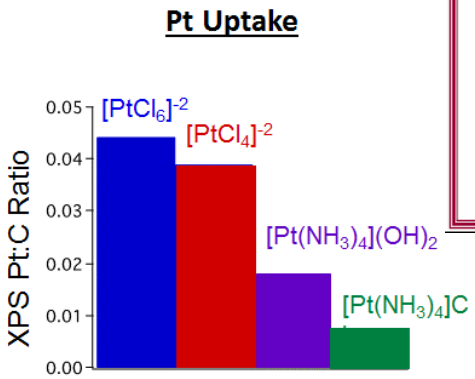
Keith Ellis his team at VCU and USC have developed methods to deposit sub-2 nm Pd particles on graphene oxide, some of which exhibit remarkably high catalytic activity. Samples are being sent to member companies for further testing.



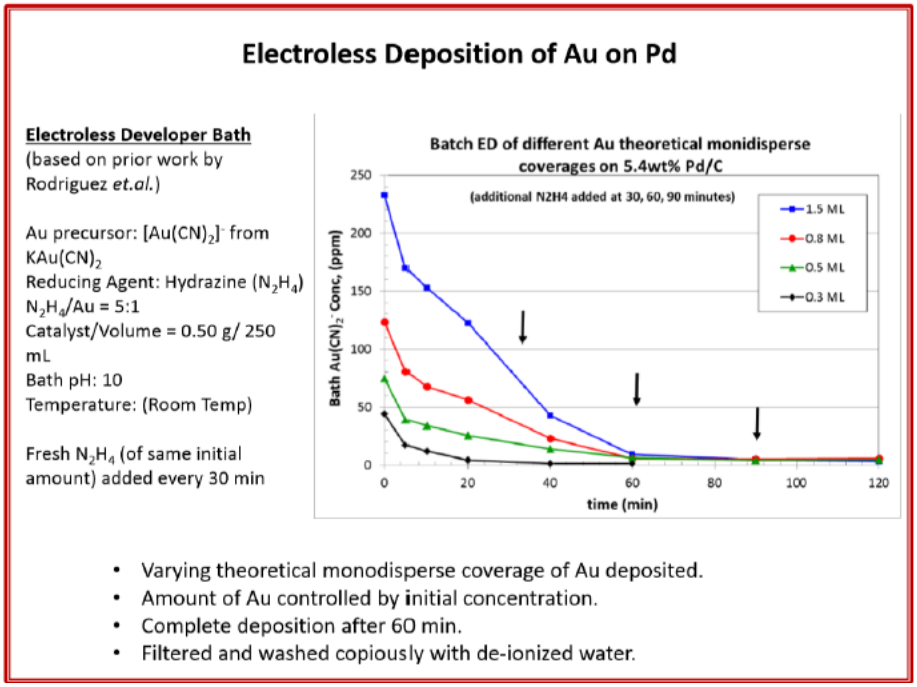
Project 4: "Real world" nanoparticle synthesis on model supports

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.





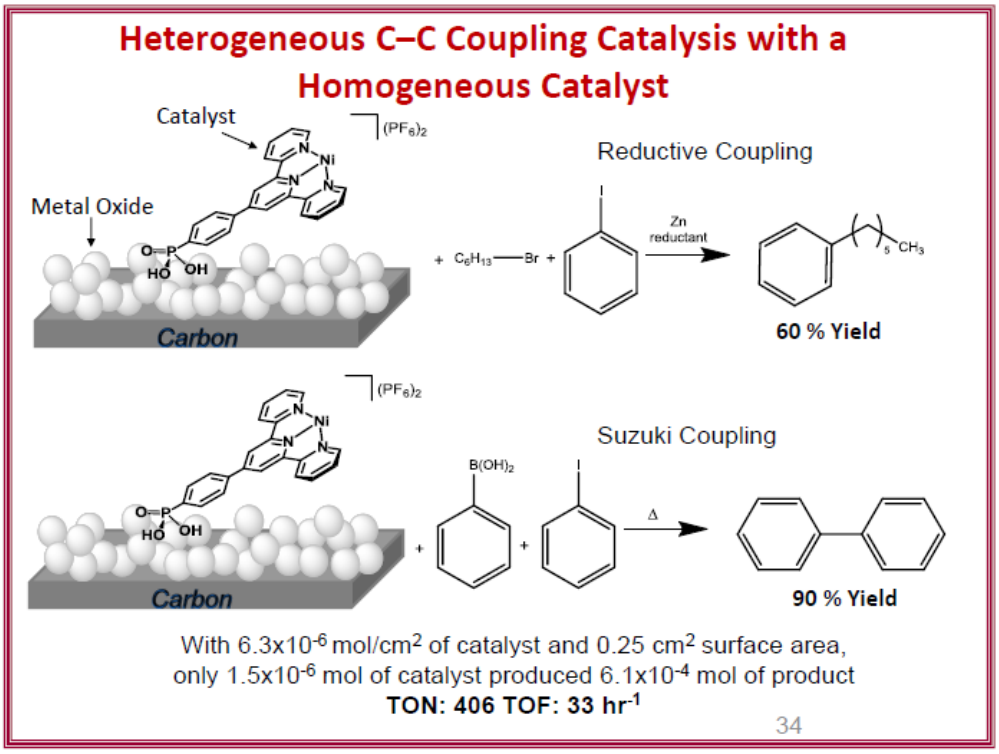
Project 5: Continuous Catalytic Oxidation in Pharmaceutical Processing



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

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/