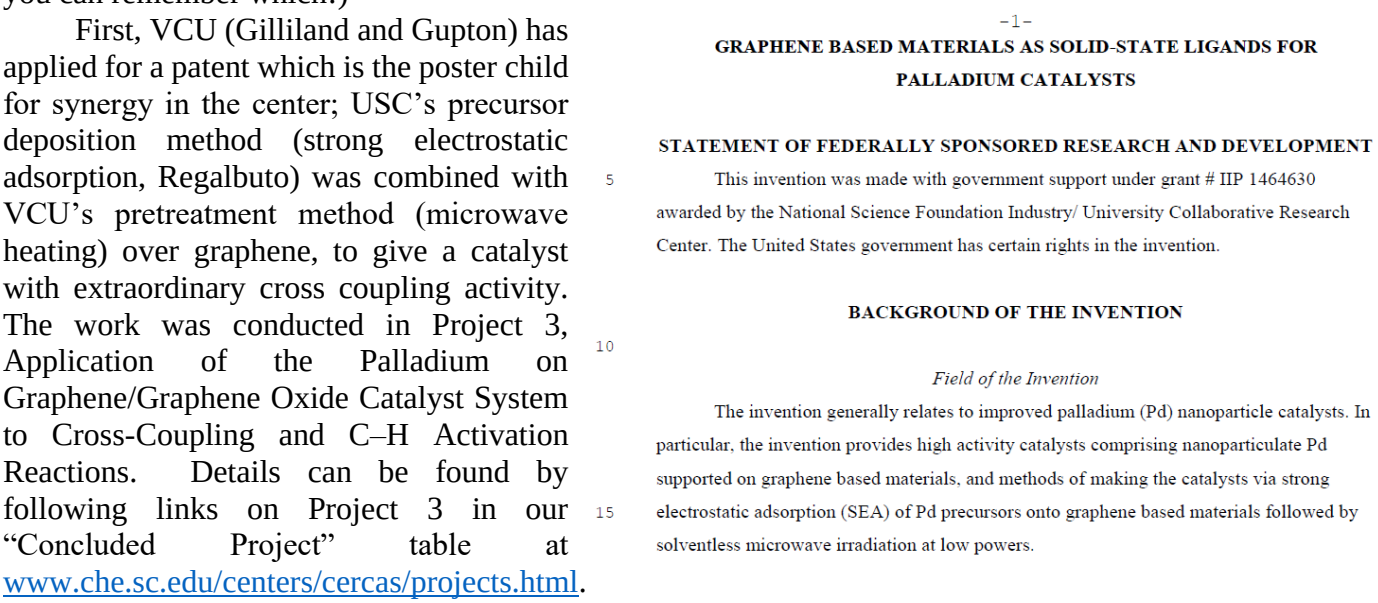
CeRCaS News Blast 10/26/18

Ring 1: Discoveries Keep Happening…

A patent application and an invention disclosure have arisen from recent and current projects (see if you can remember which!)

First, VCU (Gilliland and Gupton) has applied for a patent which is the poster child for synergy in the center; USC's precursor deposition method (strong electrostatic adsorption, Regalbuto) was combined with VCU's pretreatment method (microwave heating) over graphene, to give a catalyst with extraordinary cross coupling activity. The work was conducted in Project 3, Application of the Palladium on Graphene/Graphene Oxide Catalyst System to Cross-Coupling and C–H Activation Reactions. Details can be found by following links on Project 3 in our "Concluded Project" table at www.che.sc.edu/centers/cercas/projects.html.



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GRAPHENE BASED MATERIALS AS SOLID-STATE LIGANDS FOR PALLADIUM CATALYSTS

STATEMENT OF FEDERALLY SPONSORED RESEARCH AND DEVELOPMENT

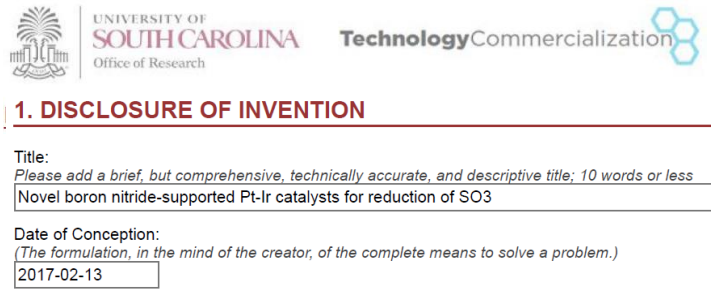
This invention was made with government support under grant # IIP 1464630 awarded by the National Science Foundation Industry/ University Collaborative Research Center. The United States government has certain rights in the invention.

BACKGROUND OF THE INVENTION

Field of the Invention

The invention generally relates to improved palladium (Pd) nanoparticle catalysts. In particular, the invention provides high activity catalysts comprising nanoparticulate Pd supported on graphene based materials, and methods of making the catalysts via strong electrostatic adsorption (SEA) of Pd precursors onto graphene based materials followed by solventless microwave irradiation at low powers.

Second, USC (Monnier, Diao, and others) has filed an invention disclosure for stable high temperature (800°C) bimetallic catalysts for SO_3 decomposition in collaboration with CeRCaS member Idaho National Lab (Ginosar) on work funded by a DOE/EERE grant to Greenway Energy LLC (Claudio Corgnale), which is associated with CeRCaS member Savannah River National Lab. This work arose partly from current project 15, Boron Nitride Supported Metal and Metal Oxide Catalysts for Selective Oxidation Reactions, but the idea of anchoring metal shells with high surface free energy cores was first explored in concluded Project 2, Enhanced Stability of Catalytic Surfaces by Bimetallic Core-Shell Structures (see www.che.sc.edu/centers/cercas/projects.html).



UNIVERSITY OF SOUTH CAROLINA Office of Research — TechnologyCommercialization

1. DISCLOSURE OF INVENTION

Title:
Please add a brief, but comprehensive, technically accurate, and descriptive title; 10 words or less
Novel boron nitride-supported Pt-Ir catalysts for reduction of SO3

Date of Conception:
(The formulation, in the mind of the creator, of the complete means to solve a problem.)
2017-02-13

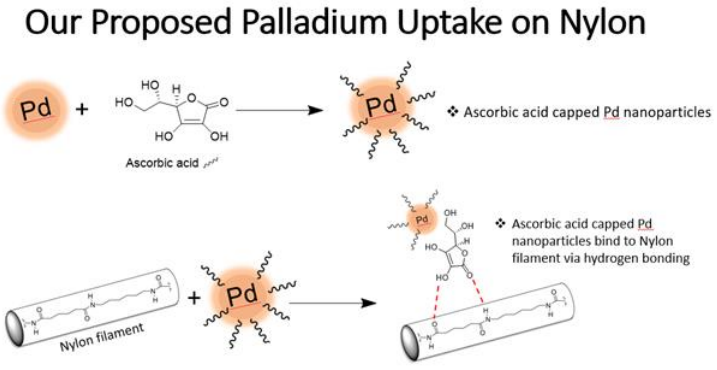
Ring 2: Six Projects are in Mid-Stream

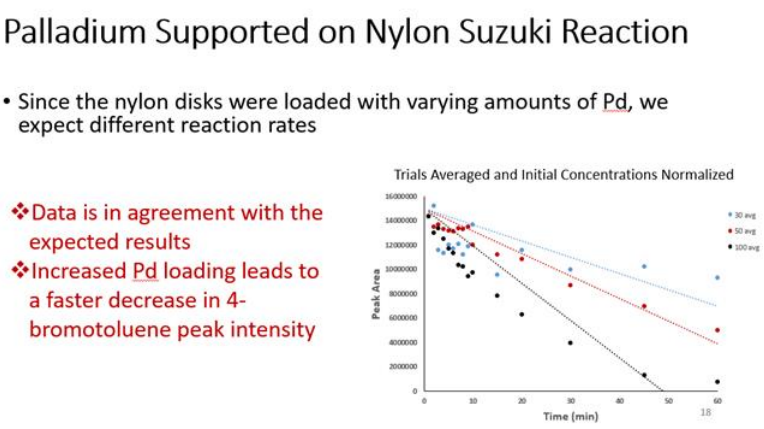
Here's the 2018-2019 project portfolio, from our home page (www.che.sc.edu/centers/cercas/):

Update Links	Project	Principal Investigators	Industrial Mentor	Next Report Date
Project 12	3D Printed Catalytic Monolith	Ferri Gupton (VCU)	(BI) (GSK) Opalka (Biogen)	**10/18** 2:00 PM
Project 13	Hydrogenation activity of Pd particles on modified carbon supports	Chen Regalbuto (USC) Gupton (VCU)	(BI) Soled Sattler (ExxonMobil) Opalka (Biogen)	**10/09** 3:00 PM
Project 14	Mechanistic Understanding of Ethane Partial Oxidation over bifunctional MoV-based catalysts	Lauterbach (USC) Carpenter (VCU)	(INL) Vityuk (BASF)	**10/15** 2:00 PM
Project 15	Boron nitride (BN) supported metal and metal oxide catalysts for selective oxidation reactions	Diao Regalbuto Monnier (USC)	(INL) Barger (UOP)	**10/19** 3:00 PM
Project 16	Solid-supported catalysts design for optimized electrocatalytic oxidation of alkenes to ketones	Gupton Castano Roper (VCU)	(BI) (GSK) Toutov (Fuzionaire)	**10/23** 3:00 PM
Project 17	Ultrasmall Bimetallic Catalysts for Selective Hydrogenation of Alkenes	El-Kaderi El-Shall (VCU) Regalbuto (USC)	Anton (SRNL) Vityuk (BASF) Weiss (ExxonMobil)	**10/31** 3:00 PM

And some highlights from them:

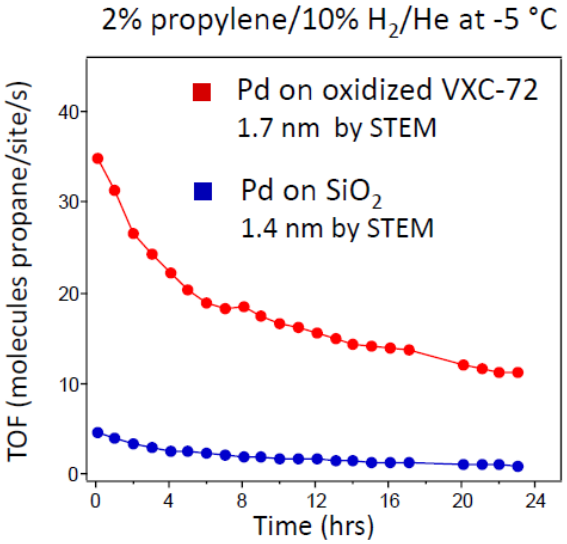
Project 12

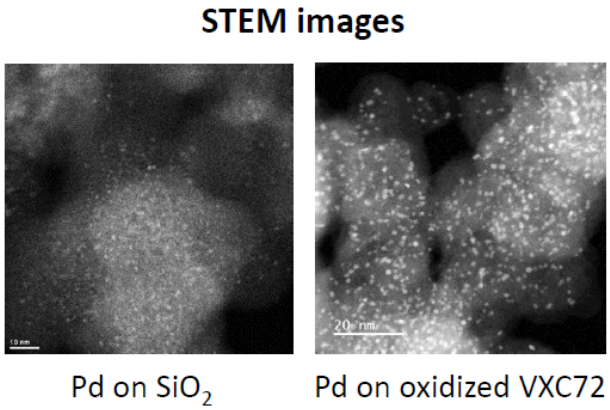




Project 13

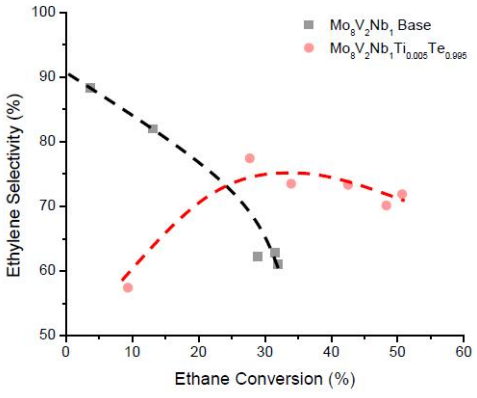
Propylene Hydrogenation: Pd on Carbon vs. Silica



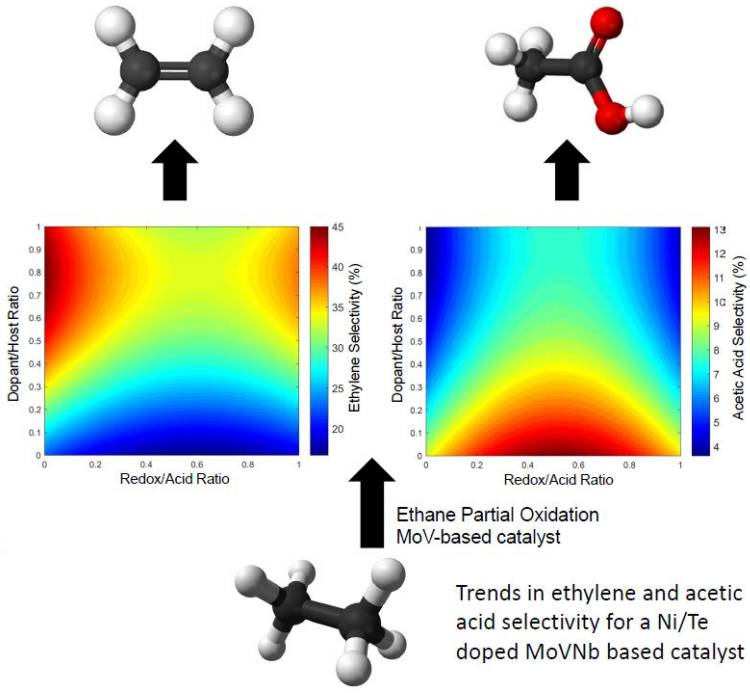


- **For similarly sized supported Pd particles prepared by strong electrostatic adsorption, the carbon support has a significant effect in enhancing hydrogenation activity compared to the oxide support**

Project 14



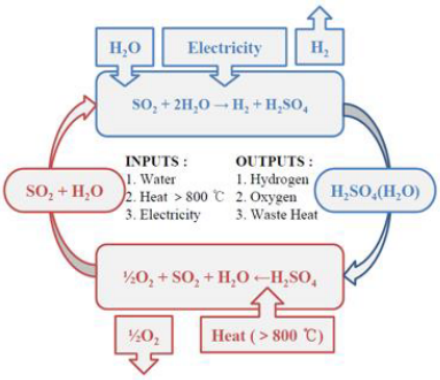
Effects of dopant addition to $Mo_8V_2Nb_1$ for ethane oxydehydrogenation



Trends in ethylene and acetic acid selectivity for a Ni/Te doped MoVNb based catalyst

Project 15

BN support Pt – Ir catalyst for H_2SO_4 decomposition



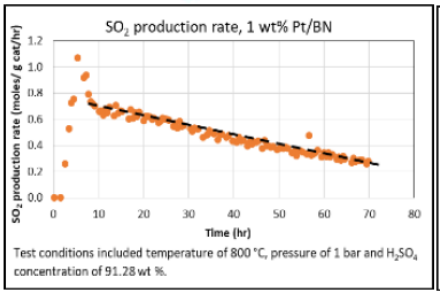
Hybrid Sulfur process for water splitting

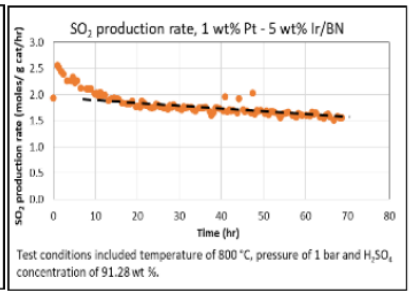
Step 1:
$H_2SO_4(aq) \rightarrow H_2O(g) + SO_2(g) + ½\ O_2(g)$
(thermochemical, T > 800 C)

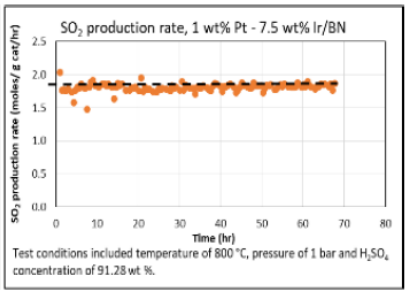
Our hypothesis:

1. **Utilize high stability and surface area of BN at >800C**
2. **Use a high SFE core to stabilize Pt shell.**

- 1% Pt – 7.5% Ir/BN shows excellent stability for 72 hrs.







Project 16

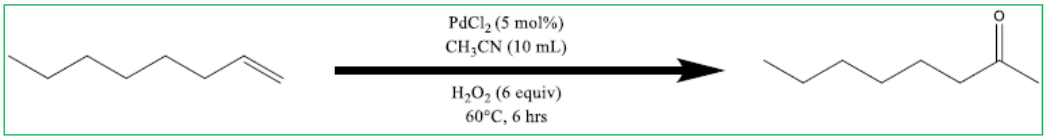
GNP-supported Catalyst performance

Preparation method	Pd loading (wt%)	Pd(II) %	Conversion (%)
Incipient wetness	2.30	73.6	91.84
Chemical reduction	4.31	68.7	87.82

Deposited catalyst ink

Standard gold electrode

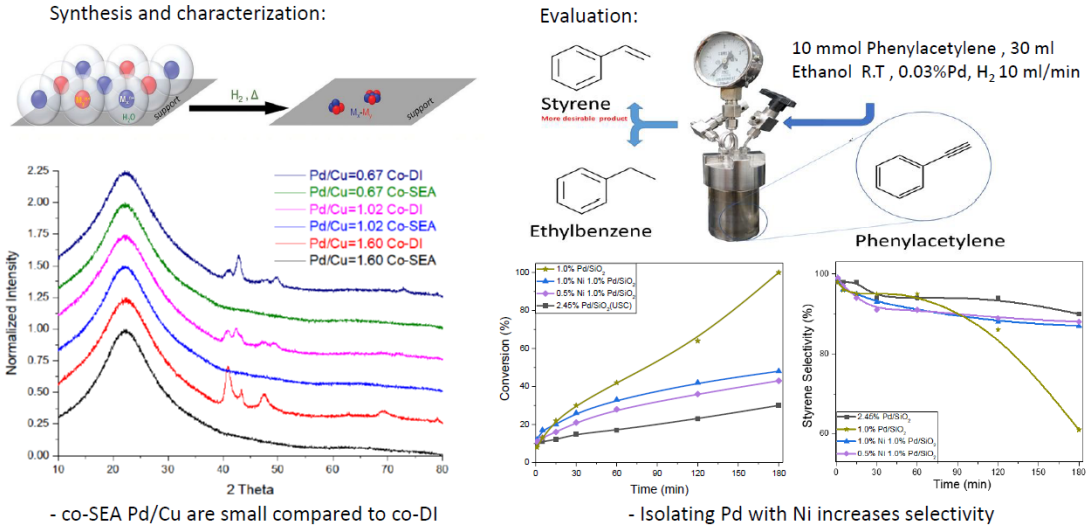
Tsuji-Wacker oxidation of 1-octene



✓ Catalysts were fine-tuned based on the Tsuji-Wacker oxidation mechanism to have optimum amount of Pd(II) species required for the reaction. The main optimization parameters were preparation method, Pd salt precursors, and microwave post-treatment after metal deposition.

Project 17

Selective Hydrogenation of Phenylacetylene by Bimetallic NPs



Ring 3: Save the Date: Fall CeRCaS Meeting (December 13-14, 2018) in Columbia.

Come and hear all the detailed project reports. Meet our students and postdocs! The Fall CeRCaS meeting will be held December 13-14 (Thursday and Friday) at the Hilton Columbia Center, a block away from "restaurant row" and two blocks west of the Capital Building. Superb amenities, comfy rooms. Discounted rates are $139 for the nights of Dec. 12-14. Hilton has provided this specific link:

http://www.hilton.com/en/hi/groups/personalized/C/CAECCHF-CERCAS-20181212/index.jhtml

or you can call 803 744-7800 and mention "CeRCaS" to get the group rate.

The meeting will begin 7:30 a.m. Thursday and conclude at noon, Friday. Come early Wednesday for a round of golf! A detailed meeting agenda will be distributed soon.

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