BNL Discovery to Deployment:

Chemistry for Sustainable Energy

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Chair, BNL Chemistry Department

State Energy Advisory Board
October 10, 2012

BROOKHAVEN NATIONAL LABORATORY
a passion for discovery

Office of Science
U.S. DEPARTMENT OF ENERGY

Topics

- BNL Energy Research in Sustainable Chemical Conversion
- Fuel Cell Electrocatalysis: Discovery to Deployment

Brookhaven Mission, Part I: *"Advance photon sciences, energy, and environment-related research and apply them to 21st Century problems of critical importance to the Nation."*

Brookhaven Energy R&D

Basic Research, Applied Research, Collaboration


Chemistry


Condensed Matter Physics & Materials


Sustainable Energy Technologies

BNL Programs
DOE Priority Research Directions

BNL Resources

ENERGY CHALLENGES: Focus Areas

- Research for Sustainable Chemical Conversions
- Science and Technology for Electric Infrastructure

Collaborators/Joint Appointments

GM, TOYOTA, Stony Brook University, Columbia University, Argonne National Laboratory, Rutgers The State University of New Jersey, UTC Power A United Technologies Company, GE, Oak Ridge National Laboratory Managed by UT-Battelle for the Department of Energy, Yale

Chemistry for Sustainable Energy R&D

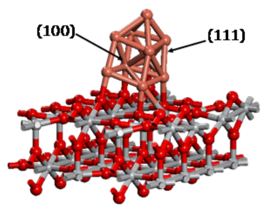
Sustainable Fuel Production

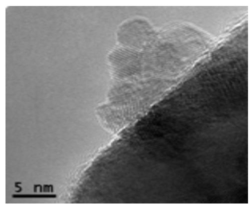
Catalysis & Photocatalysis for renewable fuels

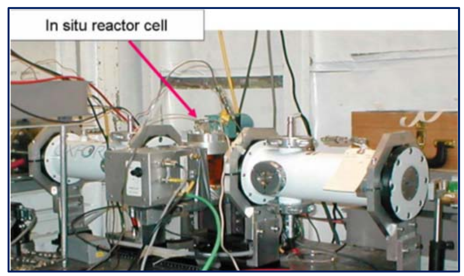
- Activate CO_2 for fuel synthesis
- Selective synthesis of C1 or higher Cn oxygenates
- Biomass thermochemical conversion to biofuels

Hydrogen as a fuel

- Water splitting catalysis – electrocatalysis & photocatalysis
- Natural gas reforming – scalable local hydrogen generation







BNL Contributions

- Molecular and Nanostructured catalysts - chemical and materials synthesis
- Mechanistic studies and In-situ characterization
  - Synchrotron Catalysis Consortium
- Computational catalysis for improved design
  - Solar Water Splitting Simulation Team (SWaSSiT)

Sustainable Fuel Use

Fuel cell electrocatalysis

- Reduce platinum, increase durability and efficiency

BNL Contributions

- Nanostructured electrocatalysts – design, synthesis and application
- In-situ experiments for fundamental understanding and improved design

University of Delaware · Yeshiva University · UOP A Honeywell Company · Oak Ridge National Laboratory · Toyota · GM · UTC Power A United Technologies Company · Stony Brook University · Yale · University of Rochester · AIST National Institute of Advanced Industrial Science and Technology (AIST) · Cornell University · Massachusetts Institute of Technology · Los Alamos National Laboratory

Critical links to BNL User Facilities: Catalysis

NSLS/NSLS II

Chemistry

CFN

Beamline ⇔ Spokespersons

Users ⇔ Collaborators

Catalysis Science Programs

SCC ⇔ PI's

Research ⇔ Co-PI's

Developers ⇔ Users

- PRT Beamlines
  - Time-resolved XRD
  - X-ray absorption
  - Photoemission
- Synchrotron Cata Consortium
- *in situ* methods
  - Reactor XAFS, XF
  - Electrochemical
  - Quick XAFS

Nanoscience capabilities
- Proximal probes
- Electron Microscopy
- Theory/computation
- Nanofabrication

Interface Science & Catalysis Theme

Developing *in situ* methods

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Catalysis Synergy

Coordinated research - World class capabilities

NSLS

Chemistry

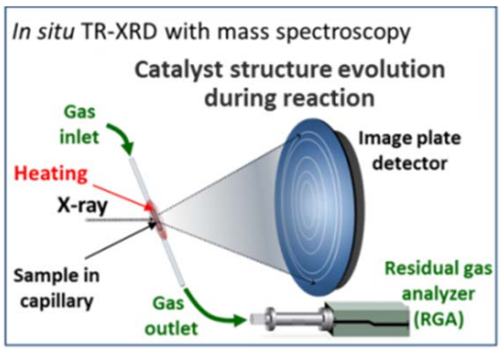
CFN

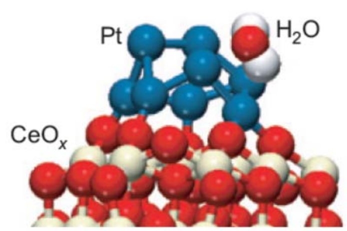
In Situ photon science

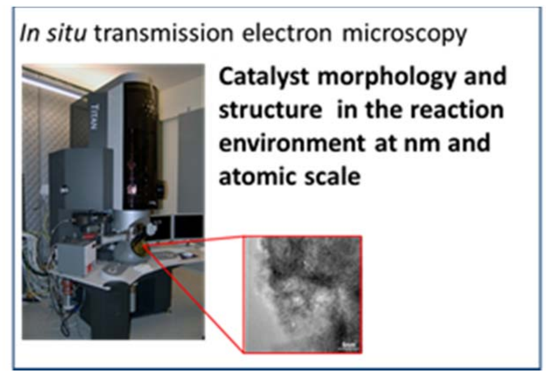
Catalyst ⟷ Model System

Computation

In Situ nanoscience







NSLS II

Theory & Computation

New York Blue

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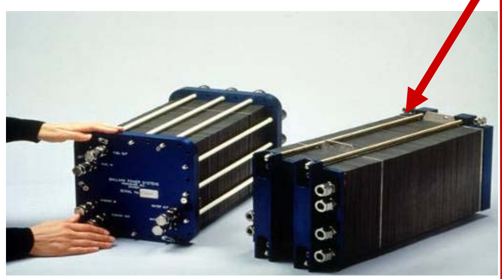
Nanostructured catalysts for improved fuel cells

Fuel Cell: ‘Ideal’ Energy Conversion

- Direct energy conversion
  - Fuel + O_2 $\rightarrow$ electrical energy
- High conversion efficiency
- H_2O product in $H_2 – O_2$ cells
  - Pollution-free with H_2
- Continuous, silent operation



Obstacles

1. Cost
   Goal: $30/kW
2. Durability
   5,000 hours, 150K miles

Require Improved Electrocatalysts

1. **Decrease platinum content**
   - in particular in **O_2 cathodes**
2. **Increase efficiency**
   - enhance CO tolerance (anode)
   - enhance O_2 reduction kinetics (cathode)

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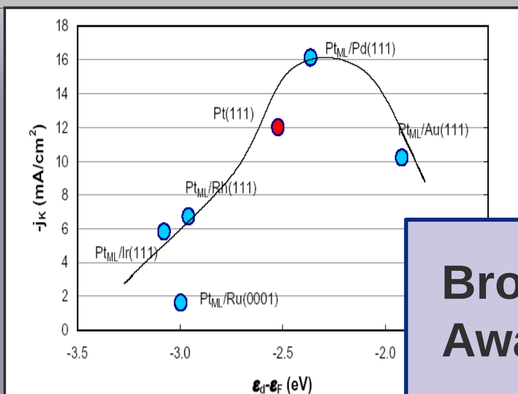
Sustainable Fuels: Catalysts for Fuel Cells

DOE – BES
Research advances

DOE (BES & EERE)
Core-Shell Nanocatalysts

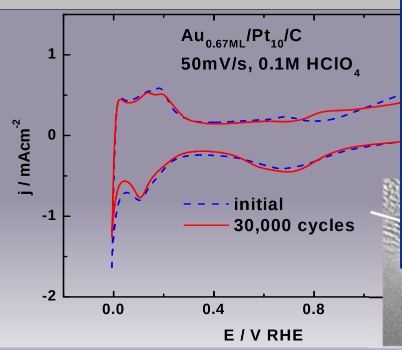
BNL-Toyota CRADA
Toward Deployment

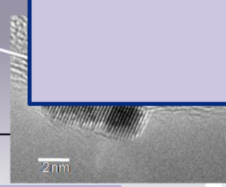
1. Pt Monolayer catalysis – high activity with ultralow Pt mass



Angewandte Chemie **44**, 2132

2. Pt stabilized against co voltage cycling by Au cl



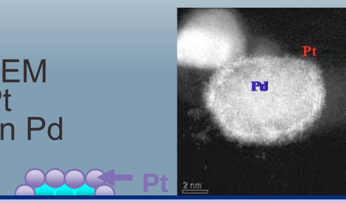


Science **315**, 220 (2007)

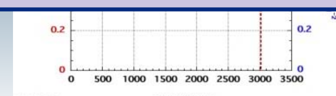
Active Pt ML shell – Metal/alloy core

Core tunes activity & durability of shell

Model and TEM image of a Pt Monolayer on Pd nanoparticle

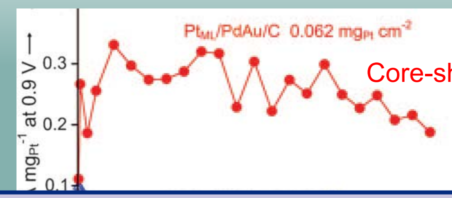


Performance



Scale-up synthesis: **Pt-ML/Pd_9Au_1/C**

Excellent fuel Cell durability 200,000 cycles



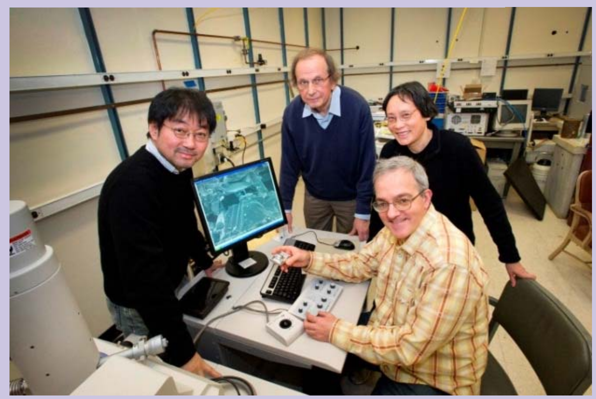
TOYOTA

Fuel Cell Catalyst readied for automotive application

N.E. CHEMCAT
Lead The Catalyst Innovations

Brookhaven Lab Chemists Win R&D 100 Award for Fuel Cell Research

Radoslav Adzic
Kotaro Sasaki
Miomir Vukmirovic
Jia Wang



2012 R&D 100
50th ANNIVERSARY

Commercial license signed 2011

Core-shell electrocatalyst development

- Basic Research: DOE Basic Energy Sciences from 1990's
  - Catalytic activity of monolayer/submonolayers of metals
  - Discovered path for fuel cell electrocatalysis breakthrough: tuning monolayer activity, and doping to increase stability.
- Basic-to-Applied Research: DOE BES & EERE 2002-2012
  - Methods for low-Pt core-shell nanoparticle electrocatalysts (3-6 nm)
  - Fuel cell testing: LANL, commercial collaborators
- Applied Research: DOE EERE & Commercial (CRADA) 2005-2012
  - Scale-up synthesis for larger tests.
  - Testing with commercial OEM and catalyst partners.
- Development: commercial licensing to NECC 2011.
  - Successful commercial synthesis at development scale
  - Sampling to automotive OEMs for FCV (e.g., to GM, Toyota, others)

Extra Slides

Hydrogen Economy - Status

- Tremendous progress worldwide in technologies for production and use during the past decade – fundamental and practical advances.
- Recent signs of commercial viability for key products
- Auto OEMs remain committed to early commercial production in 2015/2016
- Japan, Germany and others continue to plan for refueling infrastructure to meet 2015 need.
- US administration has recently indicated increased support, following a period of intense focus on battery solutions.

Worldwide Commitment to FCEVs

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

The world's leading automakers have committed to develop FCEVs. Germany and Japan have announced plans to expand the hydrogen infrastructure.

Major Auto Manufacturers' Activities and Plans for FCEVs

Toyota
- 2010-2013: U.S. demo fleet of 100 vehicles
- 2015: Target for large-scale commercialization
- "FCHV-adv" can achieve 431-mile range and 68 mpgge

Honda
- Clarity FCX named "World Green Car of the Year"; EPA certified 72mpgge; leasing up to 200 vehicles
- 2015: Target for large-scale commercialization

Daimler
- Small-series production of FCEVs began in 2009
- Plans for tens of thousands of FCEVs per year in 2015 – 2017 and hundreds of thousands a few years after
- In partnership with Linde to develop fueling stations.
- ***Recently moved up commercialization plans to 2014***

General Motors
- 115 vehicles in demonstration fleet
- 2012: Technology readiness goal for FC powertrain
- 2015: Target for commercialization

Hyundai-Kia
- 2012-2013: 2000 FCEVs/year
- 2015: 10,000 FCEVs/year
- "Borrego" FCEV has achieved >340-mile range.

Volkswagen
- Expanded demo fleet to 24 FCEVs in CA
- Recently reconfirmed commitment to FCEVs

SAIC (China)
- Partnering with GM to build 10 fuel cell vehicles in 2010

Ford
- Alan Mulally, CEO, sees 2015 as the date that fuel cell cars will go on sale.

BMW
- BMW and GM plan to collaborate on the development of fuel cell technology

Based on publicly available information during 2011

H_2Mobility - evaluate the commercialization of H_2 infrastructure and FCEVs
- Public-private partnership between NOW and 9 industry stakeholders including:
  - Daimler, Linde, OMV, Shell, Total, Vattenfall, EnBW, Air Liquide, Air Products
- FCEV commercialization by 2015.

UKH_2Mobility will evaluate anticipated FCEV roll-out in 2014/2015
- 13 industry partners including:
  - Air Liquide, Air Products, Daimler, Hyundai, ITM Power , Johnson Matthew, Nissan, Scottish & Southern Energy, Tata Motors, The BOC Group, Toyota, Vauxhall Motors
- 3 UK government departments
- Government investment of £400 million to support development, demonstration, and deployment.

13 companies and Ministry of Transport announce plan to commercialize FCEVs by 2015
- 100 refueling stations in 4 metropolitan areas and connecting highways planned, 1,000 station in 2020, and 5,000 stations in 2030.

North East/East Coast/National Hydrogen Infrastructure

Boston-Miami=1500mi
6 major cities
>100m people

Massachusetts - Billerica, Boston
Nuvera forklifts
Transit buses

Connecticut - Wallingford, Hartford, East Hartford
Sun Hydro, Proton,
UTC, U.Conn,
Transit Authority buses/station

New York - NY City, Rochester, Buffalo, Albany
NYHY2 Initiative, JFK, White Plains, Hempstead
Praxair green H2, ATK, GM stations, RIT, Plug Power station

New Jersey - Jersey City
Hess, Daimler

Pennsylvania – Allentown, Susquehanna
Air Products station, Defense Logistics station

Ohio - Engelwood
Millennium Reign Energy

WDC / Virginia **Fairfax County station**
Fort Belvoir, additional station

Tennessee
United Hydrogen

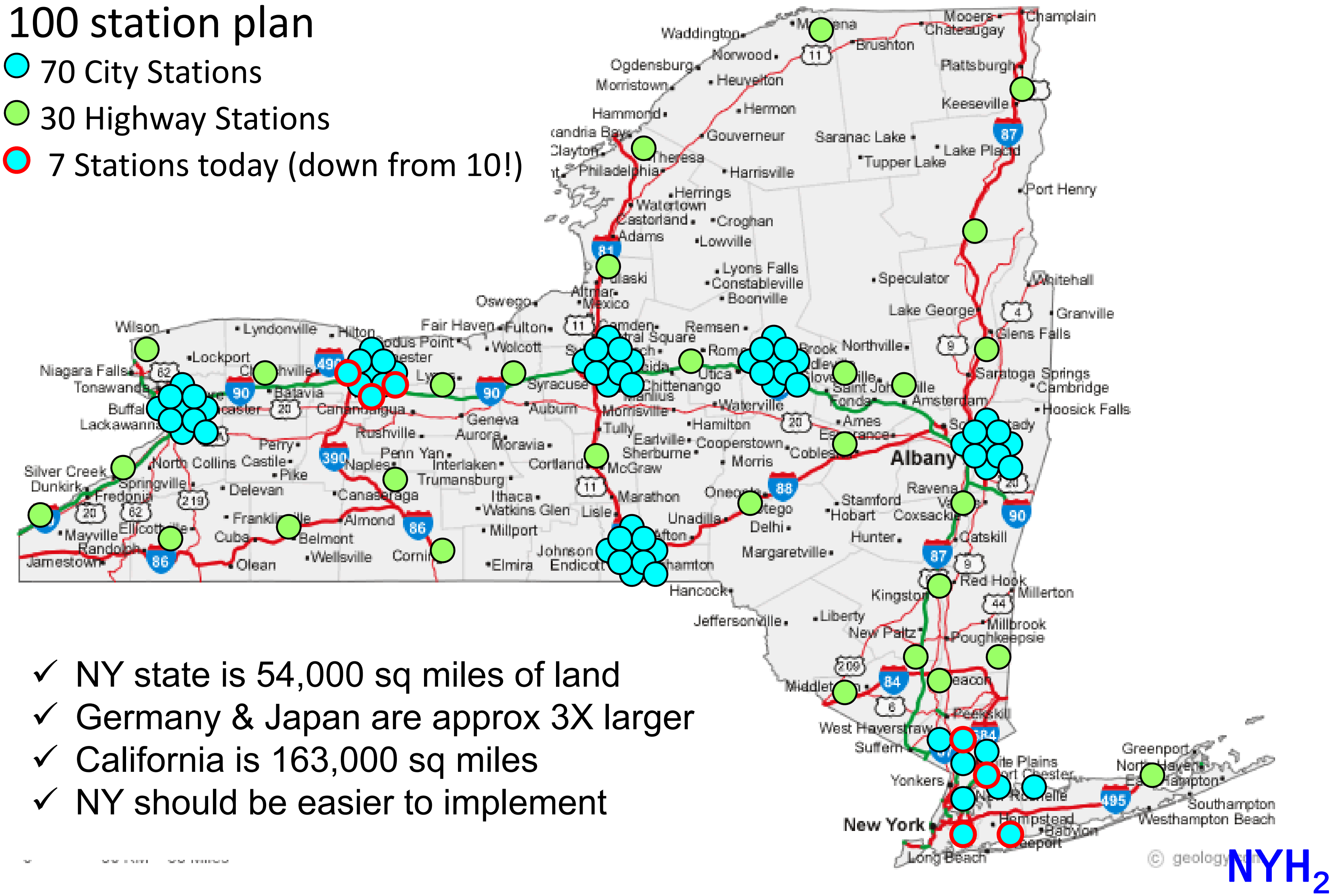
Georgia – Atlanta
United Hydrogen stations

Florida – Miami, Orlando, Cape Canaveral
NASA - station
Proton, Lumber Liquidators, home refueler

Plan for New York State Hydrogen Highway and Connecting City Plan in Support of early FCEV Deployment – 2015-2020

100 station plan

- 70 City Stations
- 30 Highway Stations
- 7 Stations today (down from 10!)



- ✓ NY state is 54,000 sq miles of land
- ✓ Germany & Japan are approx 3X larger
- ✓ California is 163,000 sq miles
- ✓ NY should be easier to implement

State OF THE States

Fuel Cells in America 2012

Chemistry for Sustainable Energy: Recent Highlights

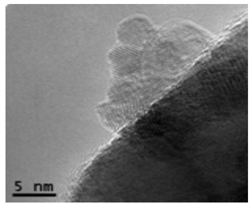
- Recent advances in catalysis for a hydrogen economy
  - Hydrogen use: Ultralow platinum fuel cell electrocatalysts
  - Hydrogen production:
    - Hydrocarbon reforming: hydrogen purification catalysis
    - Water electrolysis – new ultralow and zero platinum electrocatalysts for hydrogen evolution
  - Hydrogen storage: new catalyst for $CO_2 \leftrightarrow$ Formate interconversion to store hydrogen chemically

- BNL catalysis capabilities and expertise for the future
  - Preparing for NSLS-II
  - Scientific Recruiting

Hydrogen as a Clean, Efficient Fuel

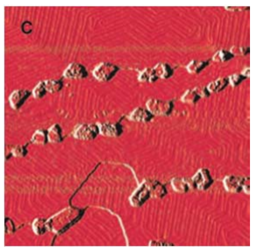
New water-gas shift catalysts for high purity hydrogen from abundant natural gas: Promising metal-doped reducible oxides (TiO_x, CeO_x)

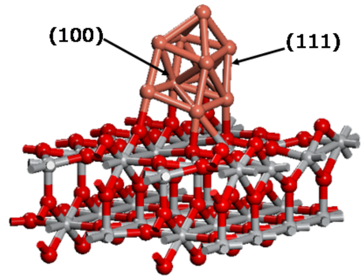
In situ powder studies



Model 'inverse' oxide/metal catalysts

CeO_x/Au(111)



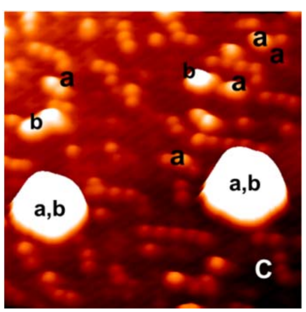


Computation - model nanocatalysts on oxides

Cu/TiO_2(110)

Bifunctional catalysts: reduced metal nanoparticle and oxide support are both important

Mixed nanoscale oxide: improved metal dispersion & activates oxide



metal/CeO_x/TiO_2 WGS catalysts show improved low temp activity

Science **318**, 1757-1760 (2007)
Proc. Nat. Acad. Sci. **13**, 4975 (2009)

Toward improved industrial catalysts for local hydrogen generation