BNL Discovery to Deployment: Chemistry for Sustainable Energy

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Chair, BNL Chemistry Department

State Energy Advisory Board
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Topics

- BNL Energy Research in Sustainable Chemical Conversion
- Fuel Cell Electro catalysis: 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

BNL Programs
DOE Priority Research Directions

ENERGY CHALLENGES: Focus Areas
- Research for Sustainable Chemical Conversions
- Science and Technology for Electric Infrastructure

Collaborators/Joint Appointments
Chemistry for Sustainable Energy R&D

**Sustainable Fuel Production**

**Catalysis & Photocatalysis for renewable fuels**
- Activate CO₂ 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

[Logos of participating institutions]
Critical links to BNL User Facilities: Catalysis

- **PRT Beamlines**
  - Time-resolved XRD
  - X-ray absorption
  - Photoemission

- **Synchrotron Catalysis Consortium**

- **in situ methods**
  - Reactor XAFS, XFs
  - Electrochemical
  - Quick XAFS

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

**Interface Science & Catalysis Theme**
Developing *in situ* methods
Catalysis Synergy

Coordinated research - World class capabilities

NSLS

In Situ photon science

Chemistry

Catalyst ↔ Model System

Computation

Theory & Computation

New York Blue

CFN

In Situ nanoscience

NSLS II

In situ TR-XRD with mass spectroscopy
- Catalyst structure evolution during reaction
  - Image plate detector
  - Residual gas analyzer (RGA)
- Sample in capillary
- Gas inlet
- Heating
- X-ray
- Gas outlet

In situ transmission electron microscopy
- Catalyst morphology and structure in the reaction environment at nm and atomic scale
Nanostructured catalysts for improved fuel cells

Fuel Cell: ‘Ideal’ Energy Conversion

- Direct energy conversion
  - Fuel + O₂ → electrical energy
- High conversion efficiency
- H₂O product in H₂ – O₂ cells
  - Pollution-free with H₂
- 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 O₂ cathodes
2. Increase efficiency
   - enhance CO tolerance (anode)
   - enhance O₂ reduction kinetics (cathode)
Sustainable Fuels: Catalysts for Fuel Cells

- **DOE – BES**
  - Research advances

- **DOE (BES & EERE)**
  - Core-Shell Nanocatalysts
  - Active Pt ML shell – Metal/alloy core
  - Core tunes activity & durability of shell

- **BNL-Toyota CRADA**
  - Toward Deployment

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

   ![Graph showing Pt Monolayer catalysis](image)

2. Pt stabilized against corrosion in voltage cycling by Au clusters

   ![Graph showing Pt stabilized against corrosion](image)

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

- Radoslav Adzic
- Kotaro Sasaki
- Miomir Vukmirovic
- Jia Wang

- 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.

  - Methods for low-Pt core-shell nanoparticle electrocatalysts (3-6 nm)
  - Fuel cell testing: LANL, commercial collaborators

  - 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

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 72 mpgge; 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

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Based on publicly available information during 2011

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<thead>
<tr>
<th>Country</th>
<th>Activities and Plans</th>
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<tr>
<td>Germany</td>
<td>H₂Mobility - evaluate the commercialization of H₂ infrastructure and FCEVs</td>
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<td>- Public-private partnership between NOW and 9 industry stakeholders including:</td>
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<td>- Daimler, Linde, OMV, Shell, Total, Vattenfall, EnBW, Air Liquide, Air Products</td>
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<td>- FCEV commercialization by 2015.</td>
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<td>Japan</td>
<td>UKH₂Mobility will evaluate anticipated FCEV roll-out in 2014/2015</td>
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<td>- 13 industry partners including:</td>
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<td></td>
<td>- Air Liquide, Air Products, Daimler, Hyundai, ITM Power, Johnson Matthew, Nissan, Scottish &amp; Southern Energy, Tata Motors, The BOC Group, Toyota, Vauxhall Motors</td>
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<td>- 3 UK government departments</td>
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<td>- Government investment of £400 million to support development, demonstration, and deployment.</td>
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<td>13 companies and Ministry of Transport announce plan to commercialize FCEVs by 2015</td>
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<td>- 100 refueling stations in 4 metropolitan areas and connecting highways planned, 1,000 station in 2020, and 5,000 stations in 2030.</td>
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### North East/East Coast/National Hydrogen Infrastructure

**Boston-Miami = 1500 mi**

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

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**Amended: New York City, Rochester, Buffalo, Albany**

NYHY2 Initiative, JFK, White Plains, Hempstead

Praxair green H2, ATK, GM stations, RIT, Plug Power station

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$_2$ ↔ 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 ($\text{TiO}_x$, $\text{CeO}_x$)

*In situ powder studies*

Model ‘inverse’ oxide/metal catalysts

$\text{CeO}_x/\text{Au}(111)$

Computation - model nanocatalysts on oxides

$\text{Cu}/\text{TiO}_2(110)$

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

Mixed nanoscale oxide: improved metal dispersion & activates oxide

metal/$\text{CeO}_x/\text{TiO}_2$

WGS catalysts show improved low temp activity

Toward improved industrial catalysts for local hydrogen generation

Science 318, 1757-1760 (2007)