Energy Sciences at BNL

John Hill
Deputy Associate Laboratory Director

January 5th 2015

Brookhaven National Laboratory
Doon Gibbs
Director

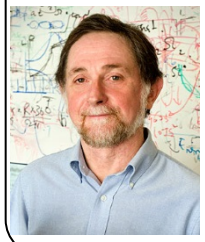
Energy Sciences Directorate
James Misewich
Associate Laboratory Director

NSLS-II
John Hill, Director
Deputy Associate Laboratory Director

CFN
E. Mendez

Chemistry
A. Harris

Condensed Matter Physics and Materials Science
P. Johnson



Sustainable Energy Technologies
J. P. Looney

EFRC/ Energy Storage Center
E. Takeuchi

Accelerator Division
F. Willeke

Photon Division
P. Zschack

U.S. DEPARTMENT OF ENERGY | Office of Science

BROOKHAVEN NATIONAL LABORATORY

Strategic Roadmap

Chemistry for Sustainable Energy

- Fuel synthesis
- Fuel use
- Chemical dynamics fundamentals

Advanced materials

- Strongly correlated electron physics
- Applications of materials

Energy Storage

- m2M EFRC
- EERE, ARPA-E
- Integrated Energy Science Center in Energy Storage

Energy Delivery and Efficiency

- Combustion efficiency
- Electric grid distribution system
- Materials for energy applications

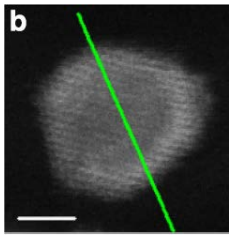
Photon Science

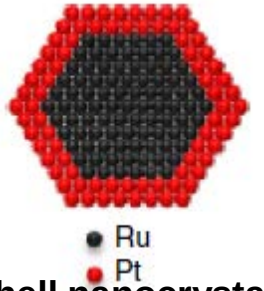
- Accelerator innovation
- World leading photon science: bio to geo to soft to hard to…
- User Community

Nanoscience

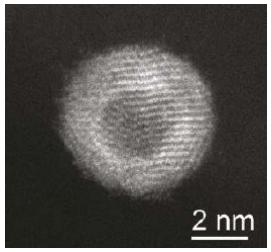
- Operando
- Nano-architectures
- Assembly
- User Community

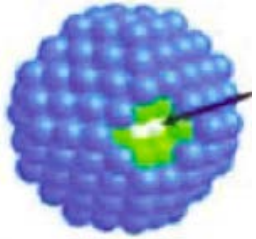
Advance: Atomic Control of Nanostructured Electrocatalysts for High Activity and Durability



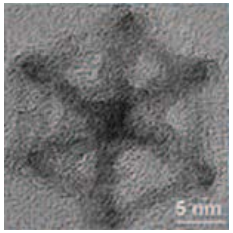


Ru@Pt core-shell nanocrystals





Hollow Pt nanoparticles



Pt_3Ni nanoframes with Pt-skin

Accomplishment

New designs and novel synthetic methods for high performance nanostructured electrocatalysts – platinum monolayer core-shell, hollow core shell, nanoframe alloy structures. Activity 10x-20x higher than platinum.

Significance

Fuel cells and electrolyzers require platinum group metal electrocatalysts to drive critical fuel-oxidation or water splitting reactions. New structures dramatically raise activity, increase durability, and reduce cost by lowering platinum group metal content. Designs are now being developed as products to improve commercial viability of fuel cells.

How it was achieved

New understanding of role of strain, surface-bulk interactions and monolayer reactivity from basic studies on model catalysts, in situ studies of structure and function by X-ray, electron microscopy and spectroscopy. New nanoscience synthetic methods for monolayer and nanorod structures to create desired designs.

Integration: Catalysis Science

Chemistry

Catalysis Science Programs

Synchrotron Catalysis Consortium

NSLS

Developers & Users

Beamline Spokespersons

Synchrotron Catalysis Consortium PIs

Users

Collaborators

Co-PI's

Beamline Synergy

Collaboration on First Experiments

in situ Nanoscience

Beamlines

CFN

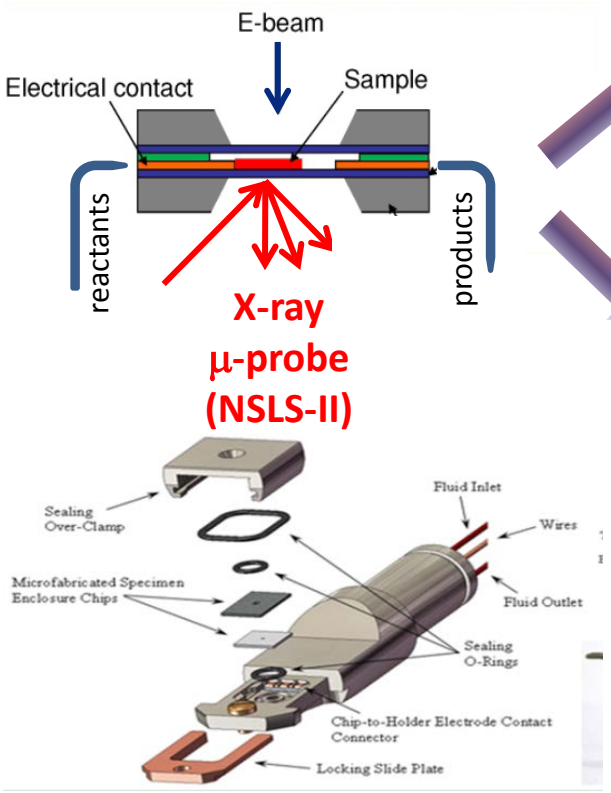
In-situ Nanoscience
Interface Science/Catalysis Thrust

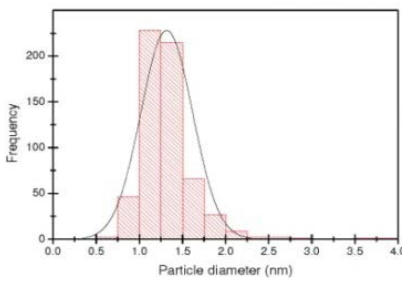
World-leading *in-situ*
Catalyst Characterization

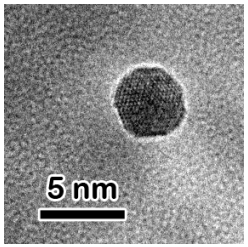
Future NSLS II

In-Situ Micro-reactor Cell: A Paradigm Shift in Catalysis Studies

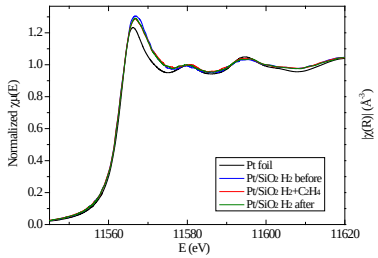
TEM (CFN)

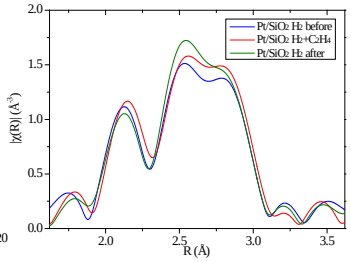






Structure of individual particles (TEM)





Global average structure & electronic structure (XANES /EXAFS)

Shape-dependent and size-dependent catalysis

Structure, dynamics and kinetics of real catalysts

Order-disorder transition in NPs

CSC will enable cross-facility access for same system *in operando* characterization

Imaging + Spectroscopy + Scattering

E. Stach, CFN: A. Frenkel, SCC/Yeshiva U
Prototype at NSLS X27A beamline
Future at NSLS-II SRX beamline

Energy Storage

Leadership—Esther Takeuchi

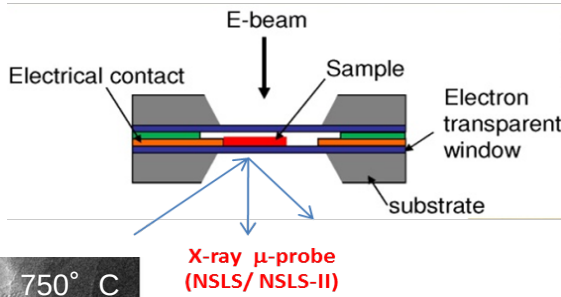
- National Academy of Engineering
- National Academy of Inventors
- National Medal of Technology
- ACS Murphree Award

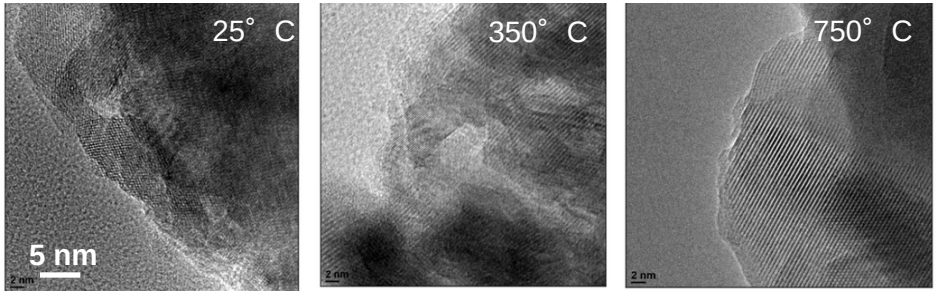
DISCOVERY MISSION

- Multifunctional materials
- Lifetime and safety issues

DEPLOYMENT MISSION

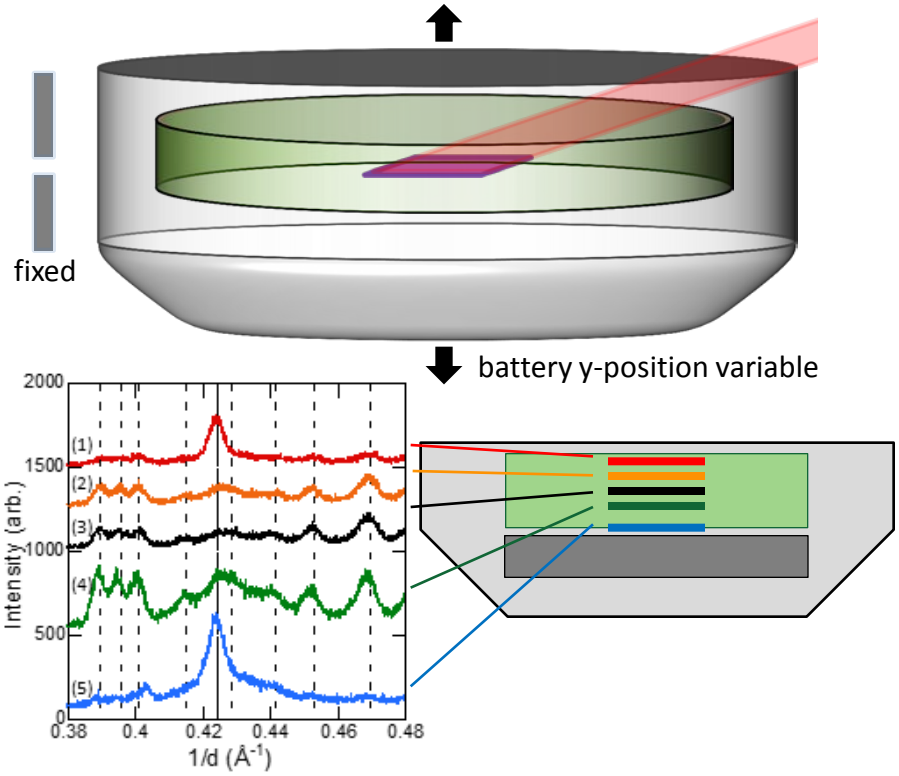
- Leveraging nanoscale tools (CFN, NSLS, NSLS-II) for electrochemical energy storage community
- Discussions on supporting DoD Energy Storage Needs
- Portal for JCESR
- Complementary to hub





Thermal cycling of the MnO_2 component in environmental TEM.

Looking inside a intact steel battery



Scientific Achievement

Xrays (NSLS-I) were employed to chemically map $Ag_2VP_2O_8$ cathodes within *intact* primary batteries at various levels of discharge.

Significance and Impact

Mapping of Ag^0 generated during reduction of $Ag_2VP_2O_8$ cathodes provides a non-intuitive, non-destructive 3D image of Ag^0 production, critical to the understanding of previously observed electrical conductivity enhancement phenomena.

Research Details

When $Ag_2VP_2O_8$ is reduced, Ag^0 nanoparticles formed within the cathode can be located by EDXRD. As discharge progresses, Ag^0 is first detected primarily nearer to the current collector, then observed nearer to the Li anode.

These results suggest when ion access and electron access are both critical to cathode discharge, the electric conductivity of the cathode can dictate the kinetic outcomes of cathode discharge. In our example, electron access was first significant, then ion access in the formation of Ag^0.

K. C. Kirshenbaum, et al. Phys. Chem. Chem. Phys. (2014)

U.S. DEPARTMENT OF ENERGY | Office of Science
BROOKHAVEN NATIONAL LABORATORY
Energy Storage Center.

Conclusion

- Energy Sciences is engaged in a broad range of research on energy related problems at Brookhaven.
- The big facilities at Brookhaven, the NSLS-II and the CFN, form a foundation for this research
- Going forward we will integrate our capabilities further so that multiple techniques – such as electrons and photon probes – can be brought to bear on the same problem.
- We see this integration as offering a competitive advantage in our research and will act as a portal to industry to address important industrial problems.