Energy Research at Brookhaven National Lab

Jim Misewich
Associate Laboratory Director
Energy and Photon Sciences Directorate

70 YEARS OF **DISCOVERY**

A CENTURY OF SERVICE

U.S. DEPARTMENT OF **ENERGY**   **BROOKHAVEN** NATIONAL LABORATORY

BNL Scientific Organizations 2018

Brookhaven National Laboratory
D. Gibbs
Director

R. Tribble
Deputy Director for Science and Technology

Nuclear & Particle Physics
B. Mueller
Assoc. Lab. Director

- **Physics** *H. Ma*
- **Instrumentation** *G. Smith*
- **Collider Accelerator** *T. Roser*
- **Superconducting Magnet** *P. Wanderer*

Energy & Photon Sciences
J. Misewich
Assoc. Lab. Director

- **Energy Science & Technology Dept.** *E. Mendez*
- **Center for Functional Nanomaterials** *C. Black*
- **Chemistry** *A. Harris*
- **Condensed Matter Physics & Materials Science** *R. Konik*
- **Sustainable Energy Technologies** *J. P. Looney*

- **NSLS-II** *J. Hill*
- **Accelerator Div.** *T. Shaftan*
- **Photon Div.** *P. Zschack*
- **EFRC** *E. Takeuchi*
- **CMS** *G. Kotliar*

Computational Science Initiative
K. Kleese van Dam
Director

- **Computer Science & Mathematics** *B. Chapman*
- **Computer for National Security** *A. Hoisie*
- **BNL Sci. Data & Comp. Ctr.** *E. Lancon*
- **Computational Science Lab** *N. D'Imperio*
- **Ctr. for Data Driven Discovery** *S. Jha*

Environment, Biology, Nuclear Sci. & Nonprolif.
M. Schoonen
Assoc. Lab. Director

- **Biology** *J. Shanklin*
- **Environmental & Climate Sciences** *A. Cialella*
- **Nuclear Science & Technology** *W. Horak*
- **Nonproliferation & National Security** *S. Pepper*

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ENERGY

Energy and Photon Sciences Snapshot

EPS by the numbers (2017)

- People: >600

- Budget: ~$171M

- Publications in Peer Reviewed Scientific Journals: 789

- Patents/Appications: 17

- Users (1600 in 2017; about 1900 in 2018)
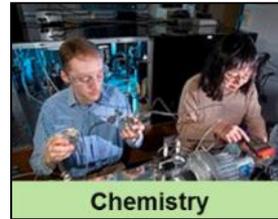
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DOE Energy Sciences Mission

Chemistry

Energy Technology

Condensed Matter Physics & Materials

BNL Core Programs

NSLS-II

CFN/Nanoscience

ISB

CSI

BNL Facilities

- **Brookhaven Focus: Materials for Energy Systems**
  - Materials for Energy (including Quantum Materials)
  - Complex Catalysts for Chemical Conversion
  - Energy Storage (partnership with Stony Brook University)
  - Energy Efficiency and Electric Grid R&D

Partners/Joint Appointments

University	*National Lab*	*Industry*	*New York State*
Columbia University	Argonne National Laboratory	GM	nyserda Energy. Innovation. Solutions.
Stony Brook University	Pacific Northwest National Laboratory	Dow	
CSH	INL Idaho National Laboratory	Toyota	NYSTAR
Rutgers The State University of New Jersey	SLAC National Accelerator Laboratory	GE	
Yale ILLINOIS	Oak Ridge National Laboratory	N.E. CHEMCAT	NY BES+
		PROTON	

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World-Leading Facilities

NSLS-II and CFN

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NSLS-II

World leading synchrotron light source

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NSLS-II: World Leading Synchrotron X-Ray Facility

>1300 Users in 2018

Delivered On-Time Under-Budget

- $912M Construction (7 beamlines)
- 28 operating beamlines in FY19
- 30 more to build for full capacity

Scientific frontiers

- Imaging science (including complementary x-ray and cryo-EM for biomaterials)
- Spectroscopy and scattering

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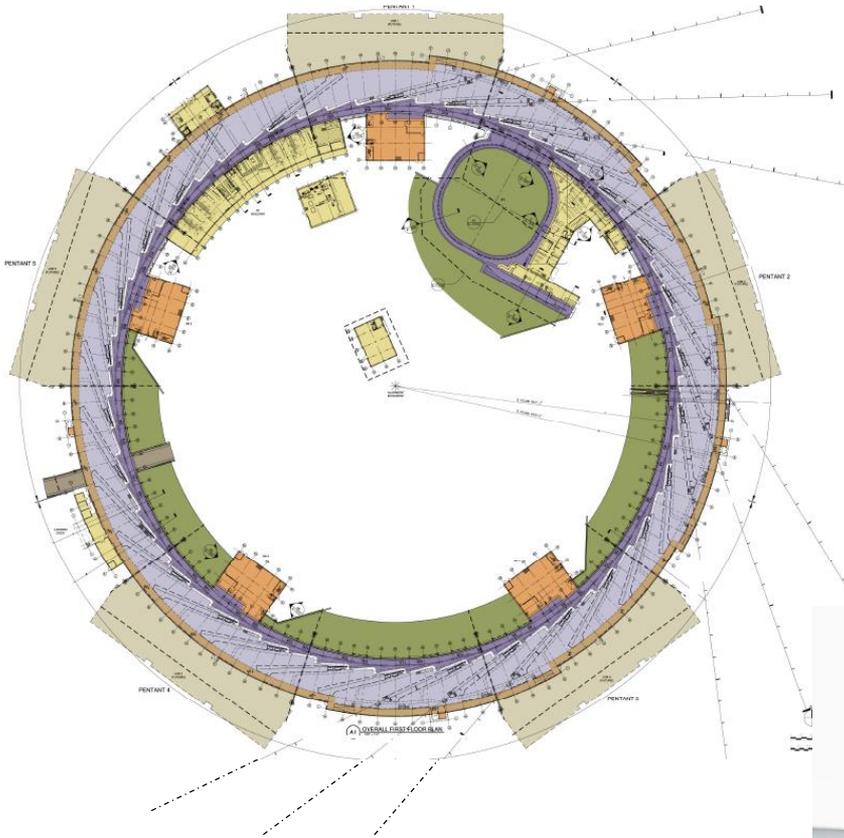
NSLS-II has a strong and productive User program

- > 1300 Users in FY18
- 30% of whom used more than 1 beamline (one used 5!)
- 55% had never used NSLS-II before
- Beamlines oversubscribed by up to a factor of 4
- Synchrotron course taught at Yale and 5 MSIs
- Innovative access modes: BAGs and multi-facility proposals (NSLS-II – CFN and NSLS-II – ORNL
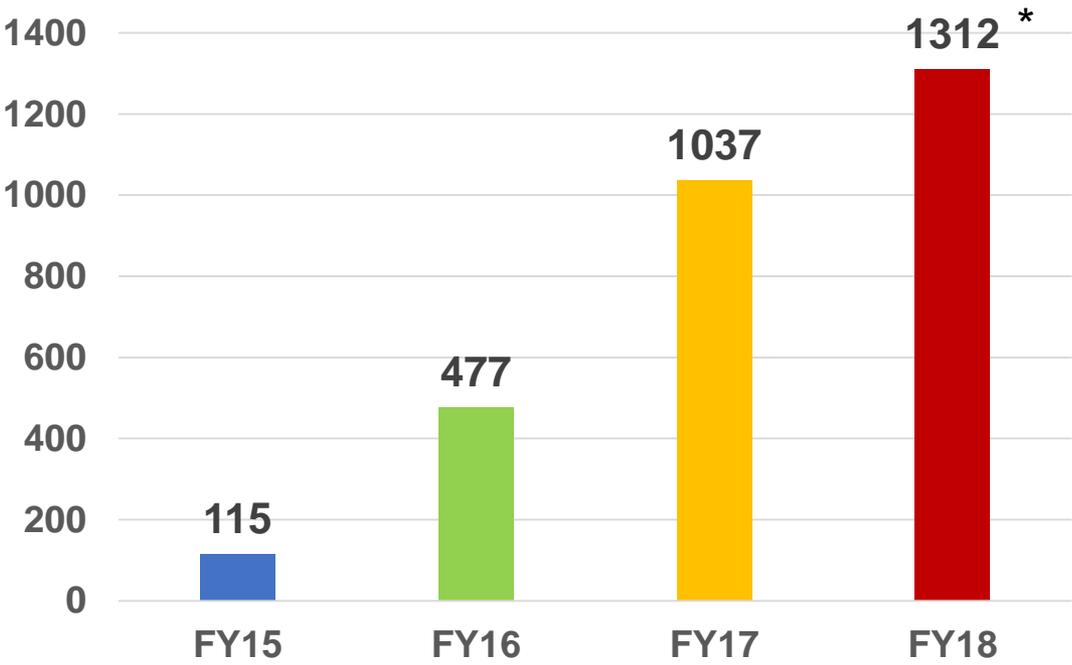
* As of August 30, 2018

Imaging of strain and stacking defects in a III-V nanowire

SEM image of nanowire with diffraction geometry (left) and cutouts from 3D images sensitive to stacking defects (right).

M.O. Hill et al.. Nano Letters. (2018)
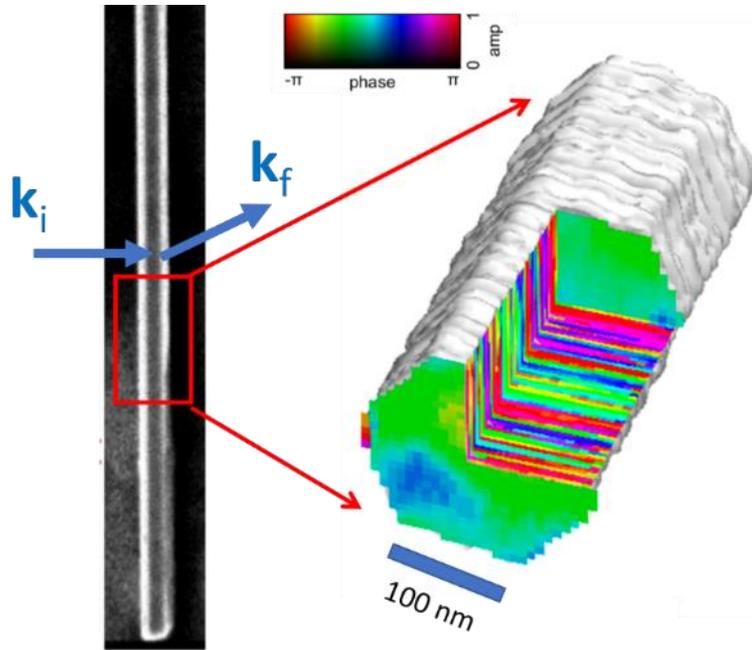
Scientific Achievement

In a single III-V nanowire, the 3D distribution of both strain and stacking defects was measured using coherent x-rays with 3nm resolution, revealing structural heterogeneity from nano- to micro-meter scales.

Significance and Impact

Structural features that determine the performance of advanced optoelectronic nanodevices can be imaged by a new coherent x-ray Bragg ptychography method suitable for studies in operando.

X-ray Imaging

Award Winning MLL design

Smallest spot in working x-ray microscope in the world (12 nm x 12 nm resolution)!
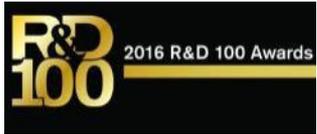
E. Nazaretski, Y. S. Chu, *et al.*

- Collaboration between NSLS-II, MIT and BU achieved the highest resolution 3D x-ray image ever taken of a life science sample.
- Showing Er tag on surface of E-coli bacterium

E. Coli Bacterium

Er Distribution

500 nm

20 nm voxel, 0.1 sec/pixel dwell
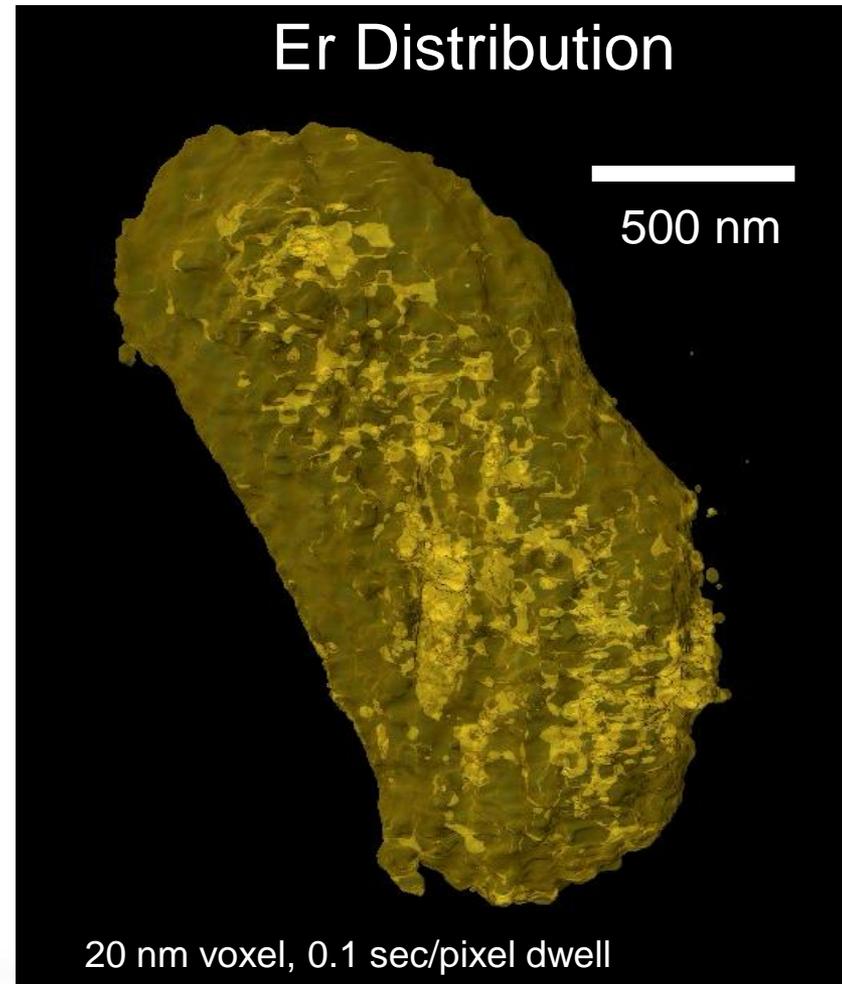
K. Allen (Boston Univ), B. Imperiali (MIT), L. Miller (BNL), whole HXN Team

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IMAGING SCIENCE: Multi-scale, multi-energy range, multi-modal
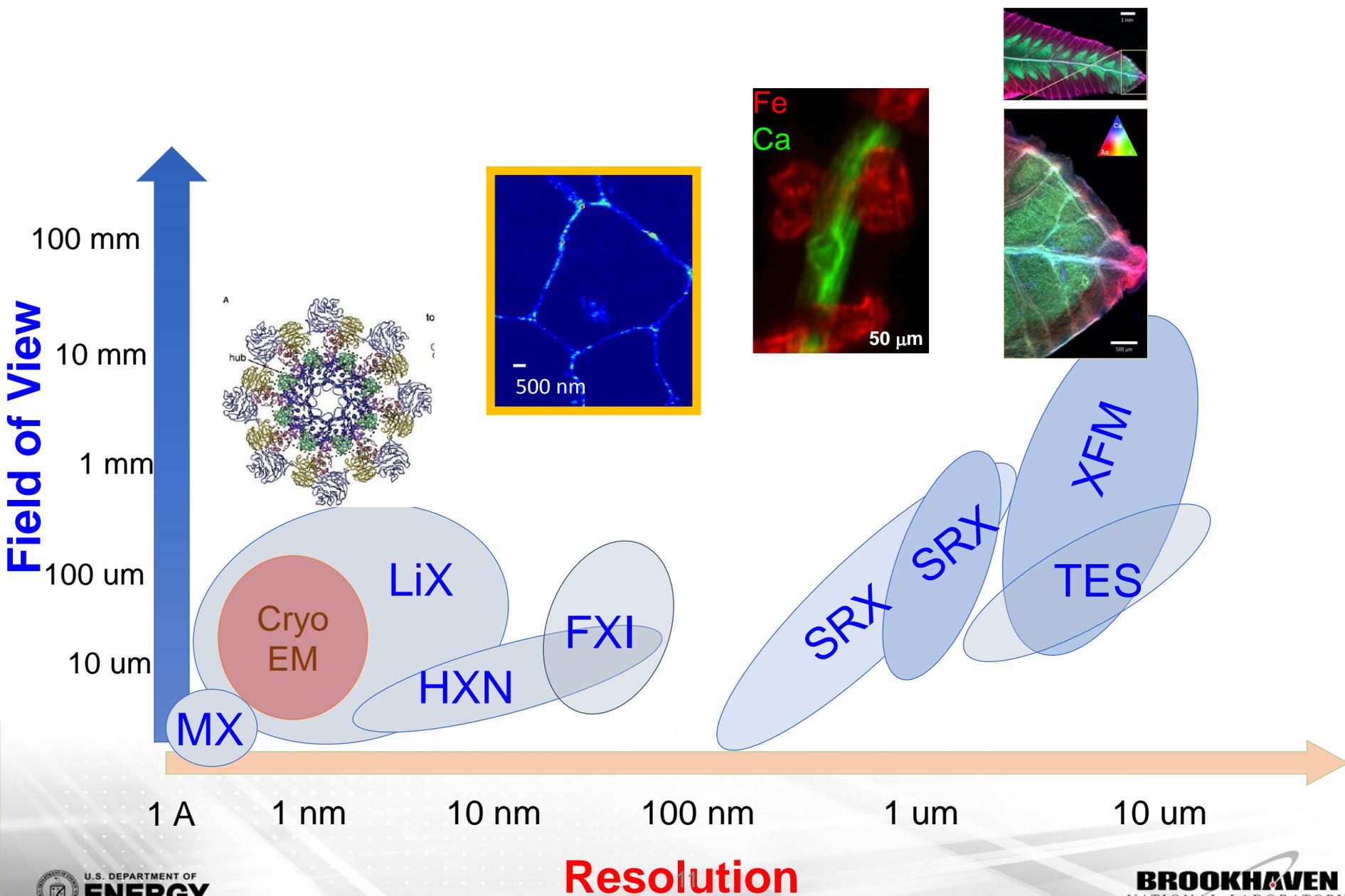
The EM Revolution

In the past three years, it has become feasible to obtain atomic resolution with cryo-EM for the first time. This is sparking a revolution in structural biology.

Ex: Splicesome
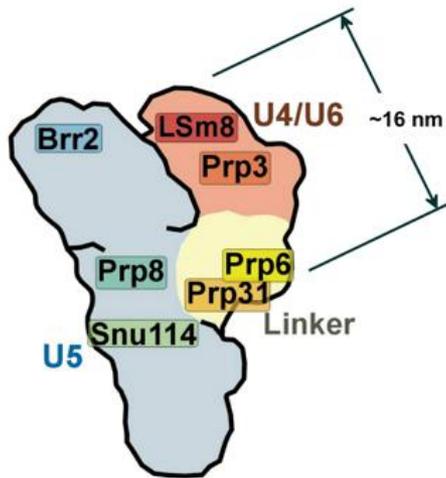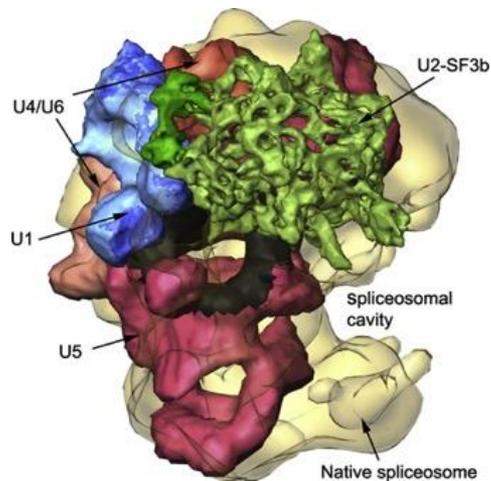
2008

2012

2015
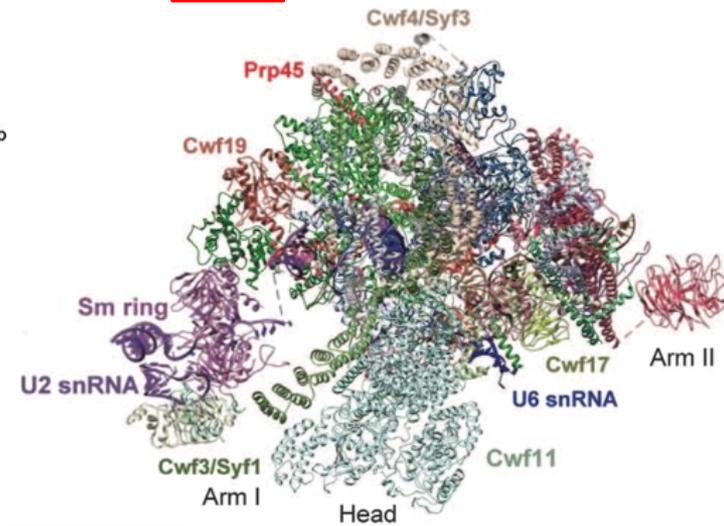
Hacker *et-al, Nature Structural & Molecular Biology* **15**, 1206 - 1212 (2008)

Frankenstein et-al Structure (2012), **6**, 1097-1106

Yan et-al Science (2015), **349**, 1182-1191

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NY gives $15M for cryo-electron microscope at Brookhaven lab

Updated May 18, 2017 8:12 PM

By Delthia Ricks   delthia.ricks@newsday.com

New York is with us
and we are building our plans and team.

Brookhaven National Laboratory on Thursday, May 18, 2017, announced that the state will allocate $15 million for a state-of-the-art cryo-electron microscope at the lab. The advanced imaging technology is expected to increase scientists' understanding of disease, with the microscope helping to discover new treatments, and boost Long Island's biotechnology and pharmaceutical industries, officials said. (Credit: Newsday)

New York State is allocating $15 million for a cryo-electron microscope at Brookhaven National Laboratory as part of a collaborative effort involving three Long Island scientific powerhouses, officials at the lab announced Thursday.

The state-of-the-art imaging technology is at the heart of a new center, the Long Island Facility for Electron Microscopy, which is to be established on the Brookhaven...

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Prep Laboratory

Screening Microscopes

LEGEND

Cryo-EM Facility

Dedicated Office Space

1 Prep Laboratory (471 SQFT)

2 Two Screening Microscopes (518 SQFT)

3 Four Cryo-EM Instruments (5,295 SQFT)

4 Connector to NSLS 2 (1,295 SQFT)

LEGEND

Cryo-EM Facility

Specialized Instrument Environment
Low RH Environment
EMI Active and Passive Sheilding
Sound Attenuation Enclosure
Vibration Class: VCE Vertical
VCF Horizontal

1   NSLS 2 Connector

2   Operators Area

3   Cryo-EM Enclosure

4   Service Room / Prep Laboratory

5   Mechanical Room

6   MDF

7   Electrical Room

8   Sanitary Block

Cryo-EM Site Plan / Facility Plan / Detailes

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UNITED STATES DEPARTMENT OF ENERGY

Cryo-EM Facility

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Center for Functional Nanomaterials (CFN)

Synthesis, assembly, fabrication of materials at the nanoscale

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The Center for Functional Nanomaterials is a national nanoscience user facility

State-of-the-art capabilities for nanoscience

- Electron Microscopy
- Nanofabrication
- Advanced Optics
- Theory and Computation
- X-ray Nanoscience Instruments
- Nanomaterial Synthesis
- Proximal Probes

The CFN supported **571 external users** in 2017

>93% highly satisfied or satisfied

CFN users and staff produced **a record 320 scientific publications** in fiscal year 2017

> 1/3 in high impact scientific journals

# of Users

366, 493, 504, 571

2011 2013 2015 2017

# of Publications

130, 263, 292, 320

2011 2013 2015 2017
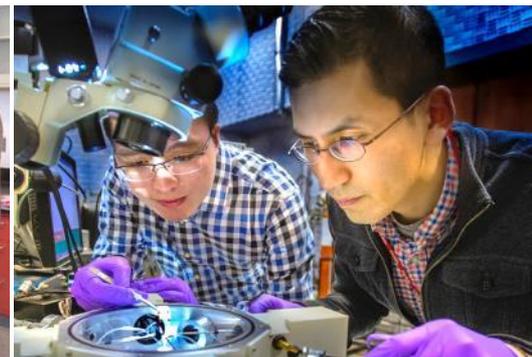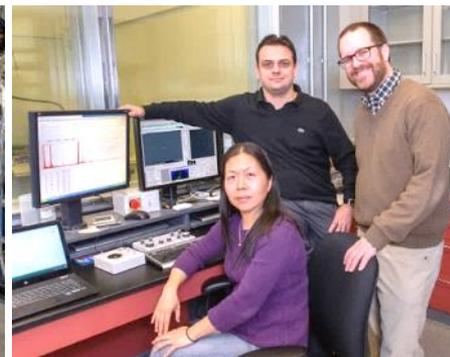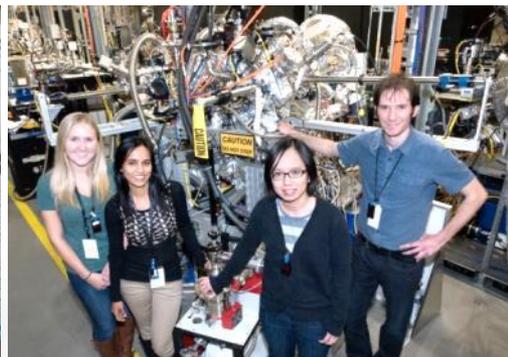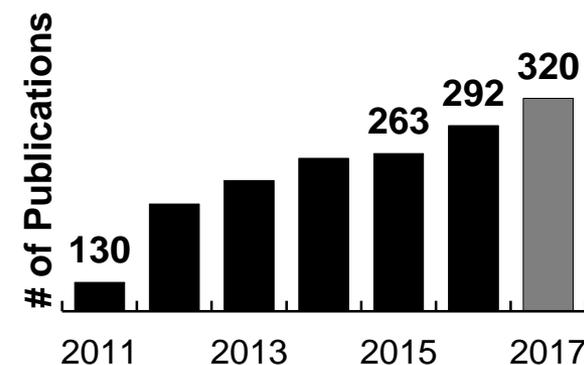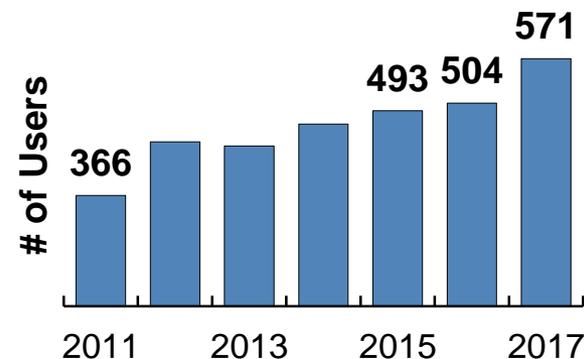
CFN researchers develop record-breaking, first-of-their-kind instruments for nanoscience

Forbes

MAY 2, 2017 @ 03:02 AM   656 👁   ⭐ EDITOR'S PICK

There's A New Record For Tiny Structures

EE|Times

News & Analysis

DoE Claims 1nm Fab Record

Electron litho unearths new properties
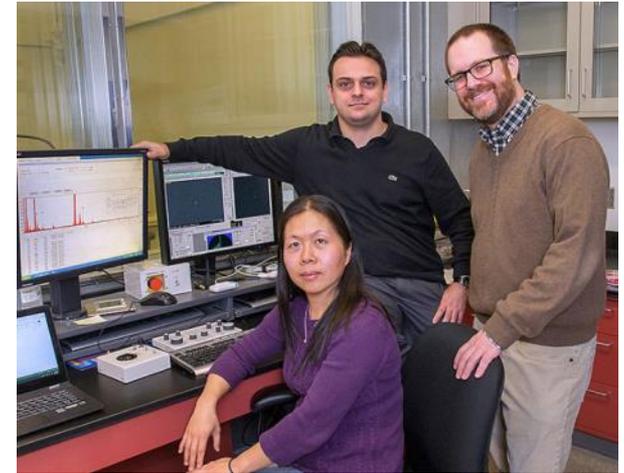
CFN scientists have set a world record for highest-resolution e-beam lithography

- A critical tool for the IT hardware industry

- A tool for patterning materials at 1 nanometer sizes (a few atoms across)

- **CFN offers this one-of-a-kind capability for use by scientists worldwide**

3 nm
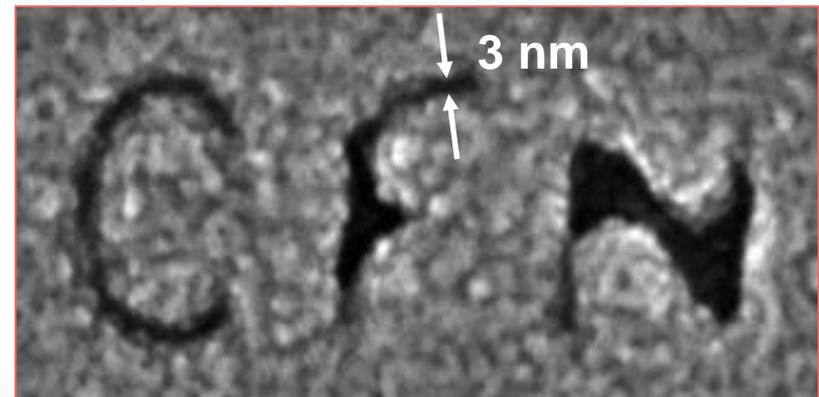
Manfrinato *et al., Nano Letters* (2017).

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CFN 'synthesis-by-assembly' of water-repellent nanotextures

A. Checco, A. Rahman, *Adv. Mat.* (2014).

Self-assembled nanotextures endow surfaces with extreme water- and fog-repellency
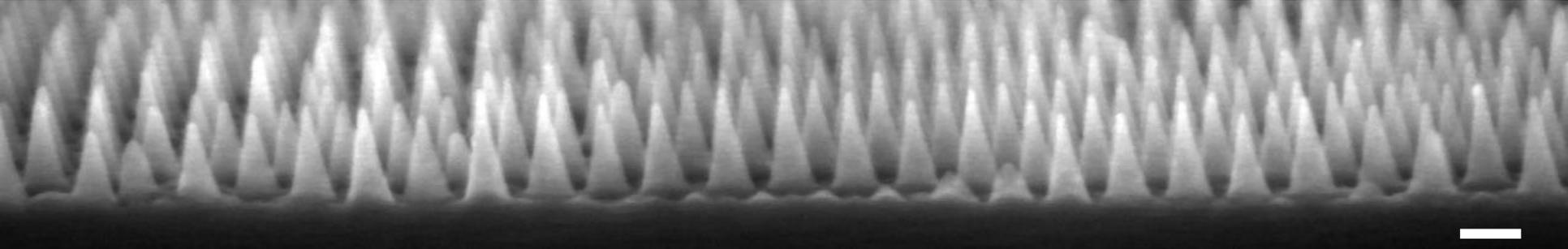
Dense nanotextures created on silicon, glass, and some plastics

flat   spiky

200 µm

e.g., falling raindrops with terminal velocity ~10 m/s
CFN User: A. Checco (SBU)
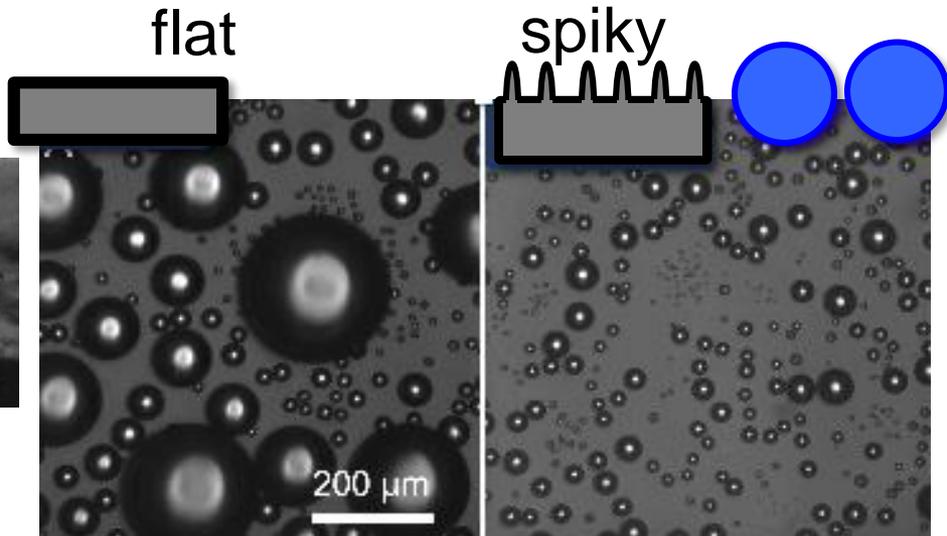
Fog repellent nanotextures
CFN User: D. Quéré (ESPCI)

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Can you see the invisible glass?
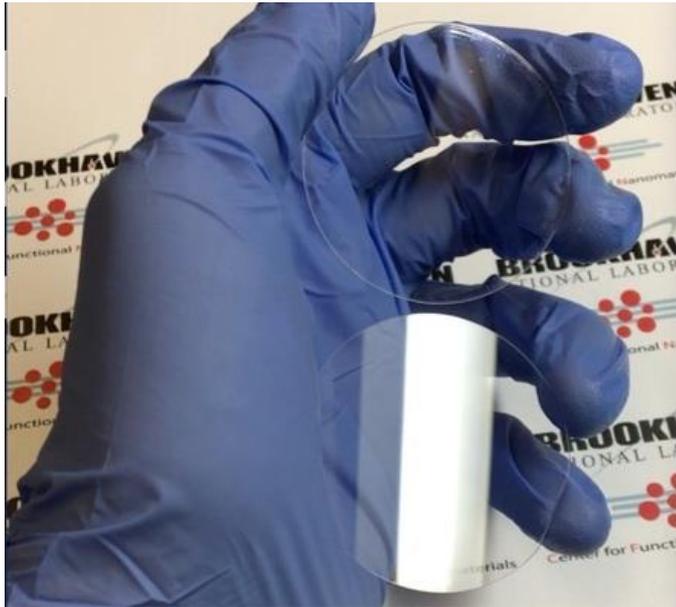
Scientific Achievement

Self-assembled surface nanotextures reduce light reflections from glass windows to <0.2% across the visible and IR, making the glass essentially invisible

Significance and Impact

These ultra-transparent windows can enhance the user experience of consumer devices, improve solar cell performance, and enable higher-power, pulsed laser applications

CFN 'invisible glass' technology optioned to start-up company (Edgehog Technologies) in 2018.

2018 Grand Prize Winner:
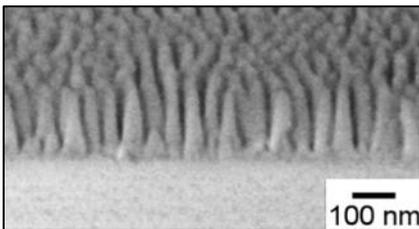
(Top) Photograph of a piece of regular glass (lower), showing the reflection of an overhead light, and a similar piece of 'invisible glass' without any reflection (upper). (Bottom) SEM image of the surface nanotexture.

Applied Physics Letters (2017)

Science

What do we DO at these facilities and in our core programs?

Catalysis

Goal

- Develop the fundamental knowledge for designed catalysts enabling sustainable chemical conversion processes – e.g., fuel synthesis from CO_2, CH_4.

Approach

- Build on BNL's discovery of enhanced heterogeneous catalysis with active metal:oxide interfaces and leadership in mechanistic studies of homogeneous photocatalysis

Determination of Nanocatalyst Structure "*on-the-Fly*" by Supervised Machine Learning
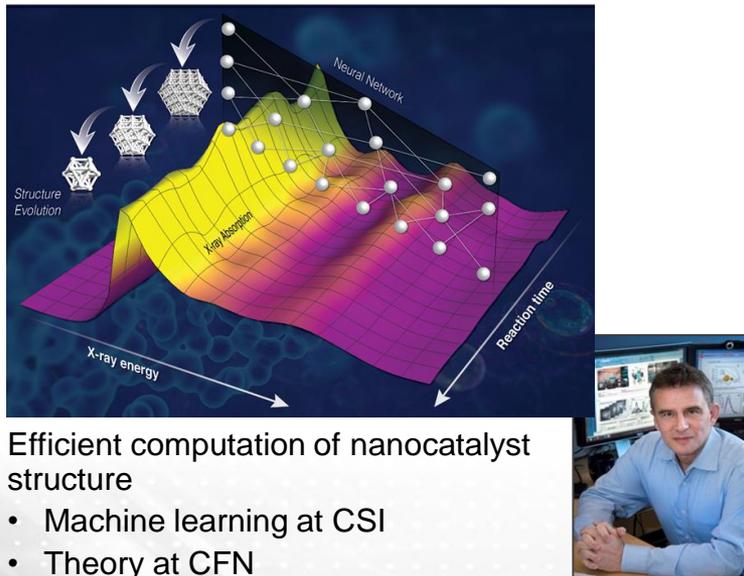
Efficient computation of nanocatalyst structure
- Machine learning at CSI
- Theory at CFN
  J. Phys. Chem. Lett. (2017)

Anatoly Frenkel

Develop Multi-modal Methods for Catalysis

In situ X-Ray and Electron Methods

$2CH_4 + 1/2O_2 + H_2O$ → $2CH_3OH + H_2$

Reaction Mechanism

Process of Deactivation

Active Structure

Catalytic Nature

●:Cu; ●:O; ○:Ce;
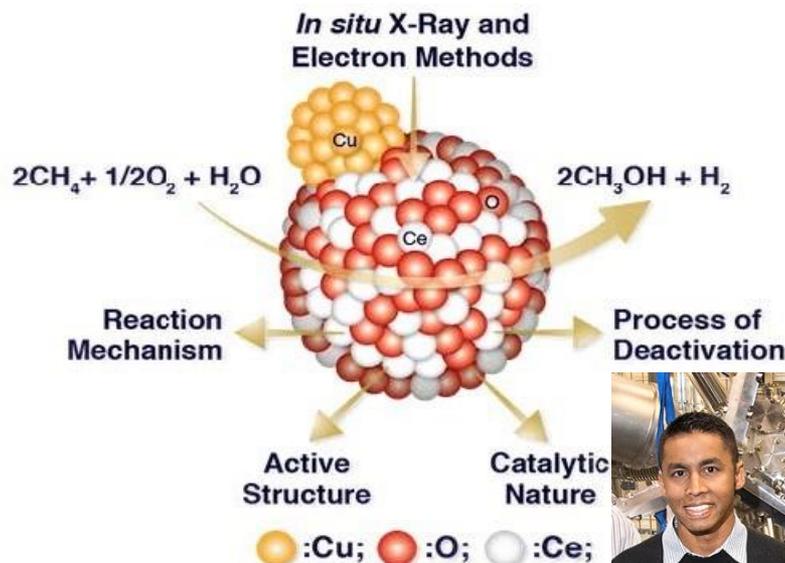
Multi-modal studies for structure and mechanism
(Early Career 2017)

Sanjaya Senanayake

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Rational Design of Catalysts for C-H vs C-C Bond Cleavage
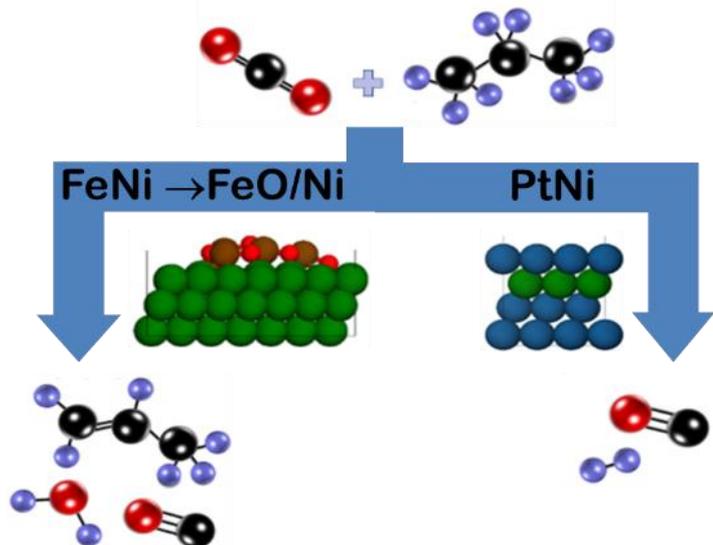
Reaction pathways over Ni bimetallics
- FeNi for C-H cleavage to produce propylene
- PtNi for C-C cleavage to produce syngas

E. Gomez, S. Kattel, B. Yan, S. Yao, P. Liu & J. G. Chen, *Nat. Commun*, (2018) 9:1398

Scientific Achievement

Theory & Experiment for rational control of CO_2 reduction with propane. Reaction pathways over Ni catalysts can be tuned by bimetallic formation for propylene (C-H cleavage) vs syngas (C-C cleavage) product.

Significance and Impact

New routes to propylene are desired due to changing feedstocks. Catalytic control of C-H vs C-C bond enables production of beneficial propylene while consuming the greenhouse gas CO_2.

Scientists used catalyst synthesis, *in-situ* measurements and theory to design and understand different catalysts for distinct conversion routes.

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Advanced Fuel Cell Electrocatalysts

BES
Basic Science

Principles and methods for monolayer electrocatalysis.
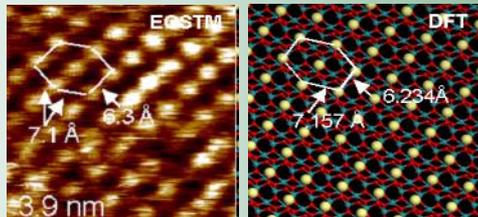
In-situ electrochemical studies of structure and catalytic activity of single atomic layers
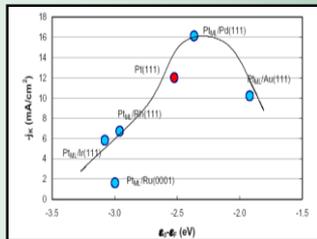
Discover and develop high activity monolayer platinum catalysts.
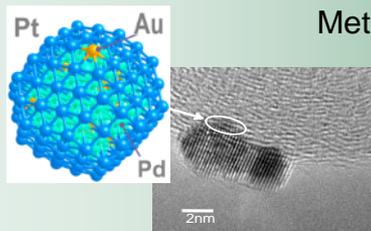
Metal alloys to improve durability

Core-shell electrocatalysts >130 publications 2001-17 >12000 citations

## EERE Fuel Cell Office
Applied Research

Core-shell electrocatalysts developed for high activity and durability with ultralow Pt mass.
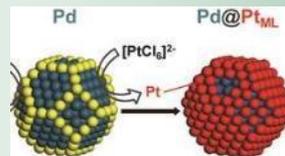
Developed syntheses for nanoscale core-shell catalysts with monolayer control.
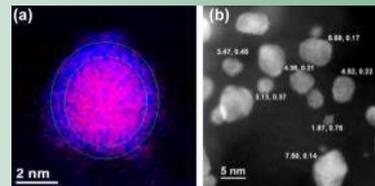
Enhanced Pt-mass weighted activity 10x. Scale-up synthesis led to membrane electrode assemblies with good performance.
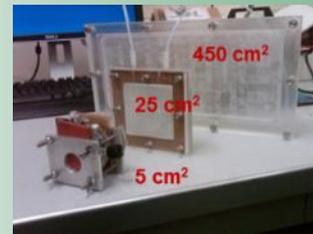
>15 US Patents ---------- R&D 100 Award

Industrial Collaboration
Toward Deployment

*Performance and durability in subsystem membrane electrode assemblies, licensing, manufacture methods*

Licensed for commercial development

Excellent low-Pt fuel cell performance
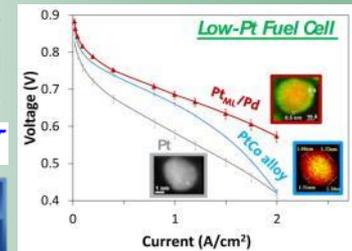
Excellent electrolyzer performance, >10x reduced Pt mass.
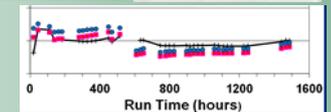
High performance, low Pt electrocatalysts ready for applications in fuel cell vehicles and hydrogen generation.

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Quantum Materials

Goal

- Leverage BNL's leadership in correlated-electron science to discover and understand the next generation of quantum materials, including those valuable for Quantum Information

Approach

- Exploit world-leading capabilities of OASIS and NSLS-II

First Science from OASIS

Systematic study of $Bi_2Sr_2CaCu_2O_{8+\delta}$

- Well-studied dome now accurately calibrated to peak at 0.18 doping
- First studies of highly overdoped regime allowing detailed studies of the pairing mechanism in this regime.
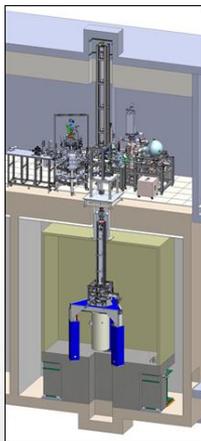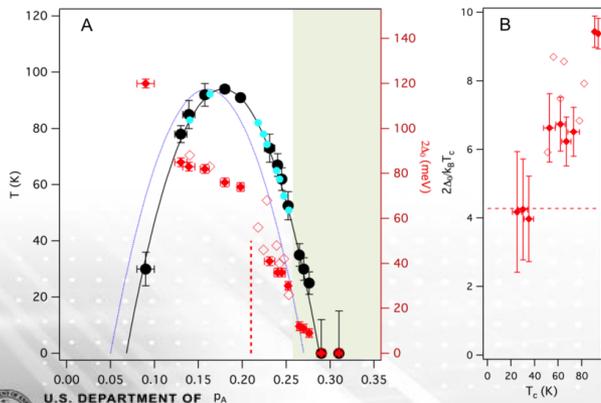
Topology and Qubits

- Customized heterostructures for topological superconductivity and quantum information science
- Resonant Inelastic X-ray Scattering of measurements of topological phonons and magnons at the SIX beamline

OASIS

LSCO

LSMO

substrate

Engineered heterostructures

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Nanomaterials Synthesis by Assembly (CFN)

Goal

- Advance the science of materials "synthesis by assembly" from components, for creating multi-functional systems with precisely defined architectures for targeted properties, including those valuable for QIS

Approach

- Employ leading scientific programs in self-assembly of soft materials and advanced nanoscience characterization at CFN and NSLS-II, especially *in situ* and *operando* measurements

Quantum Material Press (QPress)

Goal: First-of-its-kind facility for robotic synthesis of layered 2D material heterostructures by assembly; quantum properties studied at CFN and NSLS-II

Graphene
hBN
MoS₂
WSe₂
Fluorographene
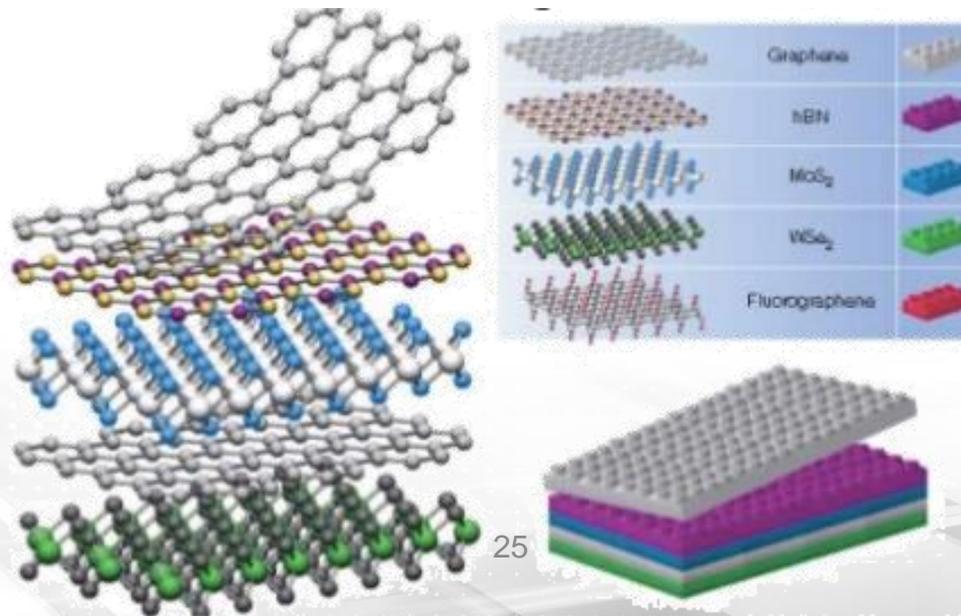
(with Harvard, MIT)

Energy Storage

Goal: Leverage BNL's facilities and expertise to understand, control and design complex battery systems

Approach: Exploit world-leading capabilities in electron microscopy and NSLS-II

EUROPEAN INVENTOR AWARD 2018

Prof. Esther Takeuchi
Stony Brook University Distinguished Prof.
BNL EPS Chief Scientist Energy S&T

Center for Mesoscale Transport Properties

Operando lithiation of Fe_3O_4 revealed:
- Onset of parasitic reactions forming surface electrolyte interphase (SEI)
- Allowed determination of contributions to heat dissipation
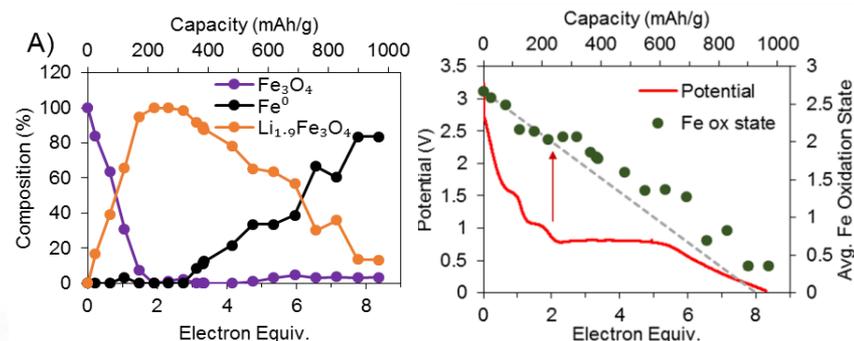
Energy Storage: SBU and BNL Leadership

U.S. DEPARTMENT OF ENERGY | Office of Science

NEW YORK STATE OF OPPORTUNITY. | NYSERDA

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy — VEHICLE TECHNOLOGIES OFFICE

Basic Research — Proof of concept — Early Stage Prototype — Product Development — Commercialization

Energy Frontier Research Center

Center for Mesoscale Transport Properties

U.S. DEPARTMENT OF ENERGY | Office of Science
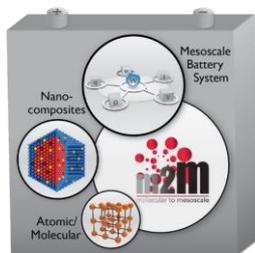
$10.4 M, 4 Y award

Mission: understand and control battery transport, molecular to mesoscale

NYSERDA-NYSTAR Match to EFRC

NEW YORK STATE OF OPPORTUNITY. | NYSERDA   NYSTAR — Empire State Development Division of Science, Technology & Innovation

10% match to in-state award

Mission: establish pouch cell prototyping capability at BNL

Coin Cell ~2 mAh   Pouch Cell 0.1 – 2.0 Ah

Industrial Program

Mission: high capacity anodes for EVs

EERE Program Portfolio

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy — VEHICLE TECHNOLOGIES OFFICE

Mission: support high impact projects to develop more energy efficient and environmentally friendly highway transportation technologies that enable America to use less petroleum

Lithium Sulfur Batt500 Seedling Project
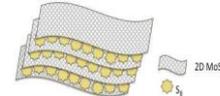
Self-forming Self-healing Solid State Lithium Battery

Enabling Extreme Fast Charging for Electric Vehicles

Target: charge in 6 minutes

Map Source: DOE Alternative Fuels Data Center's Electric Vehicle Station Locator

U.S. DEPARTMENT OF ENERGY

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Co-location with Offshore Wind R&D On Long Island

NY Offshore Wind Center

NY-ESI Energy Storage Institute

NYS-CAT Center for Advanced Technology

Manufacturing Support

Energy Efficiency: Heating and Combustion Systems

BNL has made major contributions to NYS energy and environmental challenges

BNL has helped increase efficiency of heating systems in the Northeast since the late 1970's

- demonstrated energy savings of new oil burners - 100% market penetration and savings Nationwide of $25 billion

- transition to ultralow sulfur heating oil – a 99% reduction in fine particulates with major health impacts

- developed new biomass heating system test protocols adopted by NYDEC and US EPA
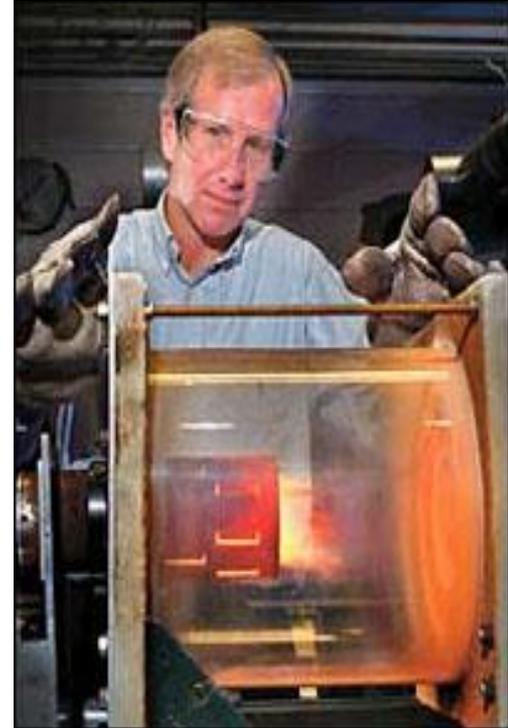
For 40 years, Dr. Butcher has been a leader in research and development of building energy systems including advanced fuels, heating and cooling systems, and advanced controls.

Energy Efficiency in Buildings

BNL is increasing its focus on building energy efficiency

Buildings applications:

- Joint DOE/NYSERDA project on performance of cold-climate air-sourced heat pumps (proposal stage)

- Energy savings potential of evaporative cooling at a DoD data center

- Thermal distribution efficiency and test methods

- Water harvesting from flue gas using a novel thermosiphon technology (ARPA-E Project w/ SBU, United Technologies)

- Hybrid condensing boiler/solar thermal system at BNL

- Advanced controls in heating systems.

- Solid oxide fuel cells for building and data center applications

- Energy savings potential of modern integrated hydronic systems with low idle losses. Field tools for predicting energy savings are now in use.

**A 60% fuel-to-electric solid oxide fuel cells under test at BNL**

BNL Grid Research: focused on NYS challenges
smart, resilient, efficient

- BNL Expertise
    - Utility operations, power-flow modeling
    - DER systems engineering
    - Meteorology and cloud science

    - Data-intensive computing
    - Open source software development
    - High-performance computing
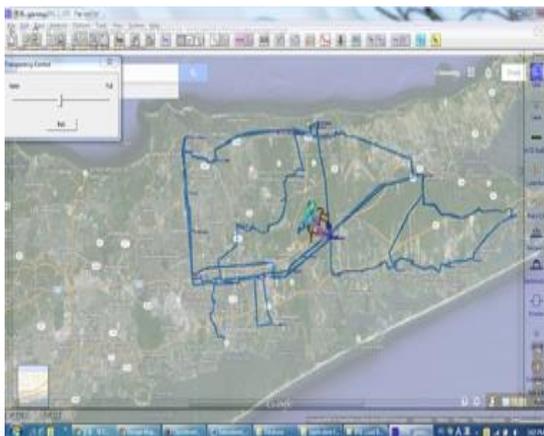
- Applying our capabilities to:
    - Power flow modeling and analysis (efficiency)
    - Storm damage prediction (resilience, restoration)
    - Automated restoration tools
    - DER, Microgrid design/optimization (resilience)

- DOE Program Efforts
    - Advanced Grid Modeling
    - Cybersecurity for Energy Systems
    - Building Technologies Office
    - Solar Energy Technologies Office
    - APRP-E

- NYS and NE Partnerships
    - NYS Utilities, NYSERDA, ESDC
    - SBU, U Conn, Purdue
    - MIT Lincoln Labs
    - NYS Smart Grid Consortium

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DOE Energy Sciences Mission

Chemistry

Energy Technology

Condensed Matter Physics & Materials

BNL Core Programs

NSLS-II

CFN/Nanoscience

ISB

CSI

BNL Facilities

- **Brookhaven Focus: Materials for Energy Systems**
  - Materials for Energy (including Quantum Materials)
  - Complex Catalysts for Chemical Conversion
  - Energy Storage (partnership with Stony Brook University)
  - Electric Grid R&D

Partners/Joint Appointments

University

COLUMBIA UNIVERSITY • Stony Brook University

CSH • RUTGERS THE STATE UNIVERSITY OF NEW JERSEY

Yale • I ILLINOIS

National Lab

Argonne NATIONAL LABORATORY • Pacific Northwest NATIONAL LABORATORY

INL Idaho National Laboratory

SLAC NATIONAL ACCELERATOR LABORATORY

Oak Ridge National Laboratory
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

Industry

GM • Dow

TOYOTA • GE

N.E. CHEMCAT

PROTON THE LEADER IN ON SITE GAS GENERATION

New York State

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