UCI-National Labs Connections

Theme 2: Renewable energy research, development and deployment

UCI

Sub-Themes:

1. Electrochemical Technologies:

- Electrocatalysis (Atanassov)
- Fuel Cells and Electrolyzers (Zenyuk)
- Batteries (Xin)
- Solar Energy/Fuels (Law)

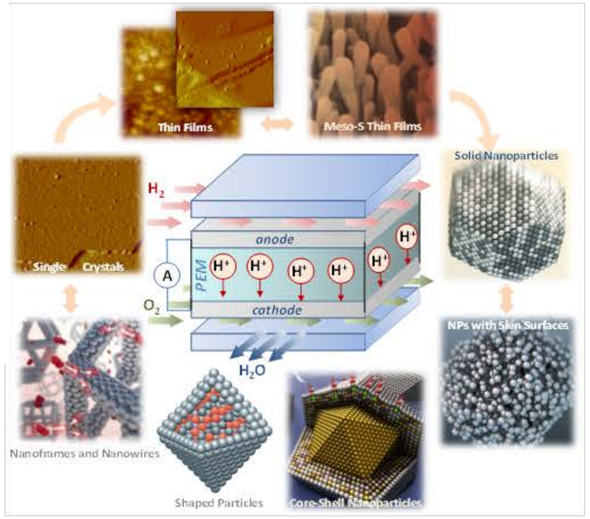
2. **Nuclear Energy** (Finkeldei)

3. **System-level Studies and Demonstration:** (Brouwer)

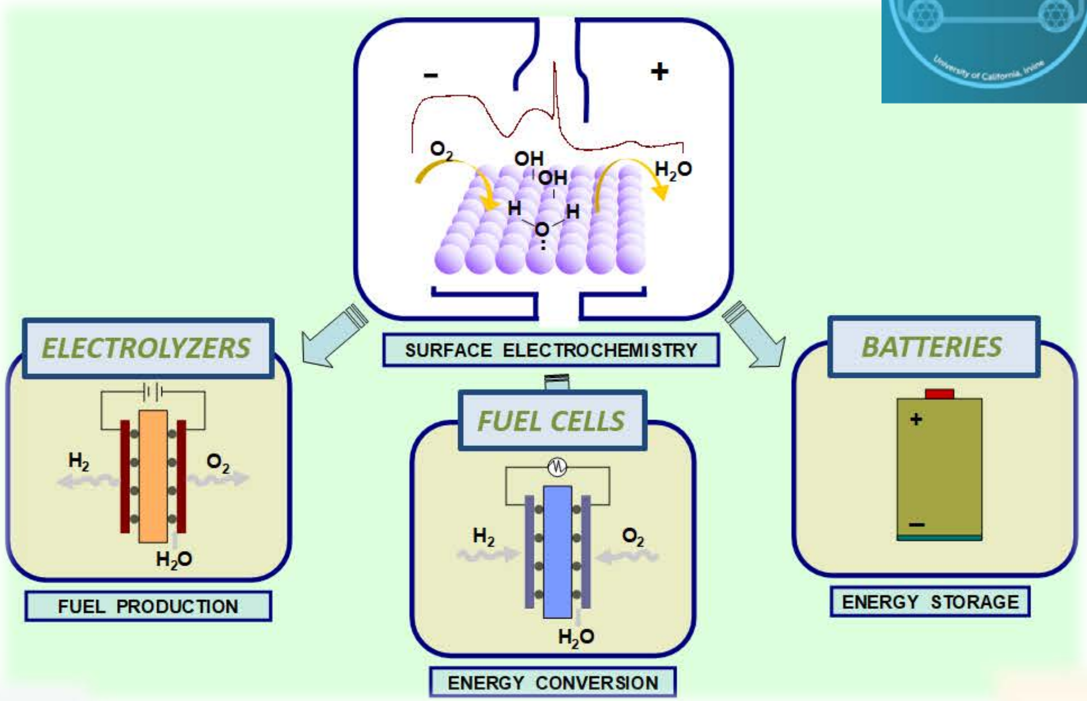
- Mobility and connectivity
- Deployment projects at UCI

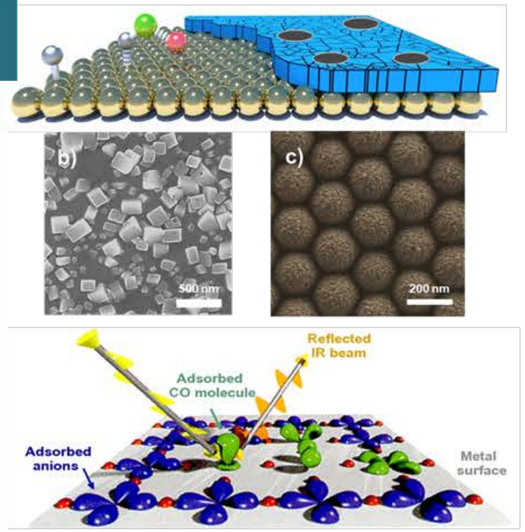
Sub-Theme 1. Electrochemical Technologies: Electrocatalysis & Electrocatalysts

Vojislav Stamenkovic, Professor, *Department of Chemical & Biomolecular Engineering*
Director, *Horiba Institute for Mobility and Connectivity²*

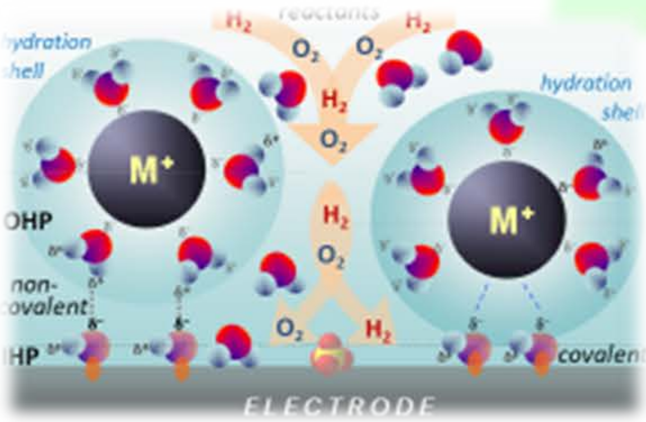


- Bottom-Up Design of Materials -



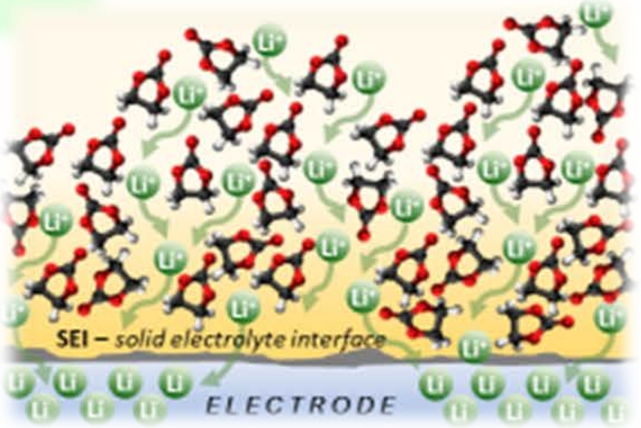


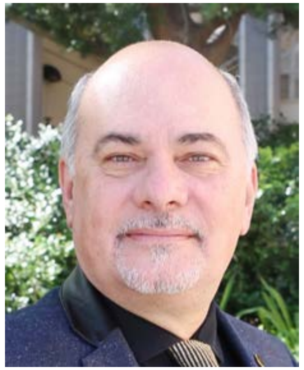
- Altered Functionality -



- Design of Electrochemical Interfaces for Energy Conversion and Storage -

from Molecular to System Level Engineering

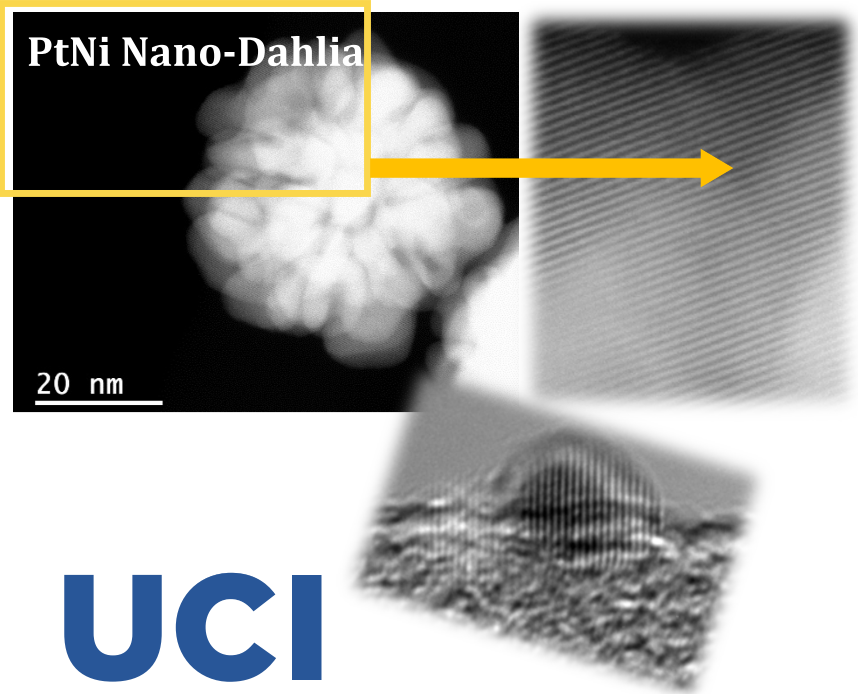


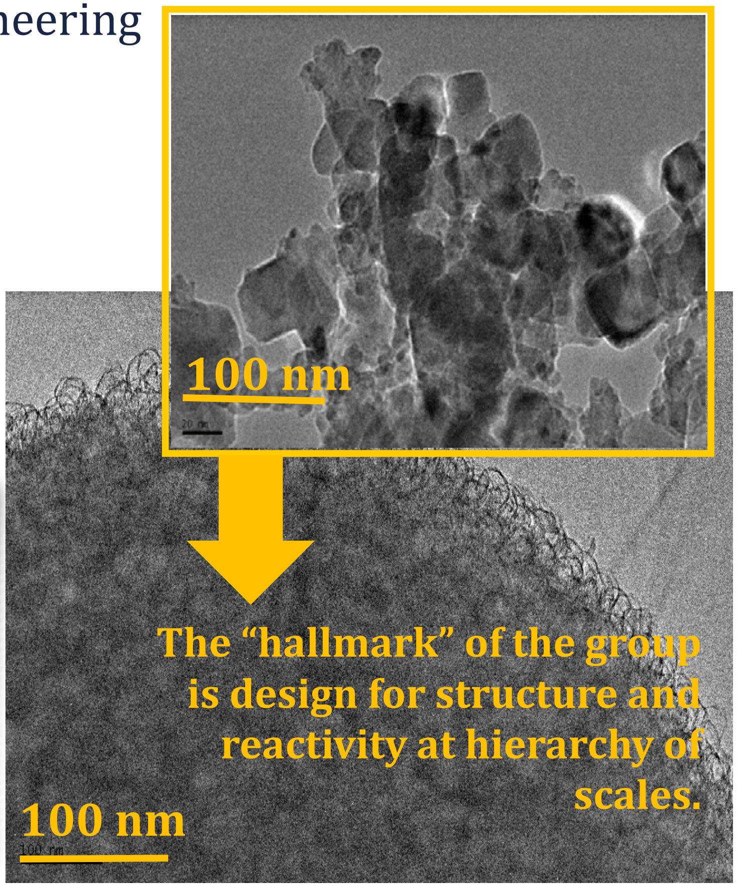


Plamen Atanassov
Chancellor's Professor of
Chemical & Biomolecular Engineering,
Materials Science & Engineering
and Chemistry

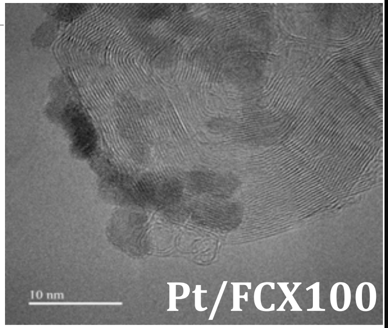
MILLION MILE FUEL CELL TRUCK
U.S. DEPARTMENT OF ENERGY

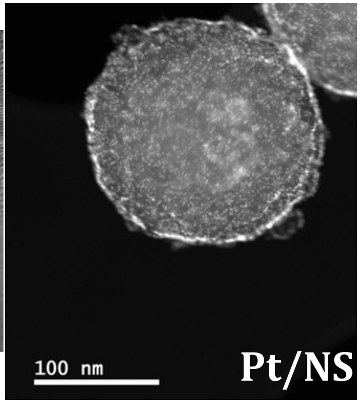
Electrocatalysts: Structured Platinum Alloys



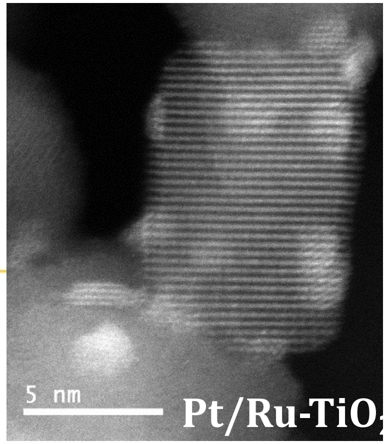


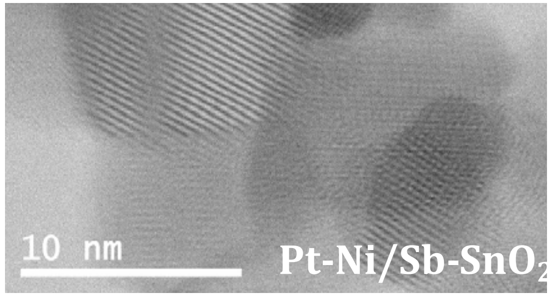
Catalyst Supports: Advanced/Functionalized Carbons





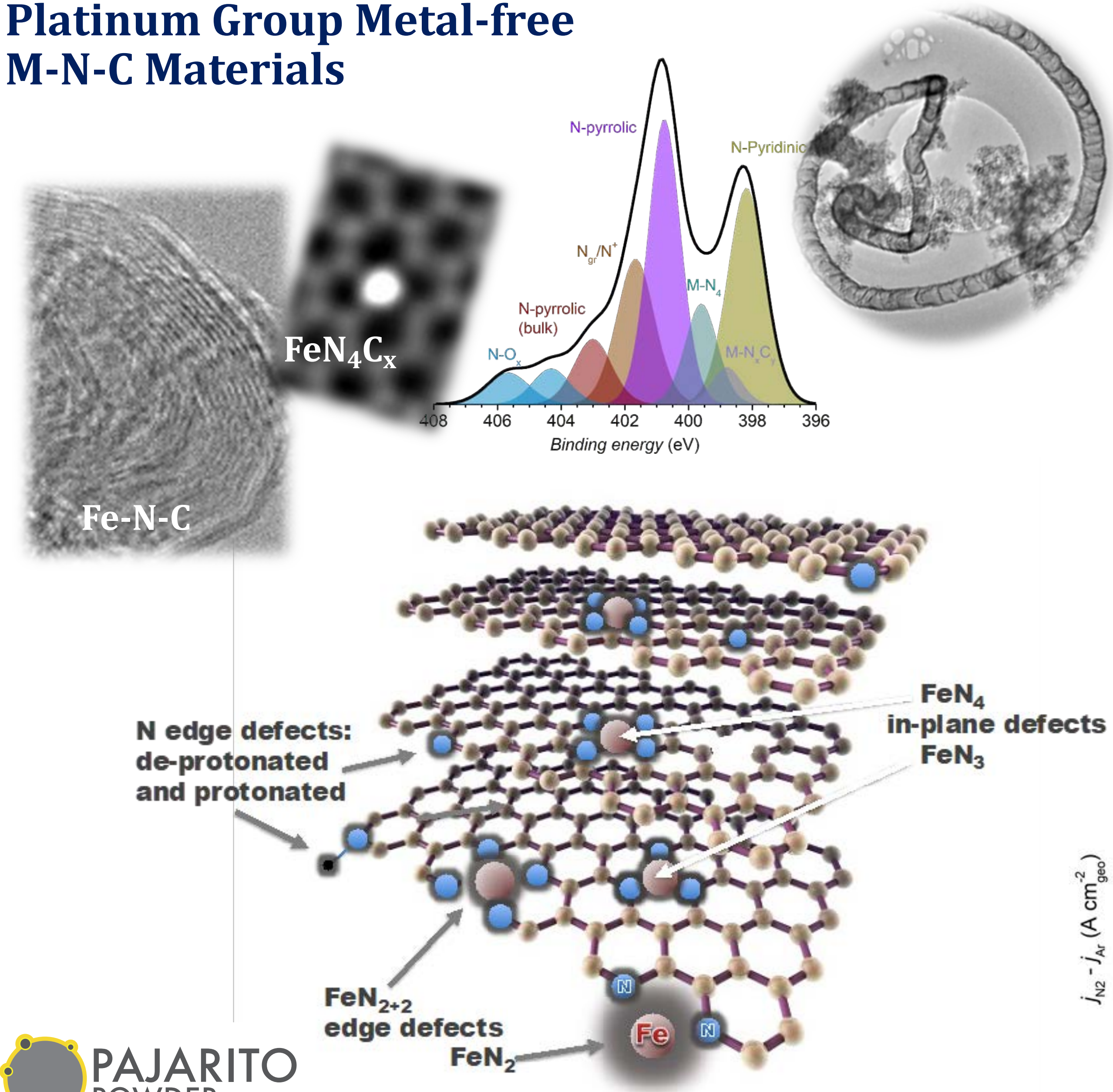
Catalyst Supports: Conductive Metal Oxides





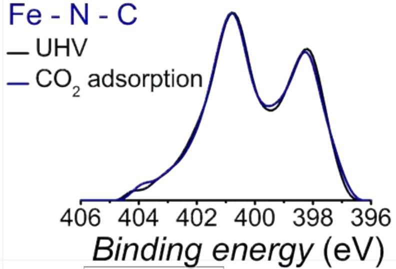
TOYOTA
CABOT
IRD
BOSCH
NISSAN
Los Alamos NATIONAL LABORATORY
U.S. DEPARTMENT OF ENERGY
Energy Efficiency & Renewable Energy
UCI

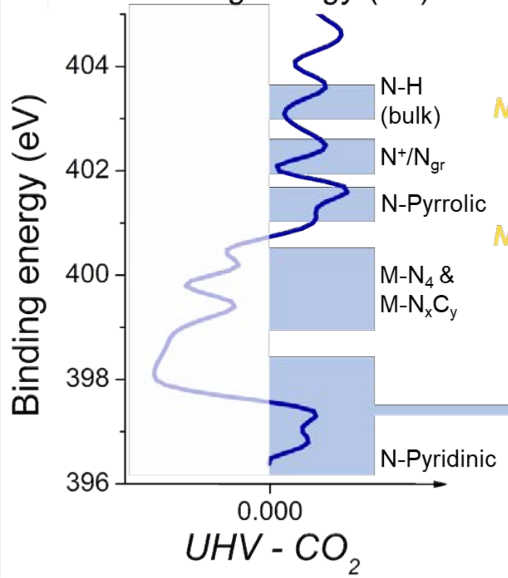
Electrocatalysts: Platinum Group Metal-free M-N-C Materials

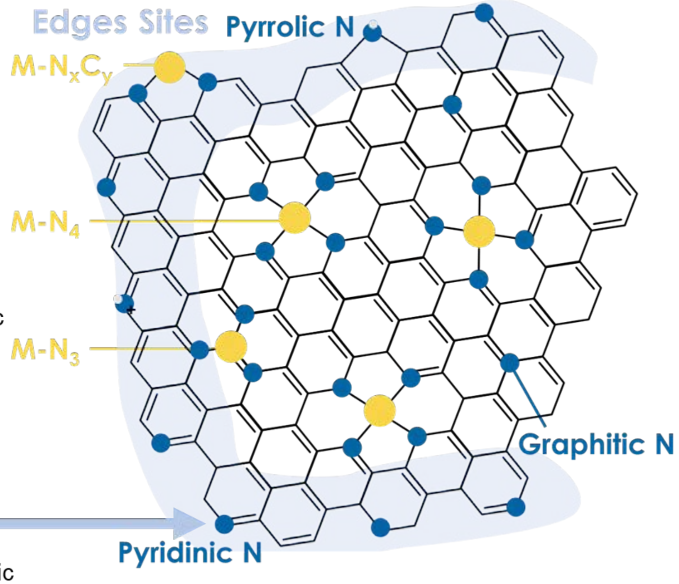


First & only commercial PGM-free catalyst

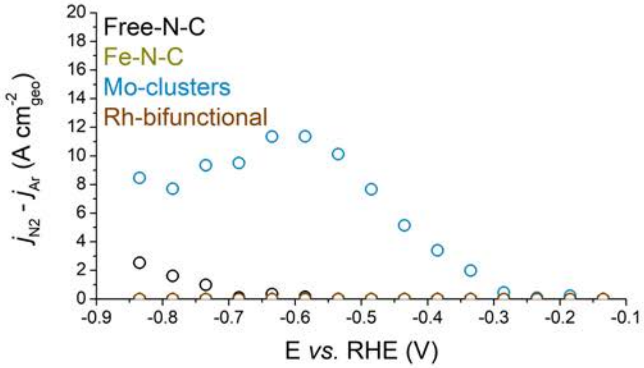
M-N-C Catalysts for CO_2 Reduction

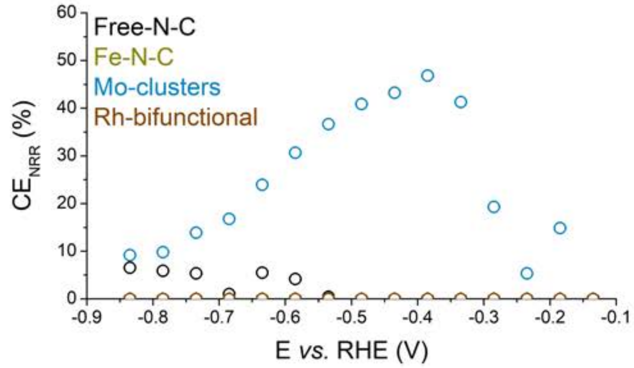






M-N-C Catalysts for NO_x Reduction





Small molecule activation by atomically dispersed catalysts

Huolin Xin
Highly Cited Researcher
MRS Outstanding Early-Career Investigator
Physics and Astronomy

Objectivs:

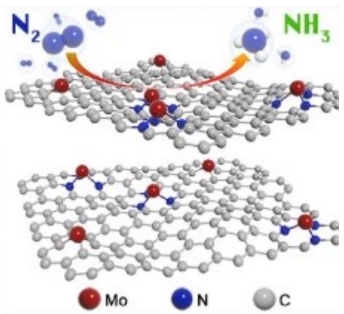
- Explore low-PGM and non-PGM catalysts for PEMFC
- Polyelectrolyte membrane design
- Tackle the low efficiency and durability issues of metal-air batteries
- Reduce reliance on fossil fuels

Potential Impact:

- Reducing carbon emission
- Producing renewable fuels
- Advancing metal-air batteries and fuel cells

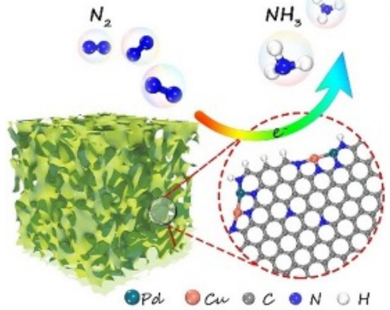
Delivered Catalyst System:

Mo SAC for NRR



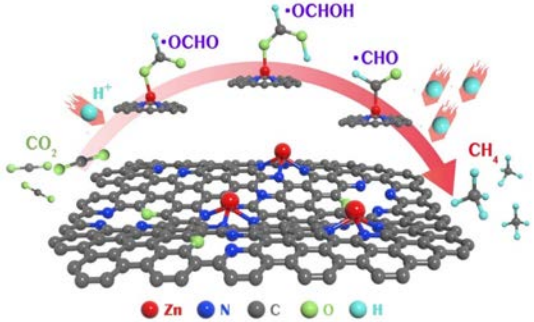
Angew. Chem. Int. Ed. Engl. 2019, *58*, 2321.

PdN_2CuN_2 sites for NRR



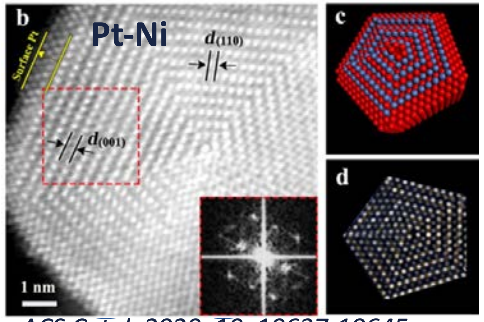
Angew. Chem. Int. Ed. Engl., *2021, 133, 349-354.*

ZnN_4 sites for CO_2RR



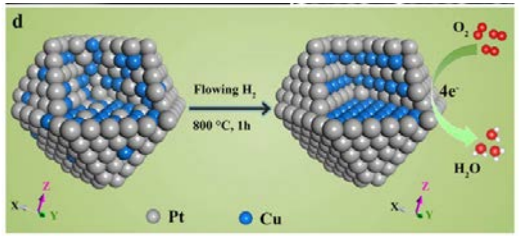
J. Am. Chem. Soc. 2020, *142* , 12563.

Ordered Pt-TM for ORR



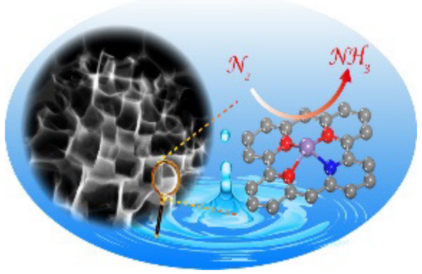
ACS Catal. 2020, 10, 10637-10645

Rhombohedral Ordered Pt-Cu for ORR



ACS Catal. 2021, 11, 1, 184–192

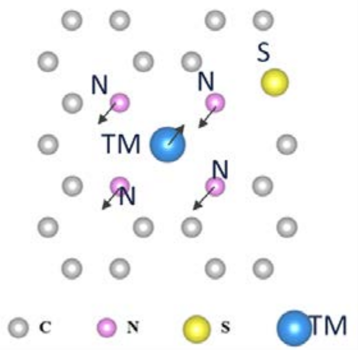
MnO_3N_1 sites for NRR



ACS Catal., 2021, 11, 2, 509–516

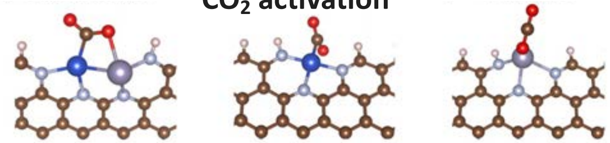
New Directions:

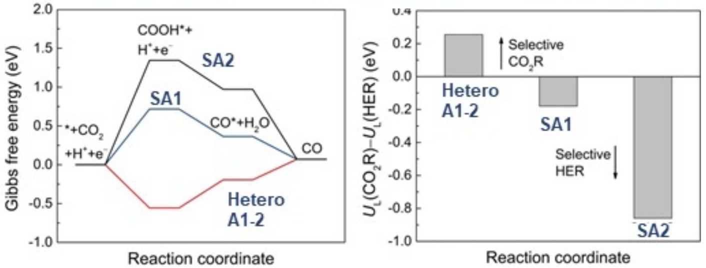
1: Altering ligand effect through second-shell anion modulation



- The average bond length between metal center and the coordinated N increases
- The metal center has increased charge
- The metal center will bind to oxygen stronger

2: Hetero-atom-dimers for CO_2 to CO electro-reduction

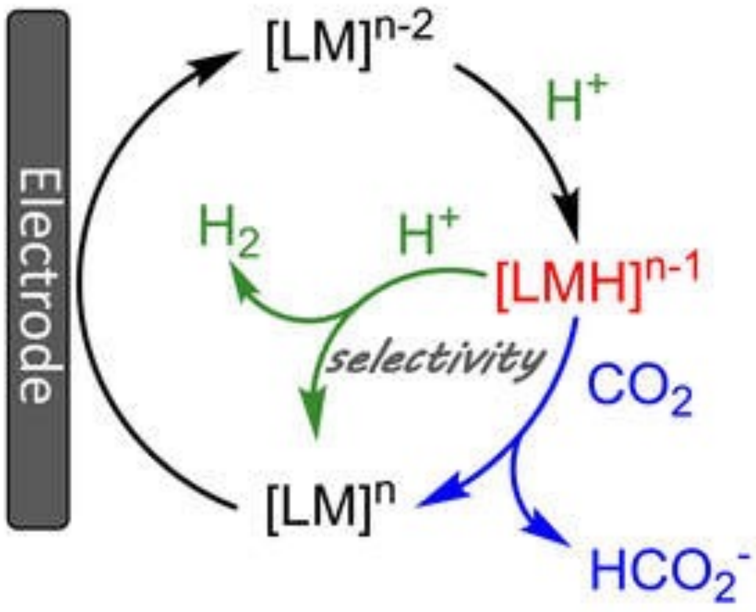




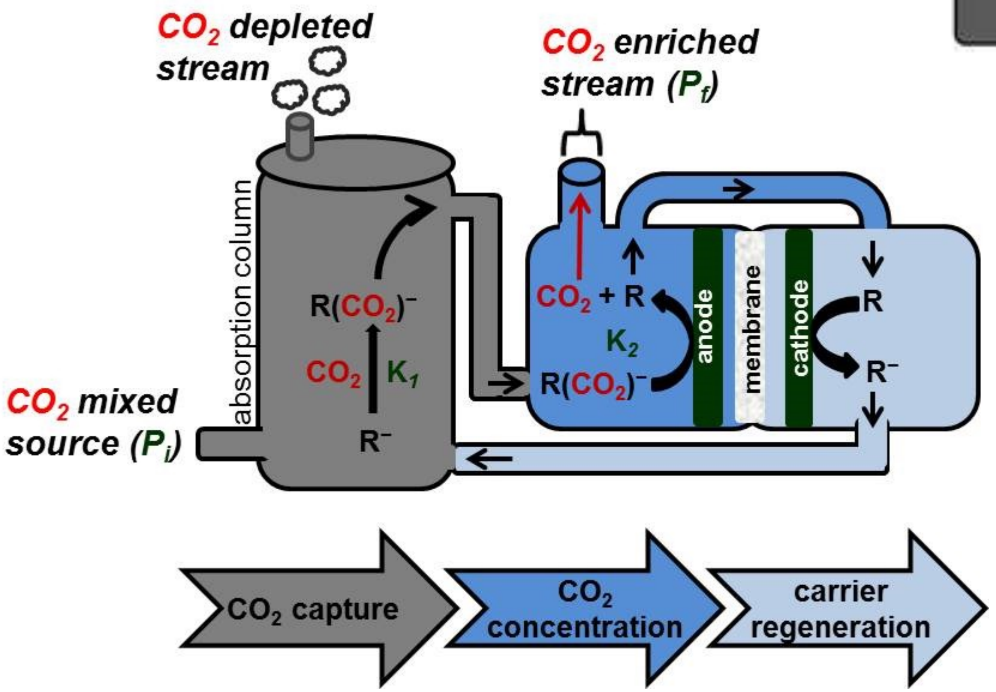
Fundamental studies on electrocatalyst mechanisms for H^+ and CO_2 Reduction

- Earth abundant molecular electrocatalysts for aqueous H^+ reduction
- Selective, low overpotential electrocatalysts for CO_2 reduction to HCO_2^-
- Reversible aqueous catalysts for CO_2/HCO_2^- redox flow batteries

- Electrochemical CO_2 capture and concentration
- Combined CO_2 capture and conversion



Prof. Jenny Yang, Chemistry



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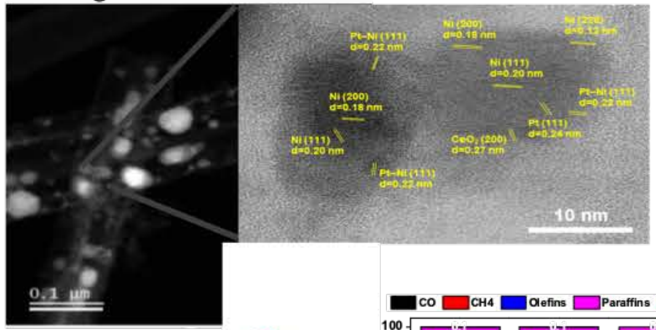
Heterogenous Catalysis for Net-Zero Carbon Reduction

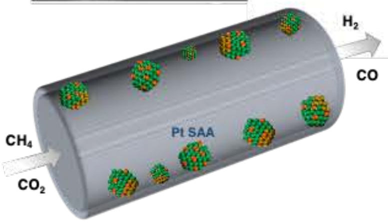
Erdem Sasmaz
Chemical and Biomolecular Engineering

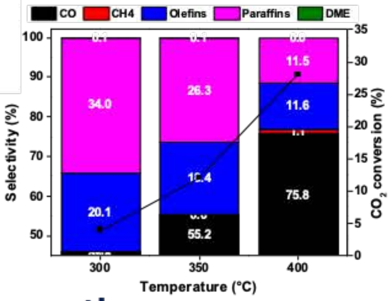
Motivation : Develop sustainable technologies to decarbonize the transportation and manufacturing sectors

CO_2 reduction to value-added chemicals

Confined yolk-shell morphologies
Pt-Ni single atom alloy catalysts



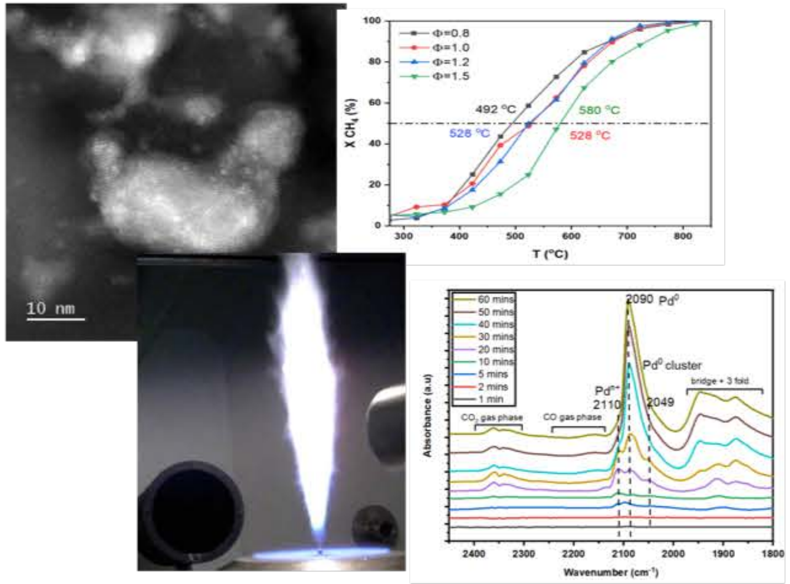




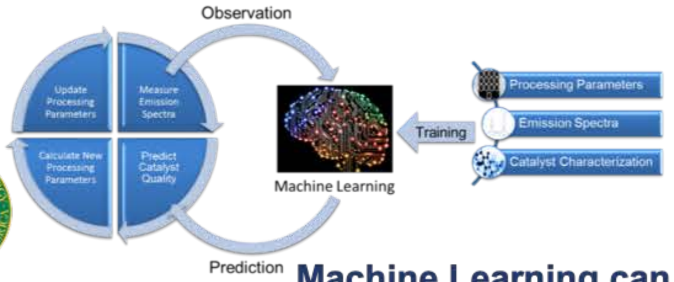
- **Minimized coke formation**
- **Enhanced oxygen transfer**
- **Improved reaction kinetics**

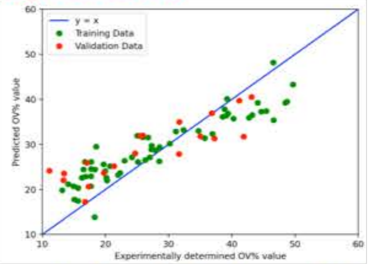
Control of Methane Emissions

634 MM ton CO_2 equivalent in 2018



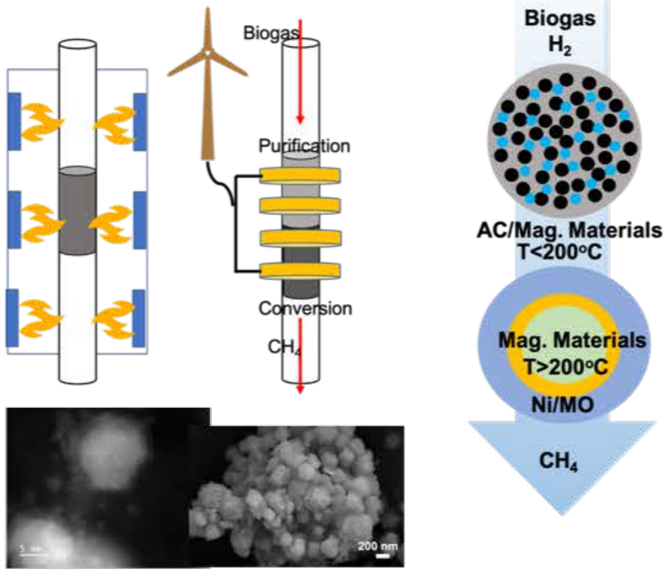
Automated nanomaterial synthesis





Machine Learning can predict catalyst quality.

Biogas Conversion and Sustainable Hydrogen Production



Novel ferromagnetic materials for radio frequency heating

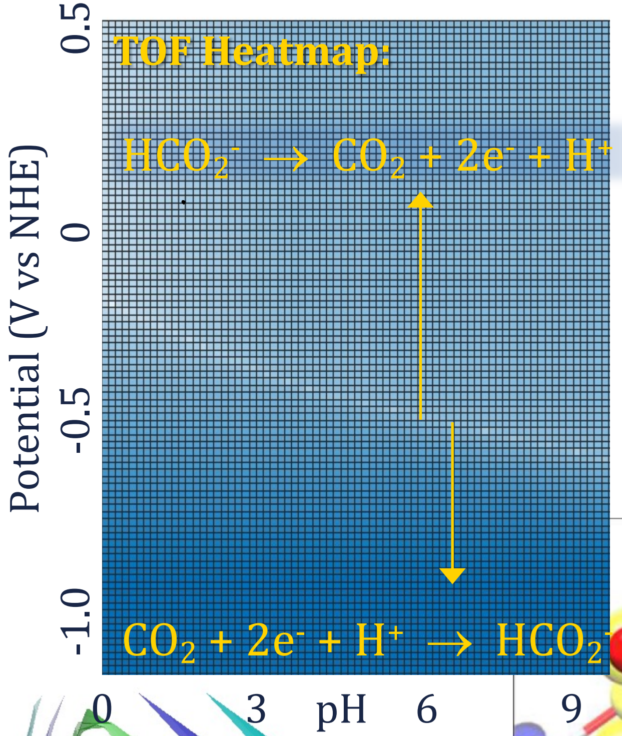
- Direct use of renewable sources for energy production
- Up to 90% energy efficiency
- Instantaneous on/off switching
- Elimination of hot-spots

Atomistic, kinetic and data modeling to understand and control reactivity

Electronic structure and mechanism
Structure-function relationships
Virtual experimentation
Materials design

Robert Nielsen

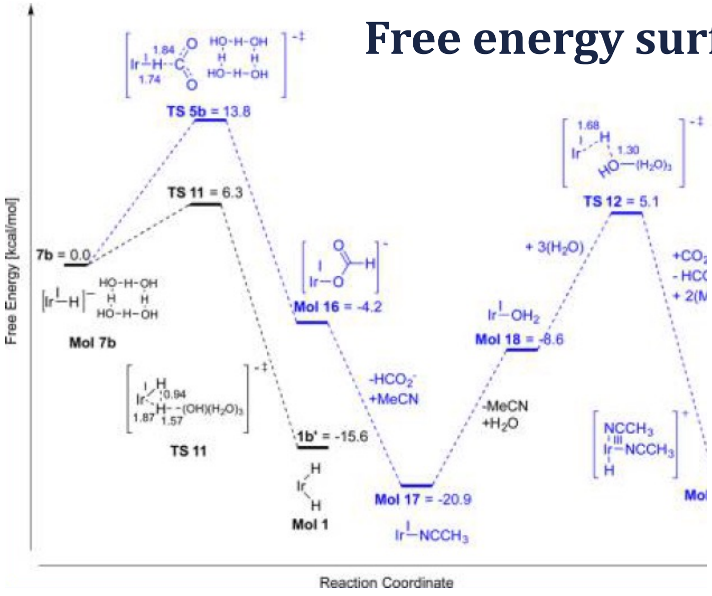
Assistant Professor, Chemical & Biomolecular Engineering

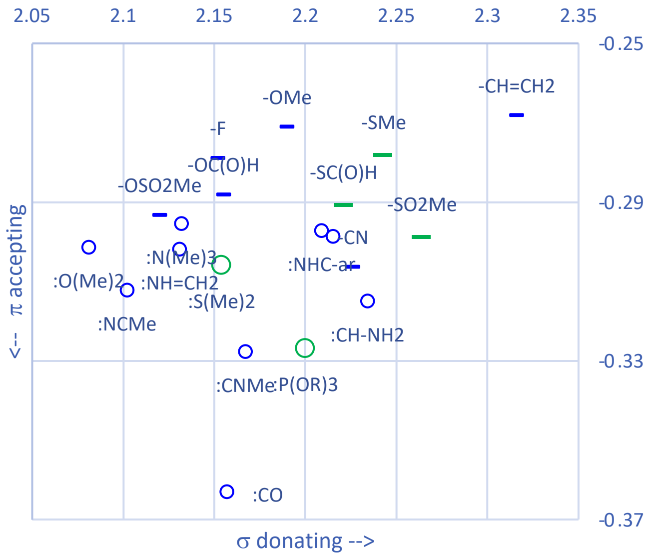


$$S_{\text{low-}\eta} = \left[\frac{k_{1\to 3}[CO_2]}{k_{1\to 6}[TFEH]^2}\right]\frac{k_{3'\to 5}K_{3/3'}[TFEH]}{k_{3\to 1}\frac{[F_3CCH_2OCO_2^-]}{[TFEH][CO_2]}} = \left[\frac{k_{1\to 3}k_{3'\to 5}K_{3/3'}}{k_{1\to 6}k_{3\to 1}}\right]\frac{[CO_2]^2}{[F_3CCH_2OCO_2^-]}$$

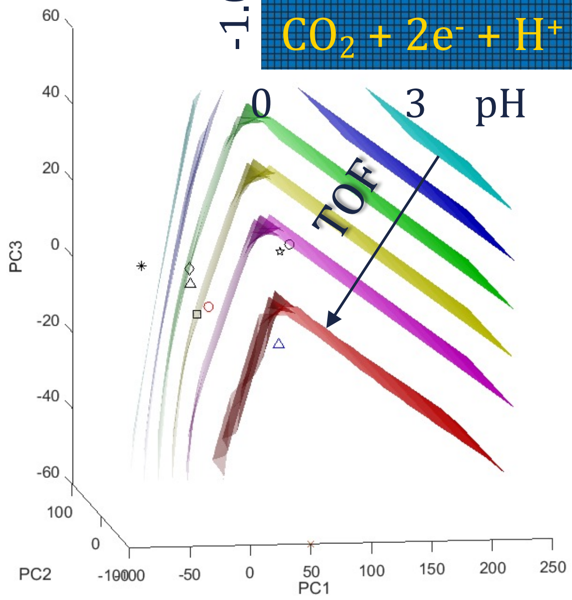
Activity and selectivities

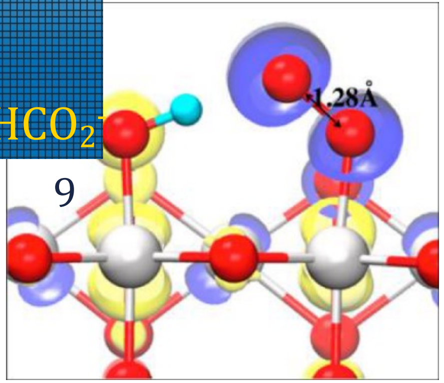
Free energy surfaces





Property descriptors





Electronic structure

Multidimensional composition-activity models

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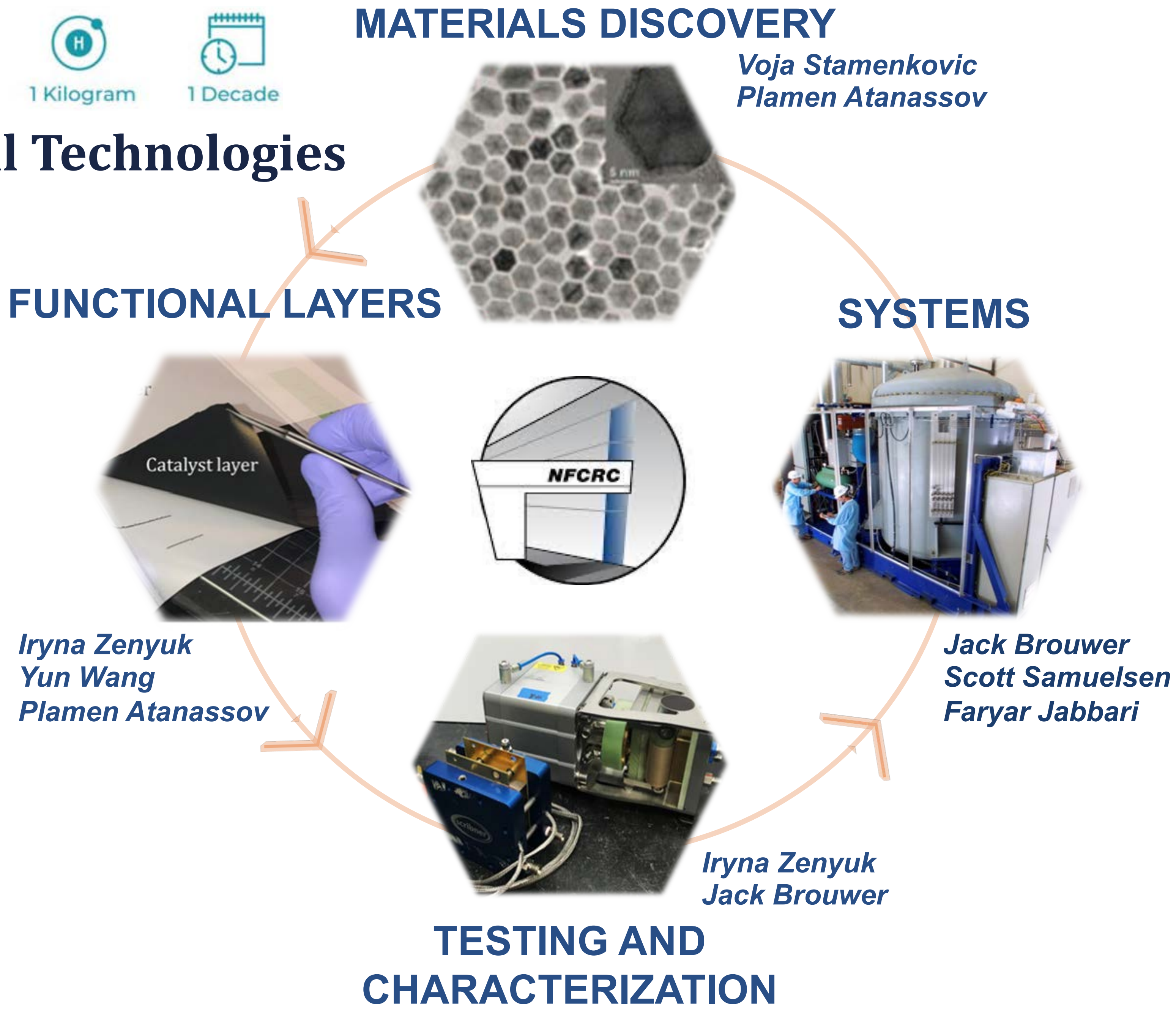
Energy Earthshots | Hydrogen

1 Dollar 1 Kilogram 1 Decade

Sub-Theme 1: Electrochemical Technologies
Fuel Cells and Electrolyzers

National Fuel Cell Research Center



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UCI Engagements with National Laboratories and Consortia in Hydrogen

MILLION MILE FUEL CELL TRUCK
U.S. DEPARTMENT OF ENERGY

Voja Stamenkovic
- Seed project from the consortia (contract for several years)

Plamen Atanassov
- Seed project from the consortia

Iryna Zenyuk
- Student sent to LANL (Jan 2022) for 1 year collaborative research (contract for 1 year)

HydroGEN
Advanced Water Splitting Materials

Shane Ardo
- $2.1M project with NREL, LBNL, SNL, LLNL

Iryna Zenyuk
- Manufacturing project with NEL Hydrogen, NREL, DeNora, ONRL

H2NEW
U.S. DEPARTMENT OF ENERGY

NREL Transforming ENERGY · INL Idaho National Laboratory · Argonne National Laboratory · Berkeley Lab · Lawrence Livermore National Laboratory · Los Alamos National Laboratory · NETL National Energy Technology Laboratory · Oak Ridge National Laboratory · Pacific Northwest · Energy Efficiency & Renewable Energy Hydrogen and Fuel Cell Technologies Office

Jack Brouwer:
- Low temperature electrolysis advisory board member

Iryna Zenyuk:
- Joined consortia through seed funding as an academic partner
- Member of durability working group (20 members, 2 from academia)

NREL
NATIONAL RENEWABLE ENERGY LABORATORY

Jack Brouwer
- CRADA for regional power-to-gas design, implementation and TEA
- California Energy Commission funded disadvantaged community microgrid that includes hydrogen
- Nuclear hydrogen recent award including INL

Sandia National Laboratories

Plamen Atanassov
- Electrochemical ammonia synthesis

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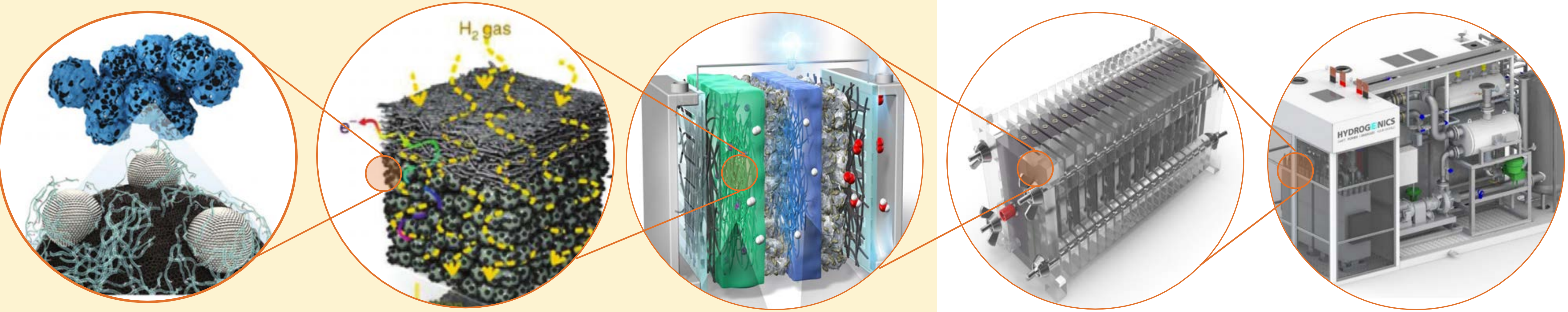
Big Questions to Solve in Hydrogen

Electrocatalyst	Catalyst layer	Cell level	Stack	Plant
10 nm	10 µm	1 cm	1 m	10 m



Fundamentals

Demonstration projects and system- level studies

- Fundamental science and engineering challenges are from nm- scale to cm-scale
- Complex scale-coupled transport and reaction kinetics problems

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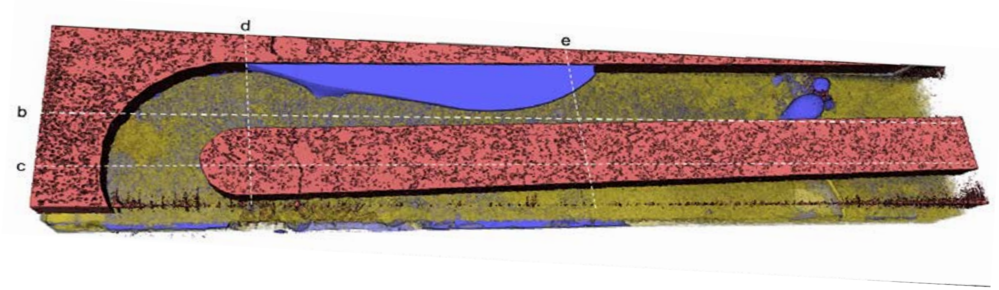
Zenyuk Group at UCI

- 7 Ph.D. students, 2 postdocs, 8 undergraduate
- 50 % fundamental and 50 % applied



Electrochemical characterization
Materials, set-up manufacturing
X-ray CT and other imaging
Multi-physics modeling

Fuel cells

Polymer electrolyte
Alkaline

TOYOTA, NSF, BOSCH, U.S. DEPARTMENT OF ENERGY, ONR, IRD, SUMITOMO ELECTRIC

Fundamentals

Heat transfer
Mass transport
Porous media
Reaction kinetics
Electrokinetics at interfaces

Electrolyzers

Oxygen evolution on anode
PTL design
Cement manufacturing

U.S. DEPARTMENT OF ENERGY, NSF, UCI

NSF

CAREER

Batteries

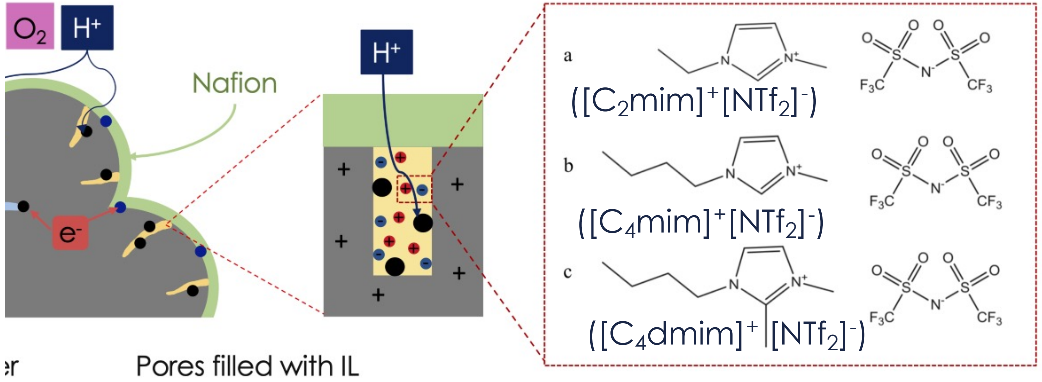
Solid polymer electrolyte

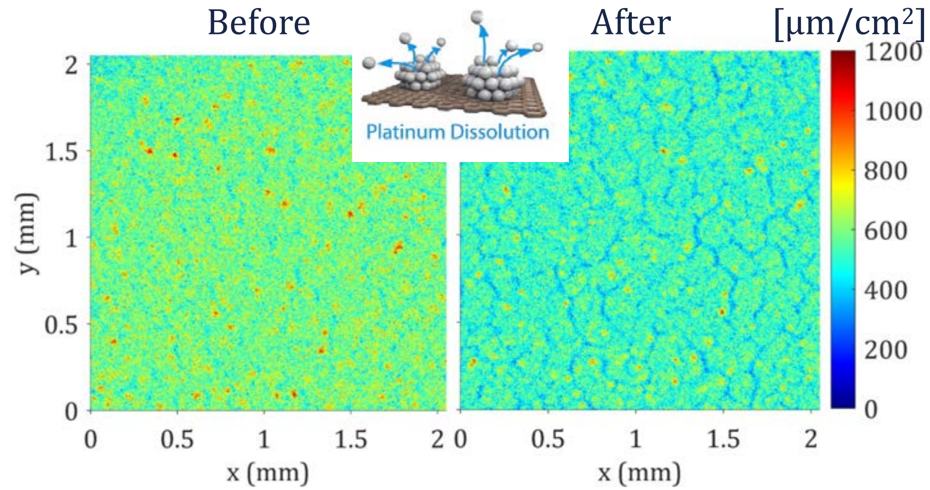
arpa·e CHANGING WHAT'S POSSIBLE

Alfred P. Sloan FOUNDATION

Activity and Durability of PEM fuel cells and Electrolyzers

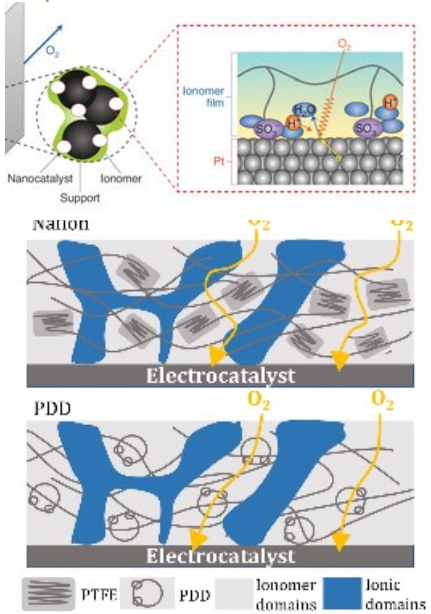
Iryna Zenyuk
Chemical and
Biomolecular
Engineering

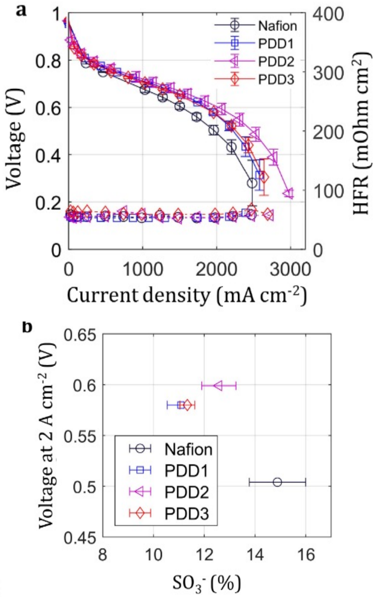


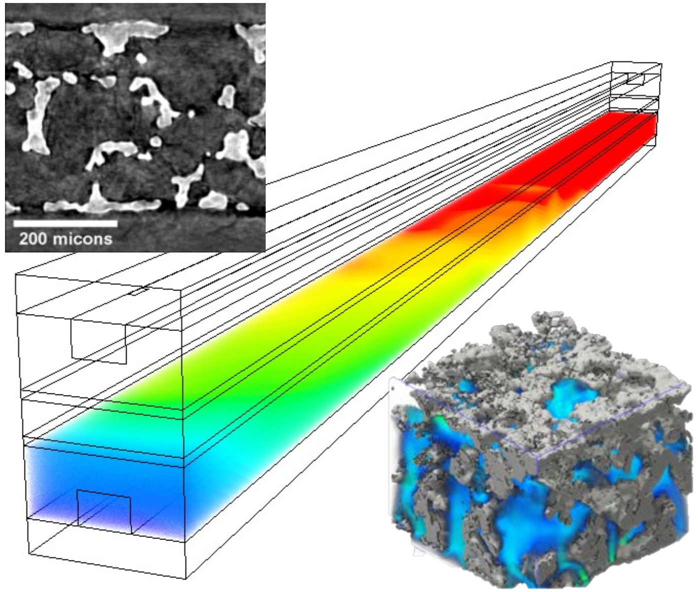


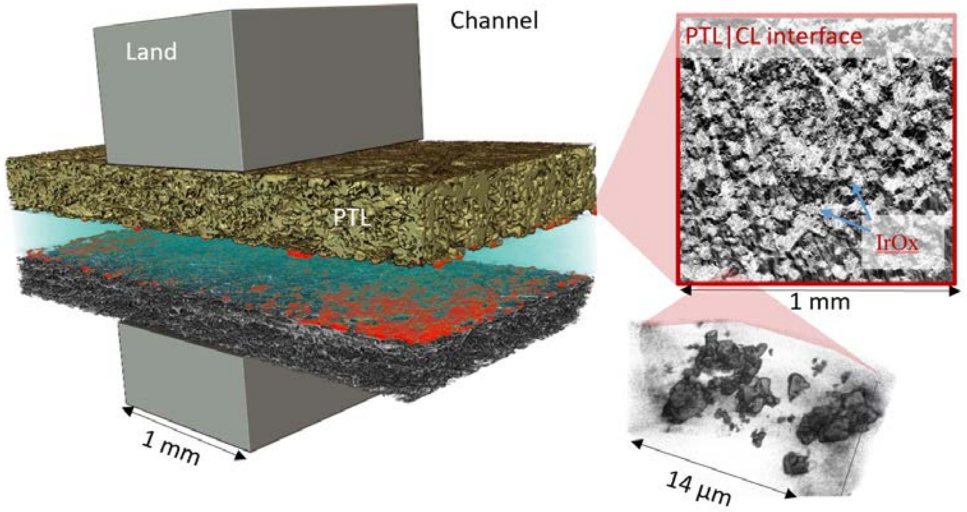
Transport in micro/meso – pores in catalyst layers

Pt catalyst degradation in catalyst layers









Ionomer- Pt interface

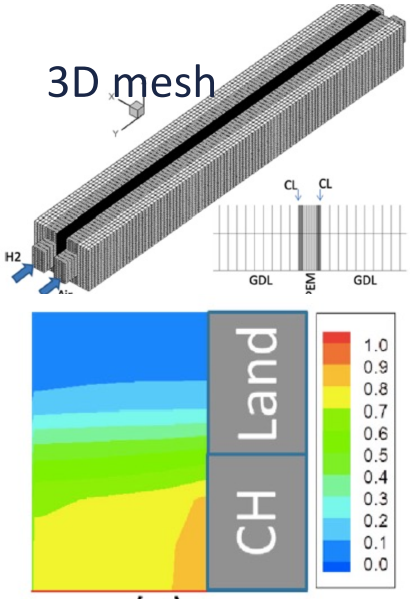
Novel flow-fields

Transport in Electrolyzers

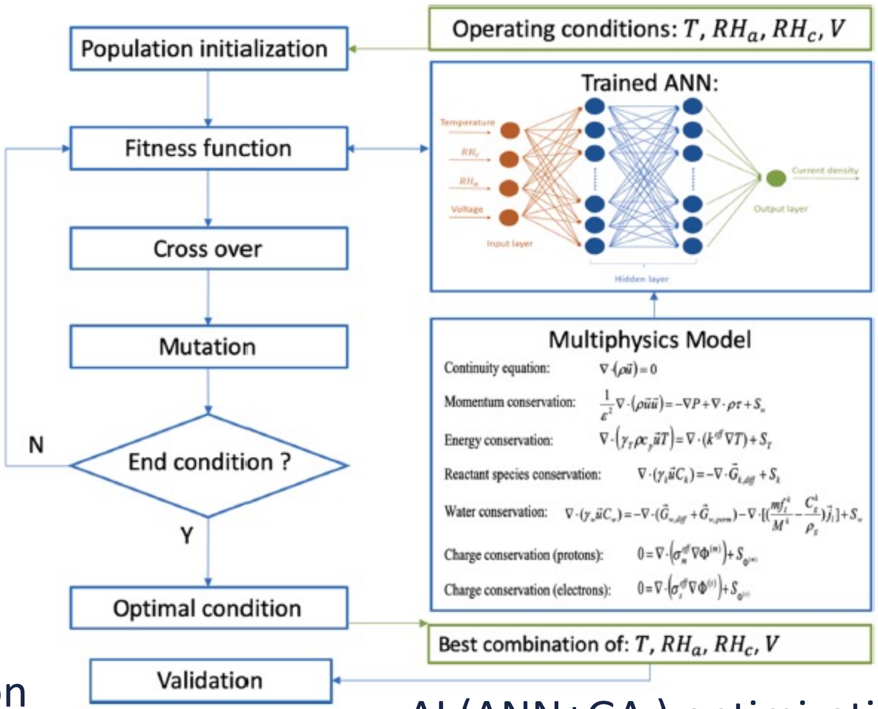
Fundamental Modeling of PEM Fuel Cell/Electrolyzer

Yun Wang
Department of Mechanical and Aerospace Engineering

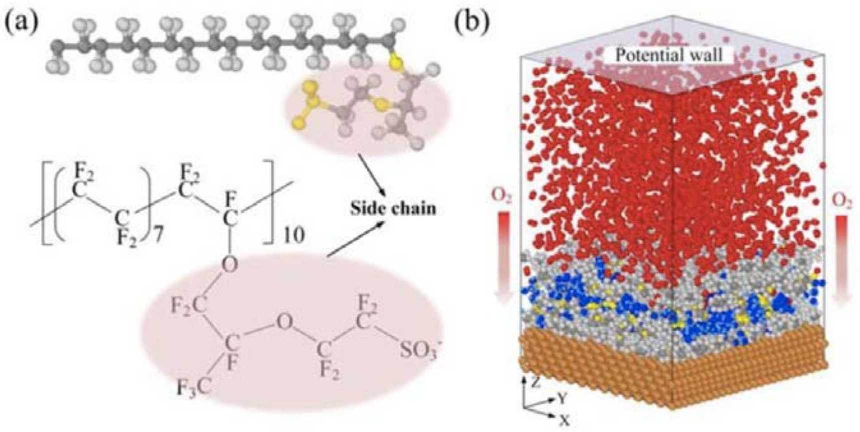
3D modeling of PEM fuel cell/electrolyzer, including catalyst layers, membrane, GDLs, and BPs;
Theories of two-phase flows in porous media/flow channels, heat transfer, dynamics, cold start, and reaction rate distribution;
Machine learning methods for fuel cells and materials/operational optimization;
MD simulation of O2 transport in ionomer thin film.



Water distribution



AI (ANN+GA) optimization



MD simulation

Impacts:

- **Optimize material/design/operation;**
- **Optimize cell dynamic control;**
- **Obtain 3D operating conditions inside a cell during operations (e.g. cold start);**
- **Define/quantify key limiting factors.**

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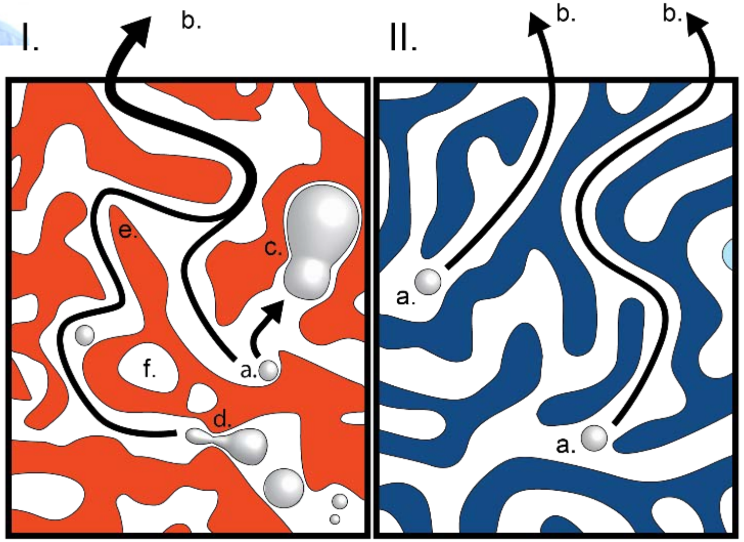
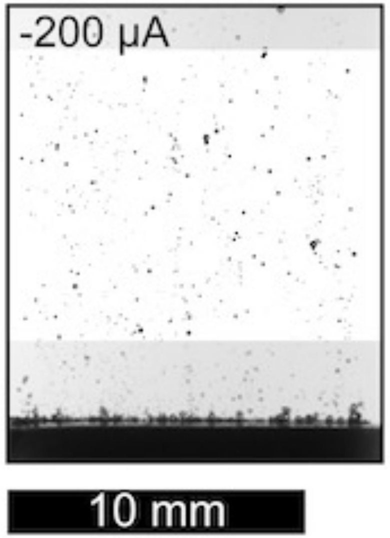
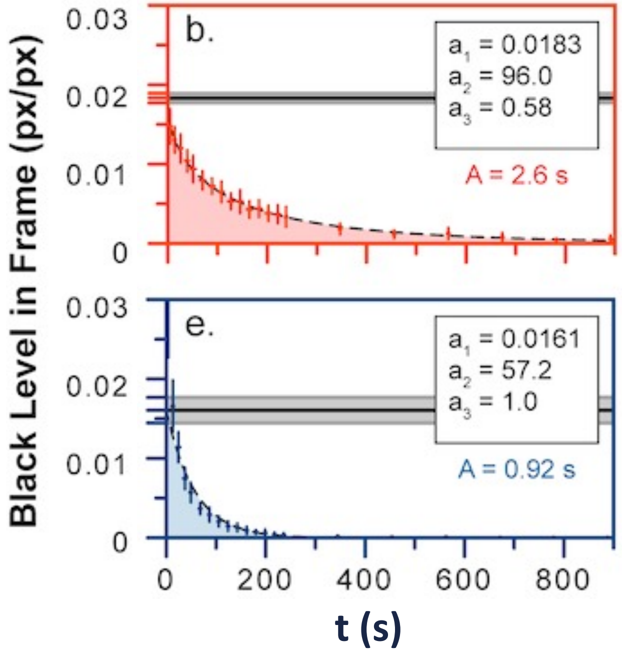
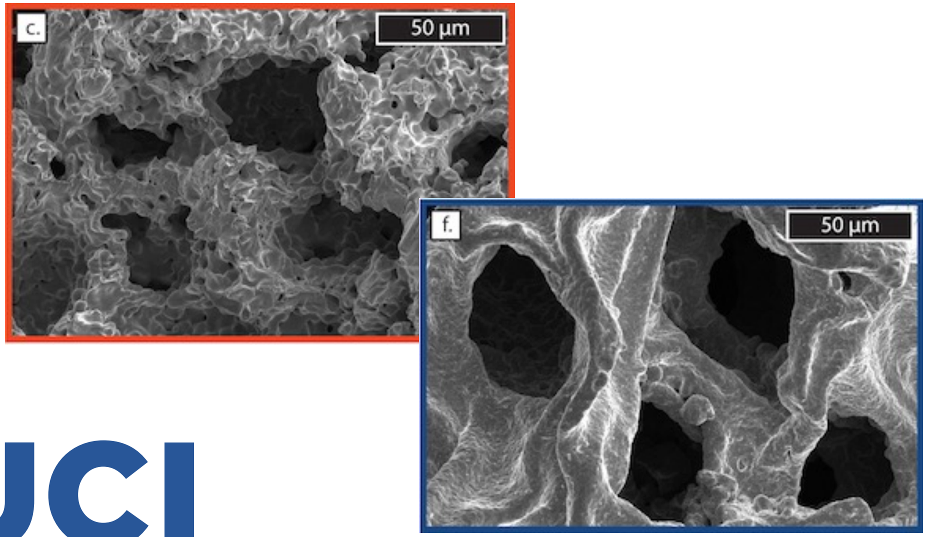
Improving the Performance of Electrolyzers via Microstructural Design

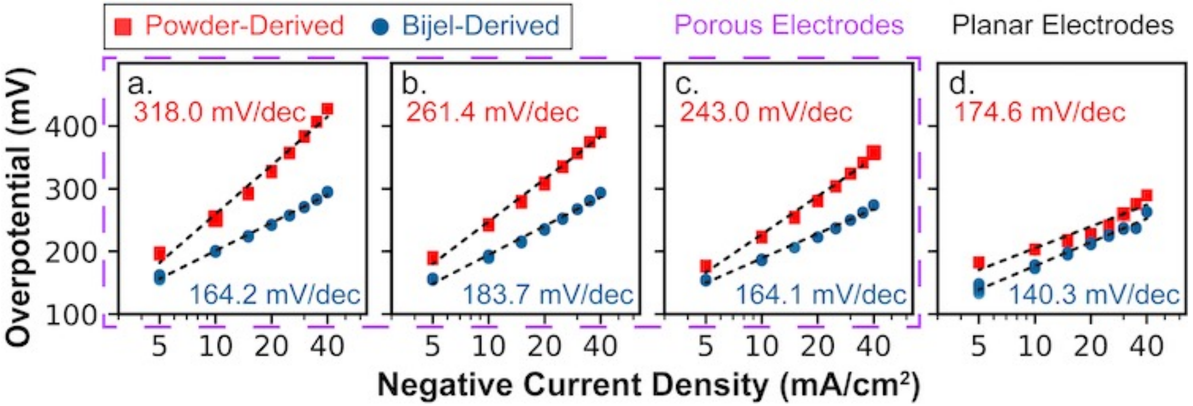
Ali Mohraz (CBE) and Daniel R. Mumm (MSE)









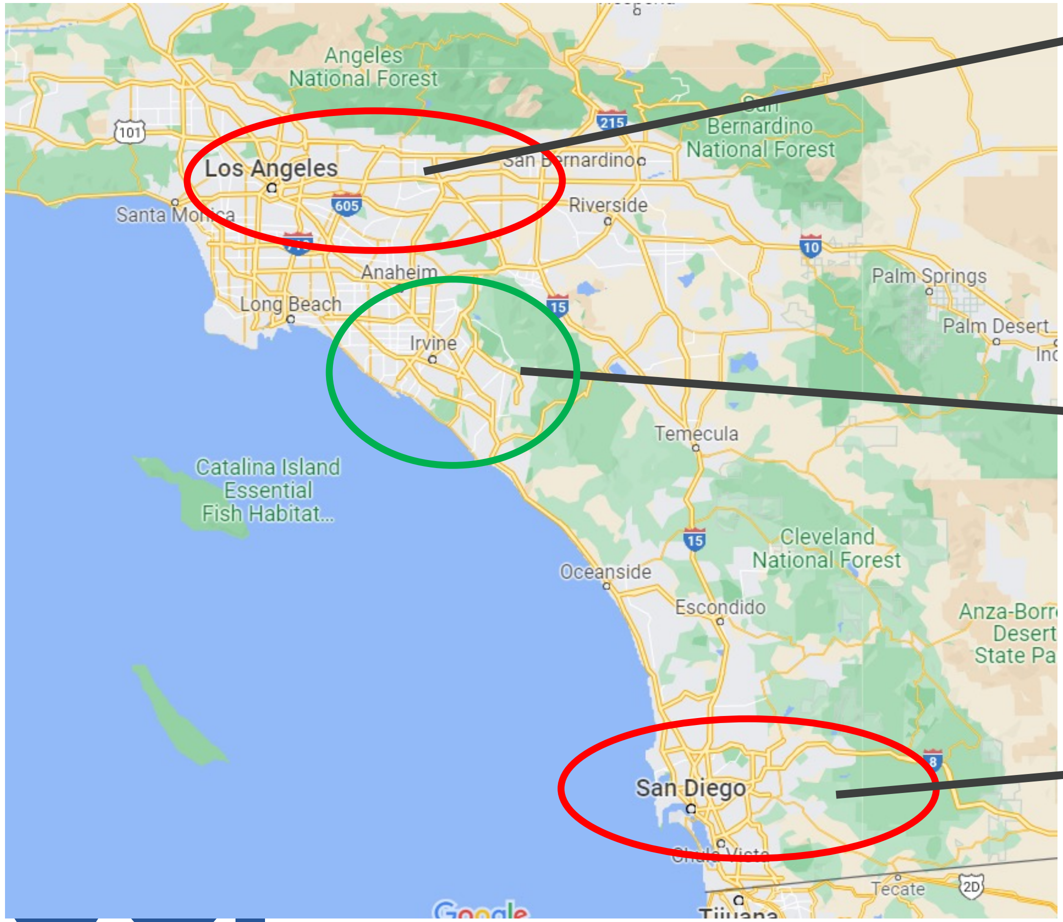


UCI

S.J. Gross, K.M. McDevitt, D.R. Mumm, A. Mohraz, *ACS Applied Materials and Interfaces* (2021)

Sub-Theme 1: Electrochemical Technologies
Batteries

Presenter: Huolin Xin, Associate Professor, Physics and Astronomy, School of Physical Sciences



UCLA and Caltech

BES funded EFRC: Synthetic Control Across Length-scales for Advancing Rechargeables

UCI

What's UCI's position in Energy Storage?

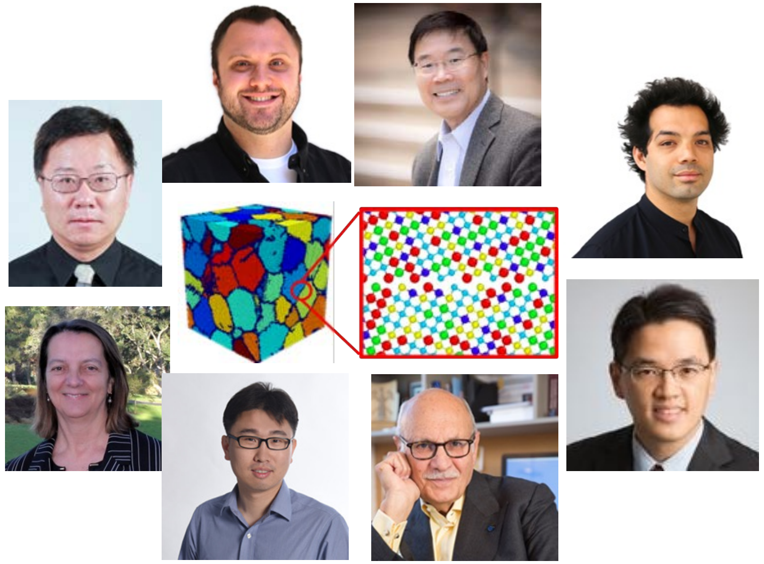
UCSD

EERE funded projects and involvement in BATT500, ReCell, etc.

A Unique Critical Mass, an NSF MRSEC Center on Complex Concentration Materials and Many Successful Battery Spinoffs

NSF funded CCAM IRG-1

- High-entropy oxide for energy storage, ionic conductivity
- Additive manufacturing

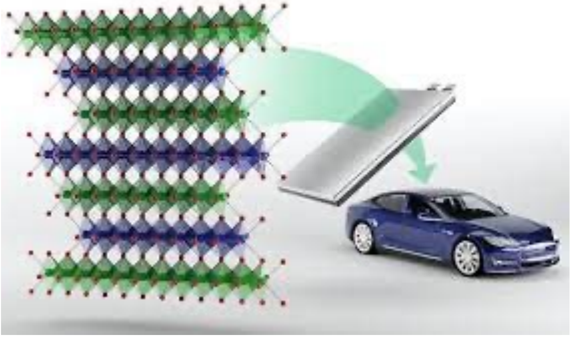


UCI https://ccam.uci.edu/

EERE VTO

No Cobalt Cathodes

$2.5 million



https://tinyurl.com/5ab3cya5

Solid-State Batteries

$5 million

https://ps.uci.edu/news/2531

Battery Startups

ENEVATE™

Prof. Marc Madou

A superstar startup in silicon anode batteries.

BATTERY **RESOURCERS**

Product offerings include:

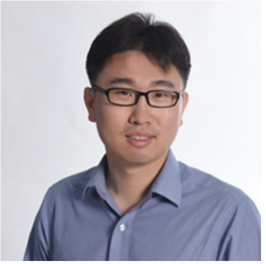
- NMC hydroxide and sintered cathode materials
  - Available in various metal ratios including: 111, 532, 622
  - Particle d50 available in both 5-6um and 10-12um
- Lithium Carbonate Li2CO3

Products currently under development include:

- High Nickel formulations including 811 and beyond
- Single Crystal Cathodes
- Battery Grade Graphite

The most successful Li-ion battery recycling startups

Prof. Diran Apelian

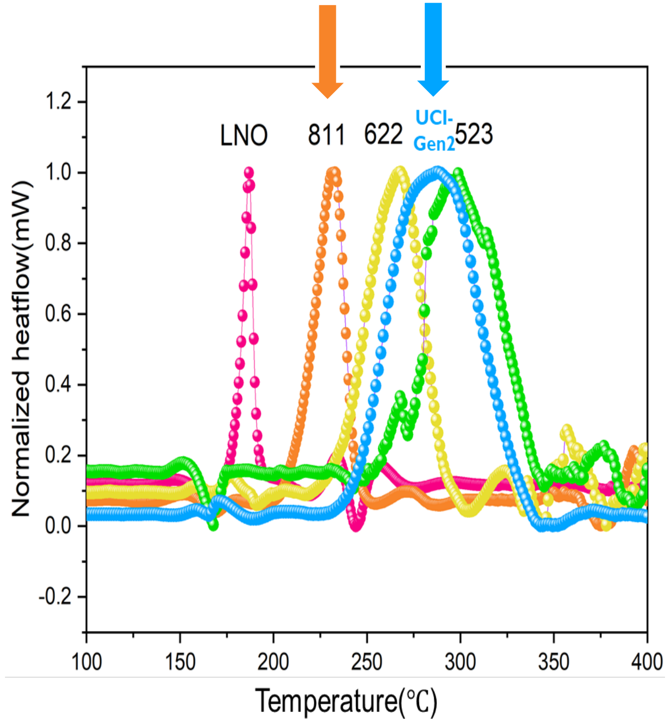


Patent-pending doping strategy enables Co-Free Cathode
Self-healing polymer electrolytes for solid-state Li^0 batteries

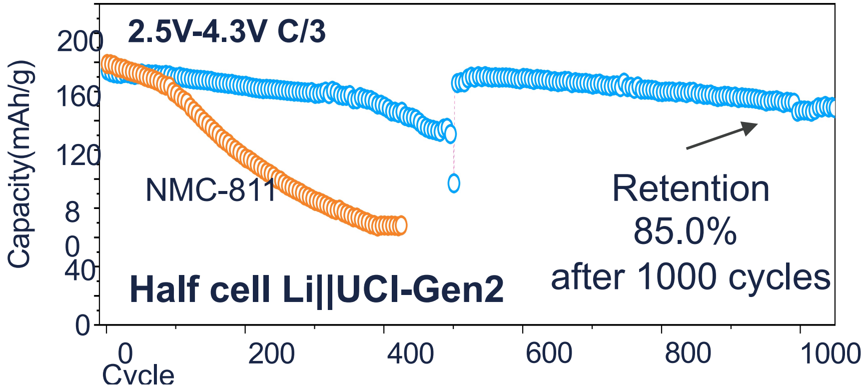
Huolin Xin
Dept of Physics and Astronomy

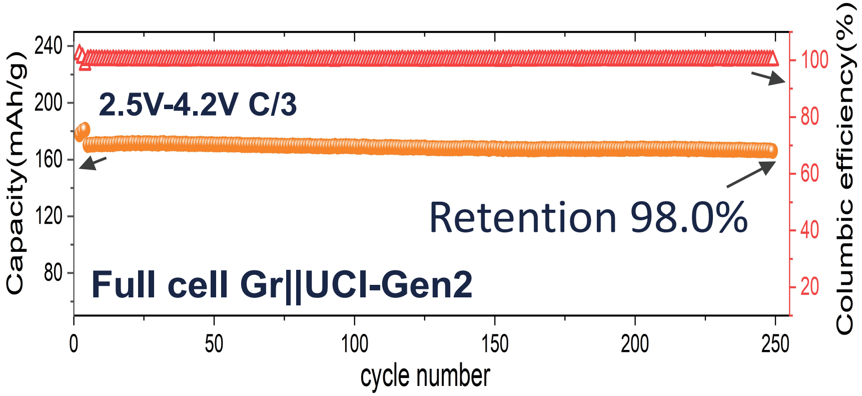
Cathode

Outstanding Thermal Stability



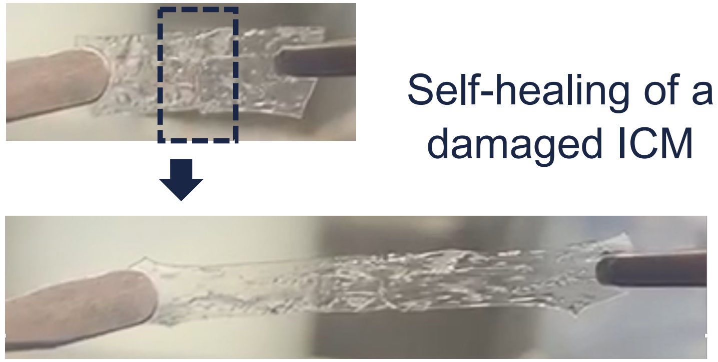
Excellent cycling performance





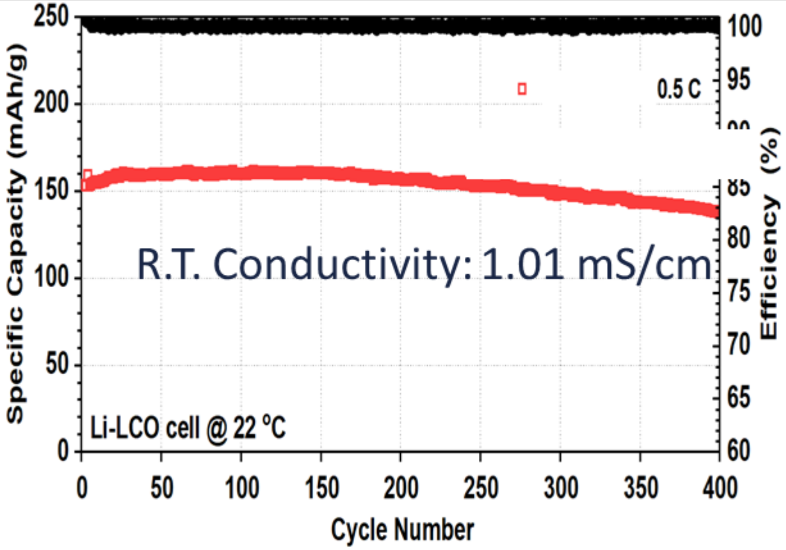
Solid Polymer Electrolyte

Self-heating and elastic:



Self-healing of a damaged ICM

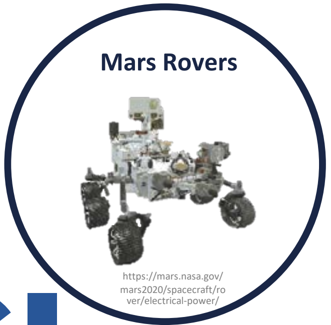
Long cycle life in Li||LCO cells at RT

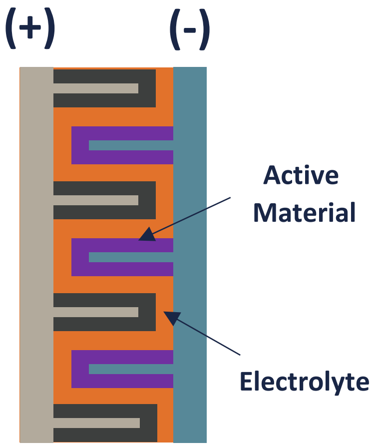


- PR and cost: cobalt free
- Safety: high thermal stability
- Performance: excellent cycle life that outperforms state-of-the-art

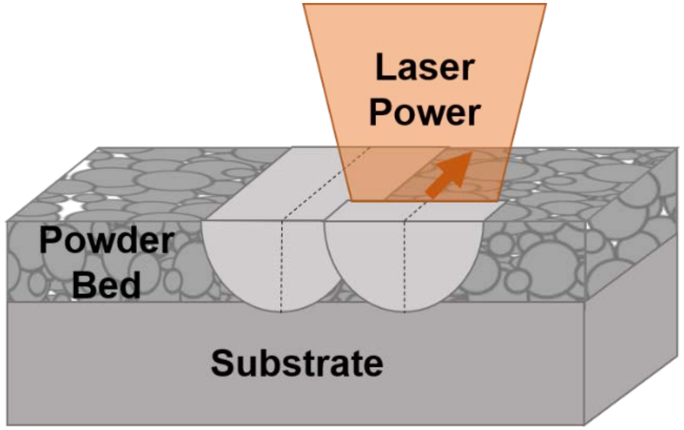
Binderless additive manufacturing of solid-state lithium-ion batteries

Julie M. Schoenung
Department of MSE





Recreated from Nanada, *et al., (2018) MRS Bulletin.*



Acord, et al. (2020) *J. Mater. Process. Technol.*

Successful 3D cathode prepared with laser powder bed fusion

Motivation

- PVDF is inactive
- Remove solvent from the manufacturing process

Impact:

- Binderless
- Complex geometry
- Multi-material printing

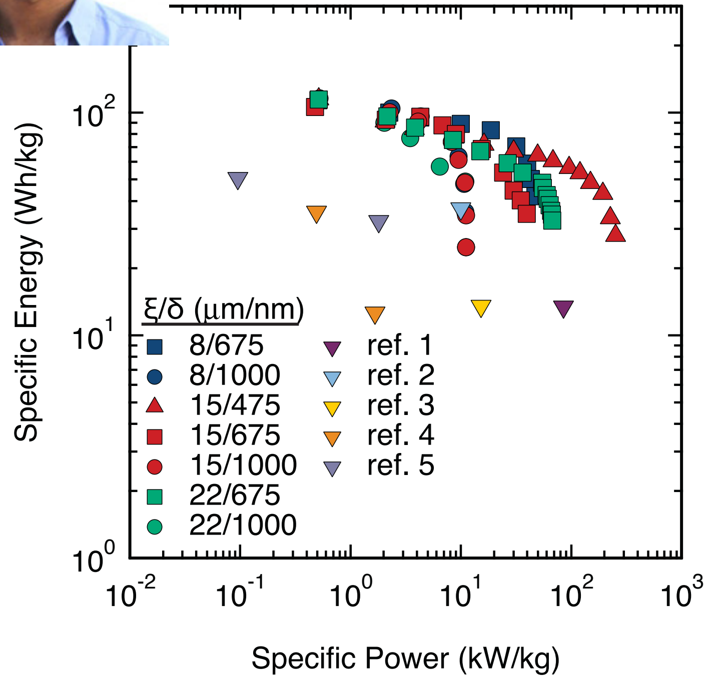
UCI

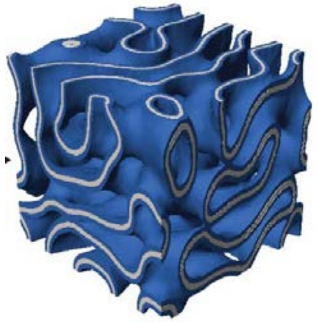
Micro-architected Electrodes for Improving Battery Performance

Ali Mohraz (CBE) and Daniel R. Mumm (MSE)

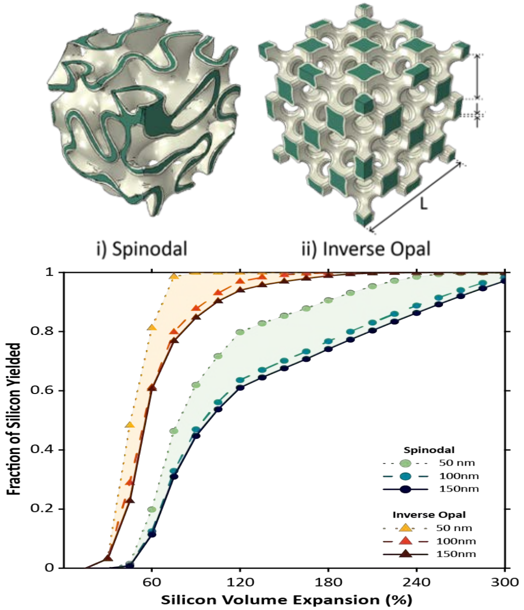
Energy- and Power-dense NiOOH Battery Electrodes

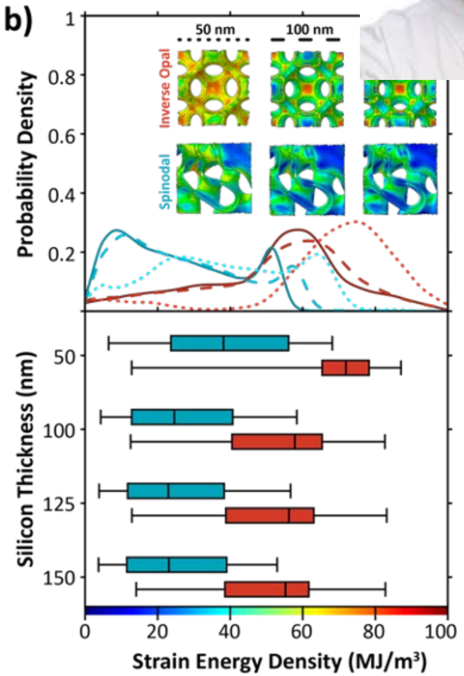
J. A. Witt, D. R. Mumm, A. Mohraz, *J. Materials Chemistry A* (2016)





Mechanics of Electrode Failure in Li-ion Batteries

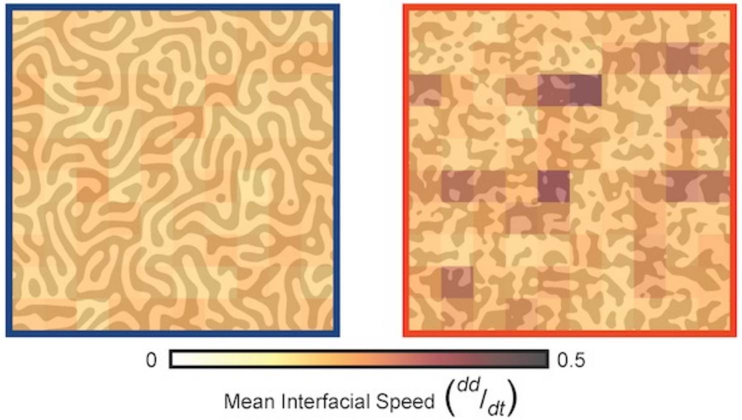


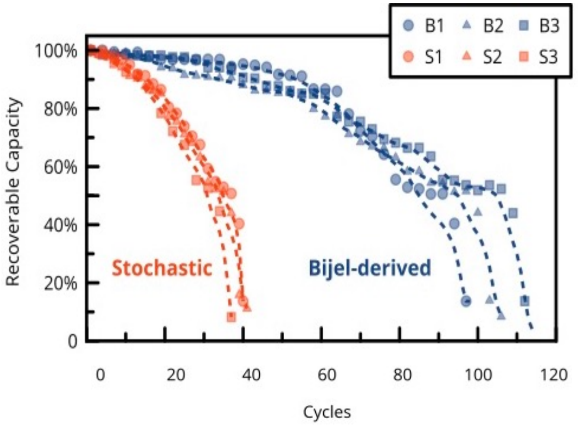


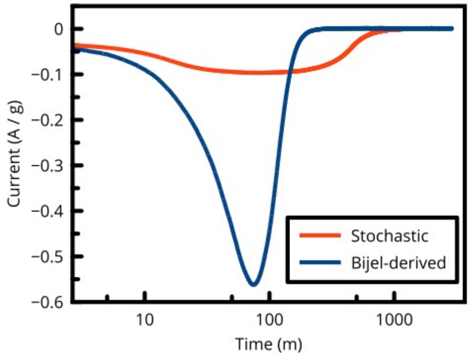
with Lorenzo Valdevit (MSE)

Improved Cycling in Zn-Air Battery Electrodes

K.M. McDevitt, D.R. Mumm, A. Mohraz, *ACS Applied Energy Materials* (2019)







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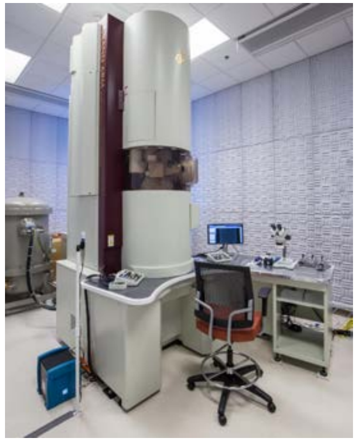
World-class facilities enables fundamental diagnostic studies

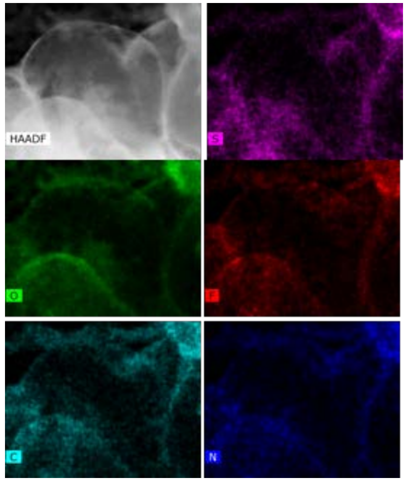
2 aberration-corrected S/TEMs

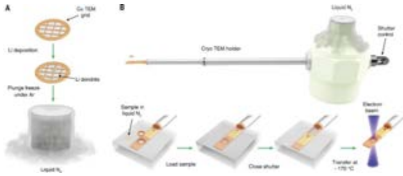
3 Cryo-EM instruments



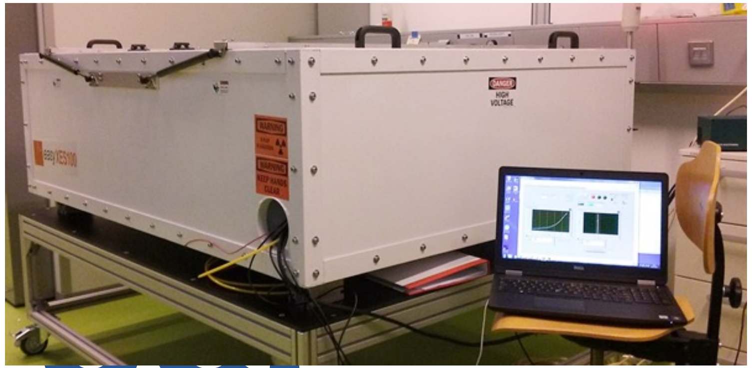


SEI Imaging



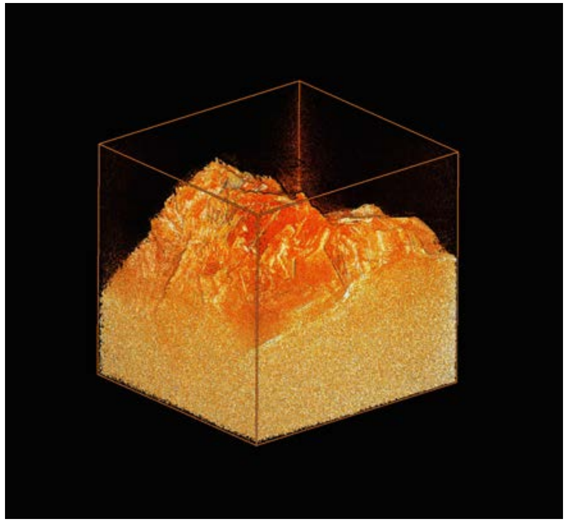
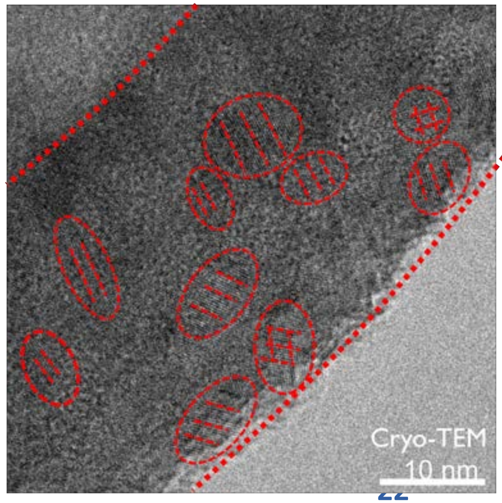


Benchtop X-ray absorption fine structure (XAFS) and X-ray emission spectrometer (XES)



ZEISS Xradia 410 Versa

Operando TXM Tomography

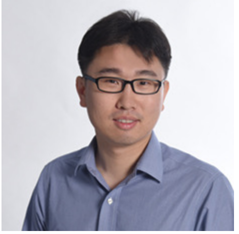



A critical mass is reached to pursue an EFRC

Ionic conductivity/solid electrolytes

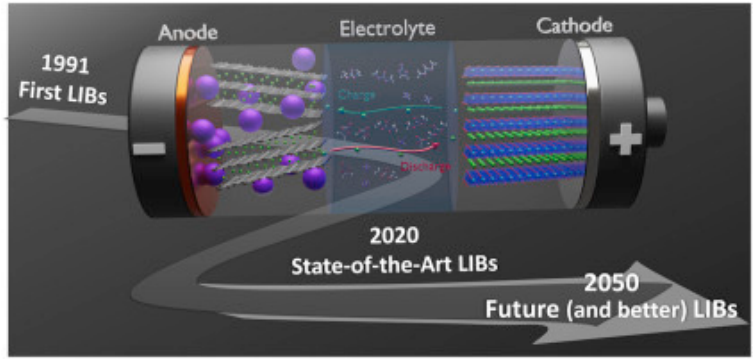



Cathode materials




Si, Li^0, and ultrafast-charging anode materials





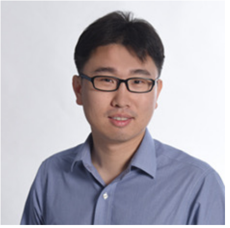
Recylcing and manufacturing


Diagnostics/Characterization





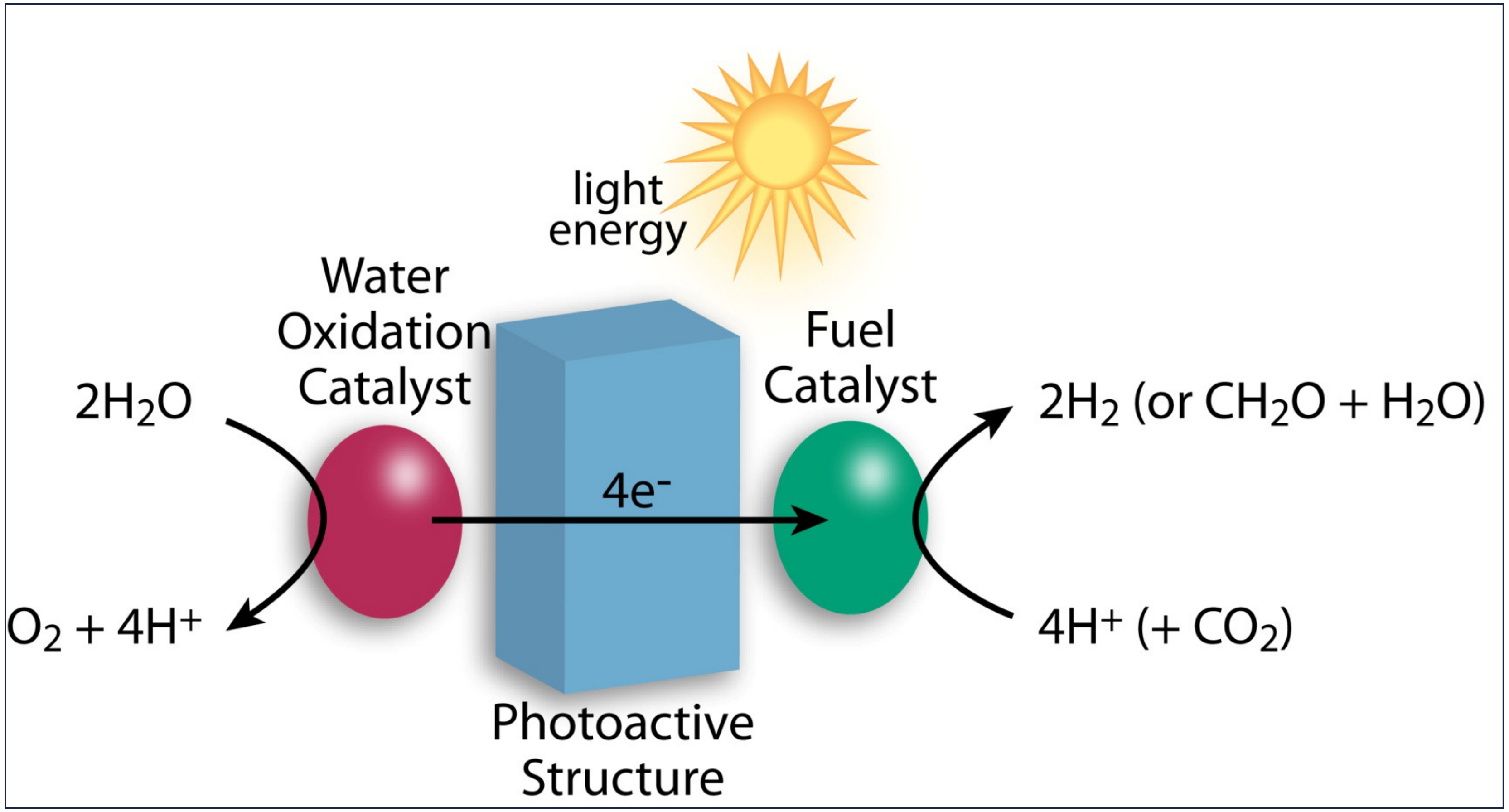
Beyond Li-ion batteries

UCI

Sub-Theme 1: Electrochemical Technologies
Solar Fuels and Electricity

Solar fuels (artificial photosynthesis): fuels from water, CO_2, and sunlight

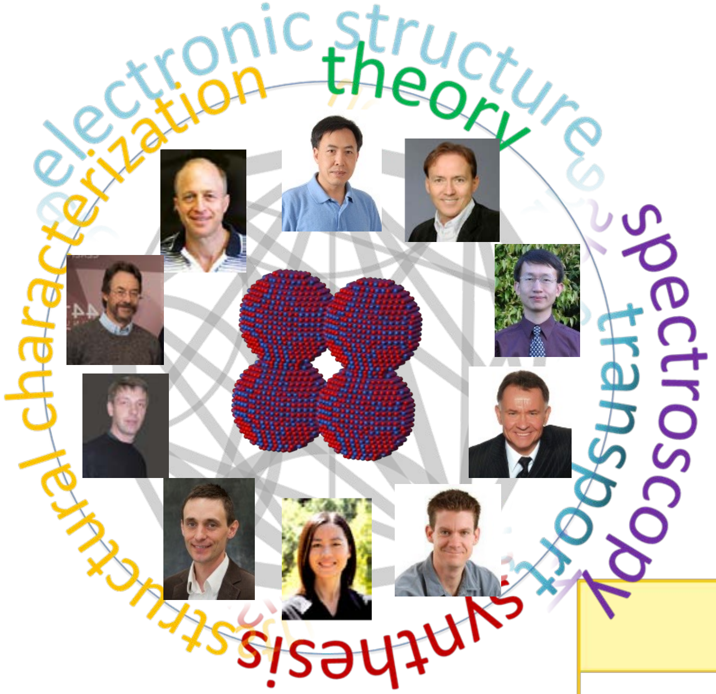


Adapted from Hurst, J. K. Science, 2010.

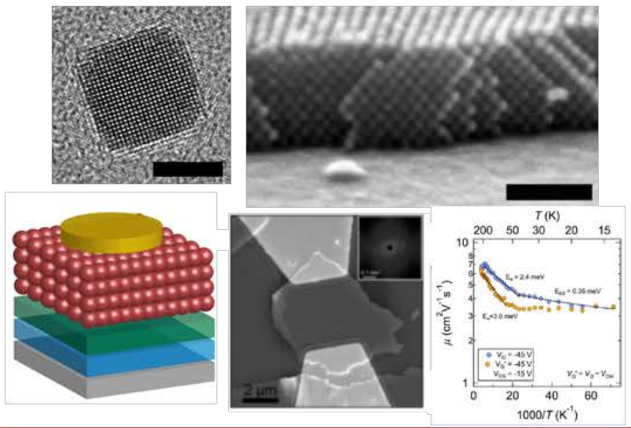
Law Research Group

Materials Chemistry for Solar Energy Conversion

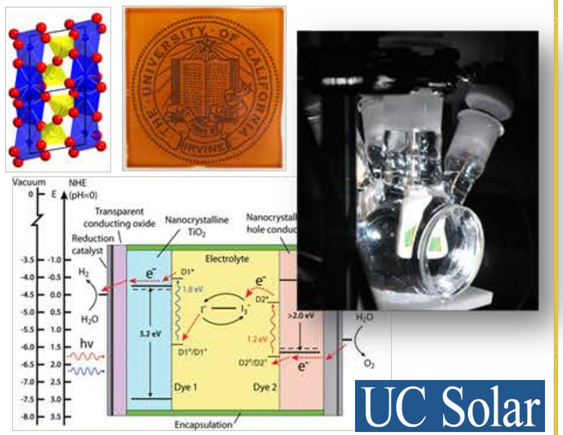
UC NATIONAL LABORATORY FEES RESEARCH PROGRAM



Quantum Dot Solids

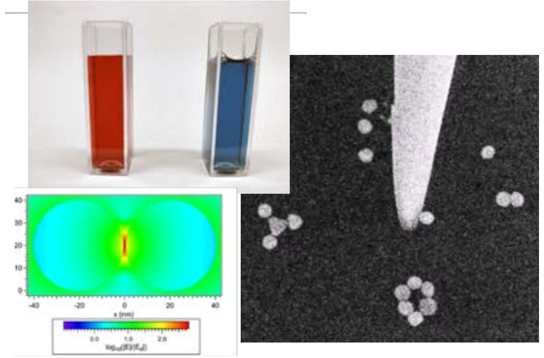


Solar Fuels



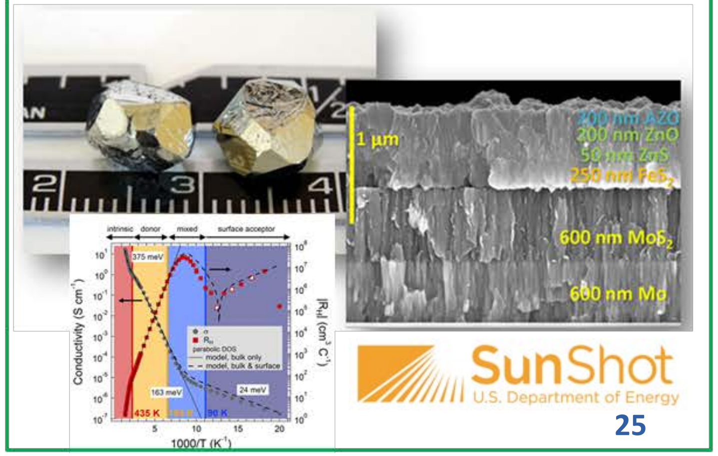
UC Solar

Plasmonics



CaSTL CENTER
Chemistry at the Space-Time Limit

Earth-Abundant Absorbers



SunShot
U.S. Department of Energy

Los Alamos
NATIONAL LABORATORY
EST. 1943

BERKELEY LAB

Cal

UC DAVIS

NIST

UCI

UCSD

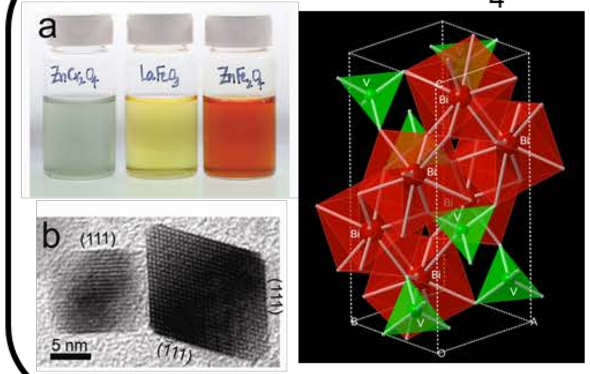
Photoanode Materials Development

Deep dives to understand the fundamentals of promising photoanode materials: $BiVO_4$, $Mn_2V_2O_7$, $FeWO_4$ …

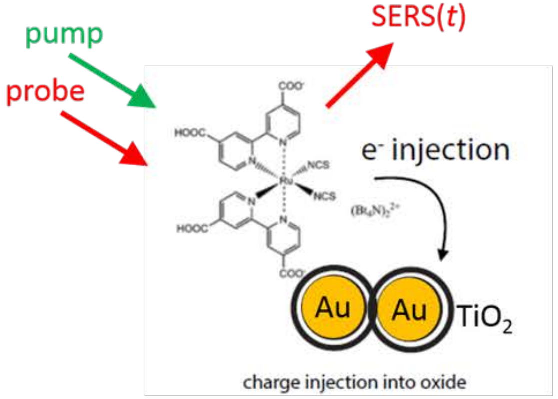
UC Solar

UCI

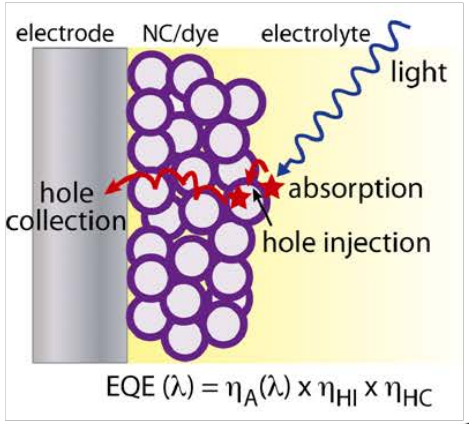
Materials Discovery



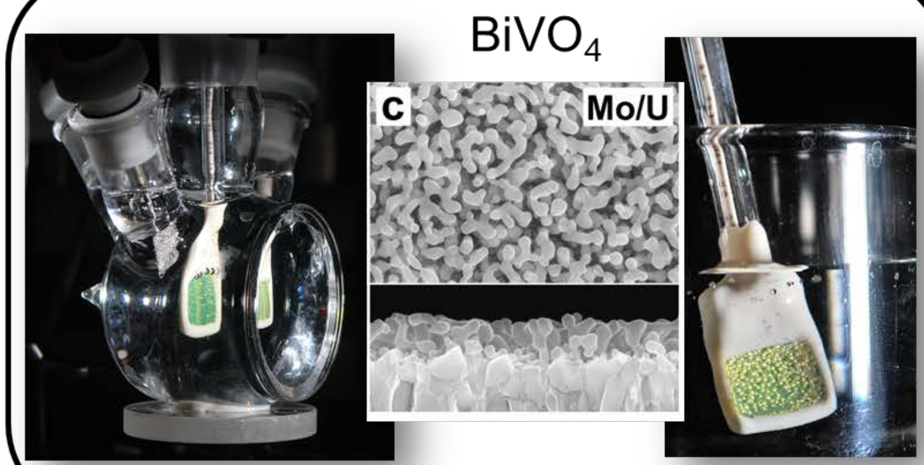
Charge Transfer



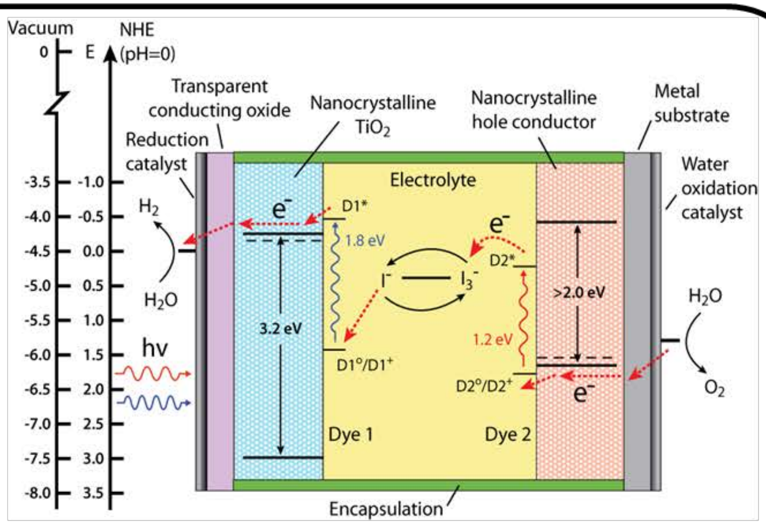
Transport



Photoelectrochemical Cells



Device Architectures



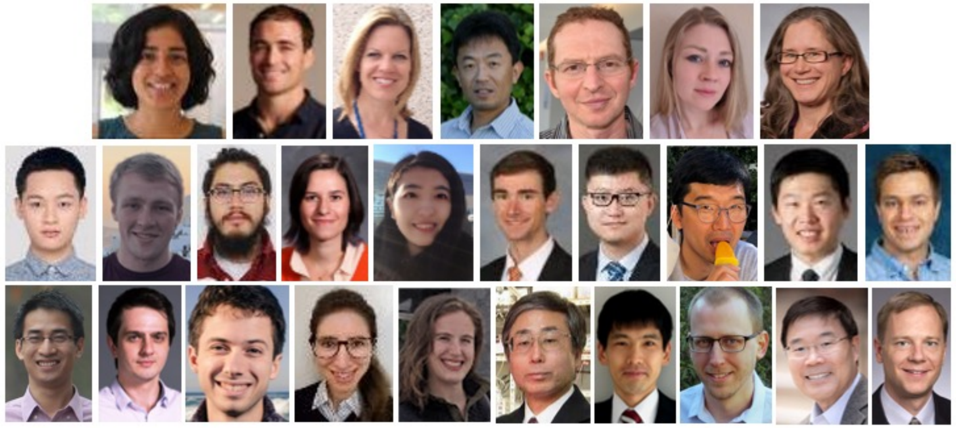
Energy Environ. Sci. 9, 1412 (2016).
Chem. Mater. 33, 7743 (2021).

Photocatalytic Solar Water Splitting

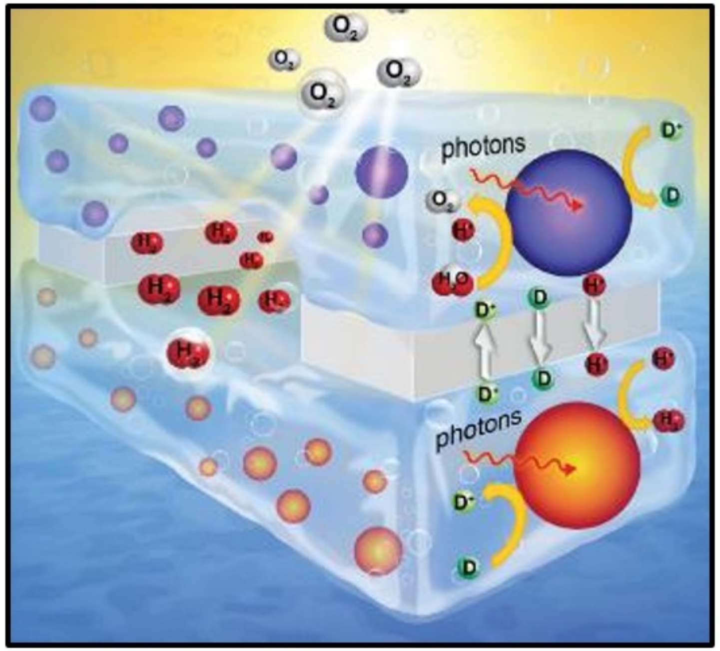
U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

HydroGEN Advanced Water Splitting Materials

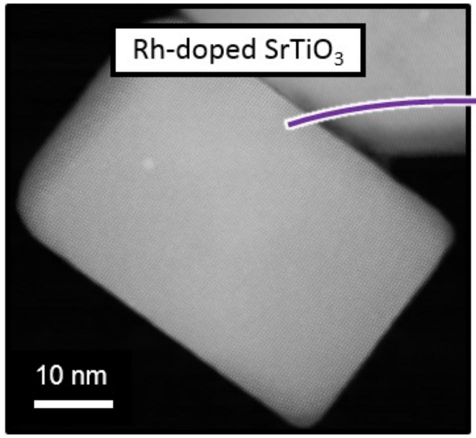
Energy Materials Network U.S. Department of Energy

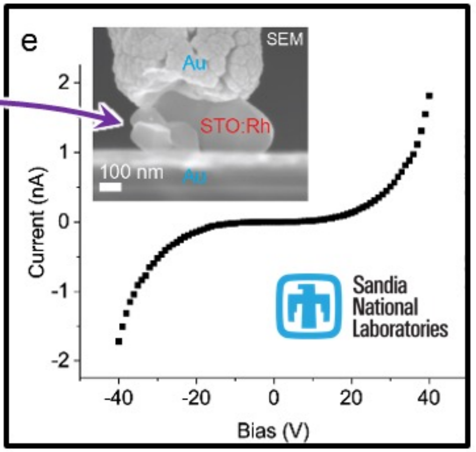


Columbia University · University of Michigan · Tokyo University of Science since 1881 · California Institute of Technology 1891 · Shinshu University Founded 1949 · NREL Transforming ENERGY · Lawrence Livermore National Laboratory · Sandia National Laboratories · BERKELEY LAB Bringing Science Solutions to the World · STRATEGIC ANALYSIS INC



- New reactor designs with inherent separation of product H_2/O_2
- Stacking enables more efficient tandem serial light absorption, and shorter distances for mass transfer
- Incomplete sunlight absorption per particle leads to larger theoretical efficiencies
- Reaction selectivity enabled by <10 nm oxide coatings





We routinely characterize dopant distributions and I-V characteristics of single composite nanoparticles

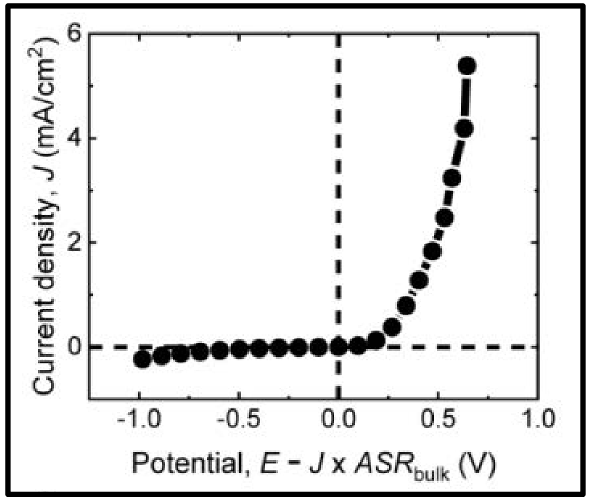
UCI

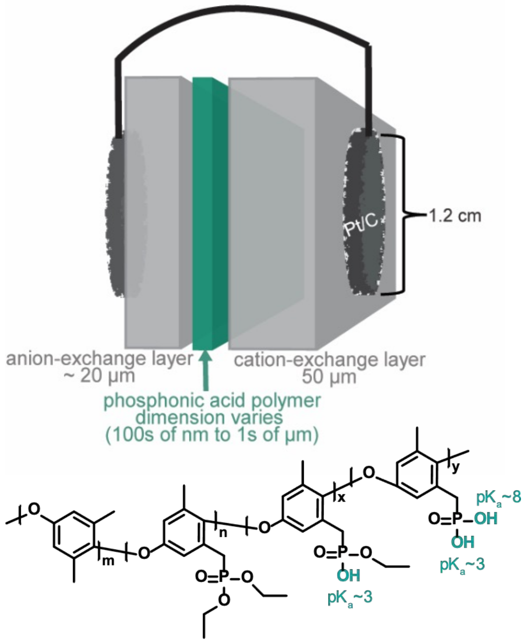
Ardo, Keene, Phun, *U.S. Patent*, 2019, US20200140293

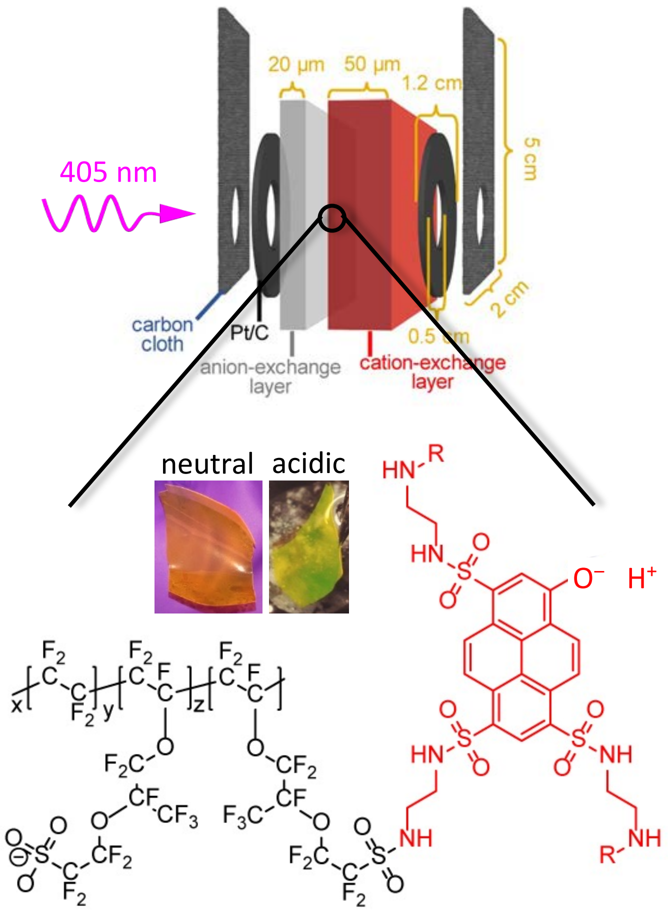
Ardo, et al., *Energy Environ. Sci.*, 2018, *11*, 115; *Energy Environ. Sci.*, 2018, *11*, 2768; *Energy Environ. Sci.*, 2019, *12*, 261

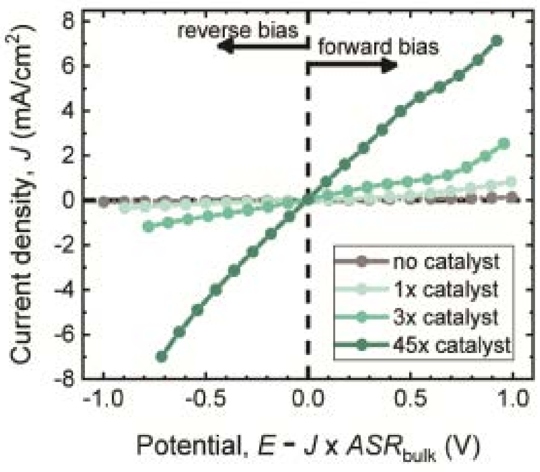
Bipolar Membranes as Diodes, Conductors & Solar Cells

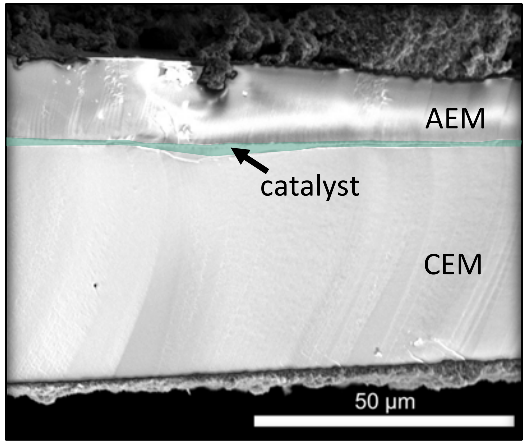
- Water is a protonic semiconductor
- **Polymer bipolar membranes** are inherently good protonic diodes
- Covalent modification of polymers with **recombination centers** results in conductive bipolar membranes
- Covalent modification of polymers with **reversible photoacid dyes** results in photovoltaic action











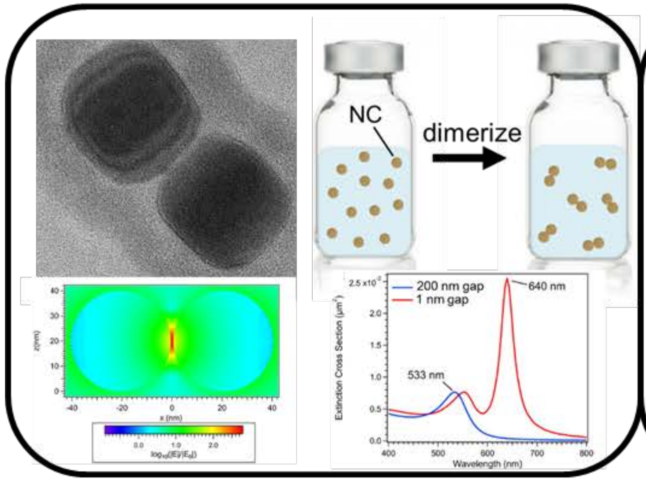
UCI

Ardo, Schwartz, Liu, Cardon, White, Tkacz, et al., *U.S. Patents*, 2018, US20180065095; 2019, US20190217255; 2020, US20210046423
Ardo, et al., *JACS*, 2017, *139*, 11726; *Joule*, 2018, *2*, 94; *Joule*, 2021, *5*, 2380; *Energy Environ. Sci.*, 2021, *14*, 4961

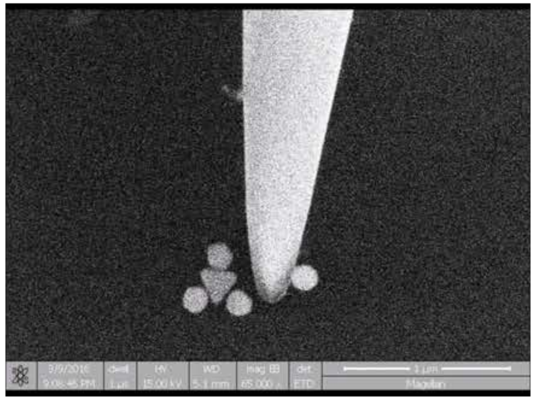
Plasmonic Photocatalysis

Precise plasmonic structures to study the mechanisms of plasmon-driven photocatalysis (*fields/hot carriers/heat*) for important reactions – H_2, NH_3, CO_2RRs

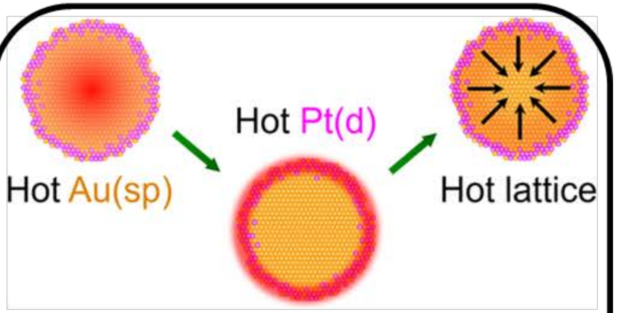
Plasmonic Dimers



Custom NC Assemblies

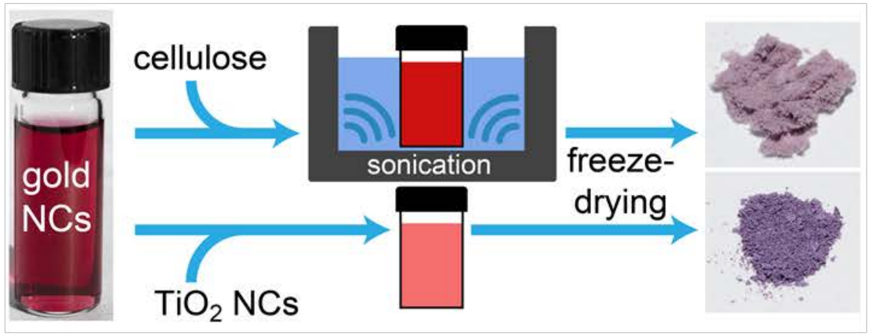


Photophysics



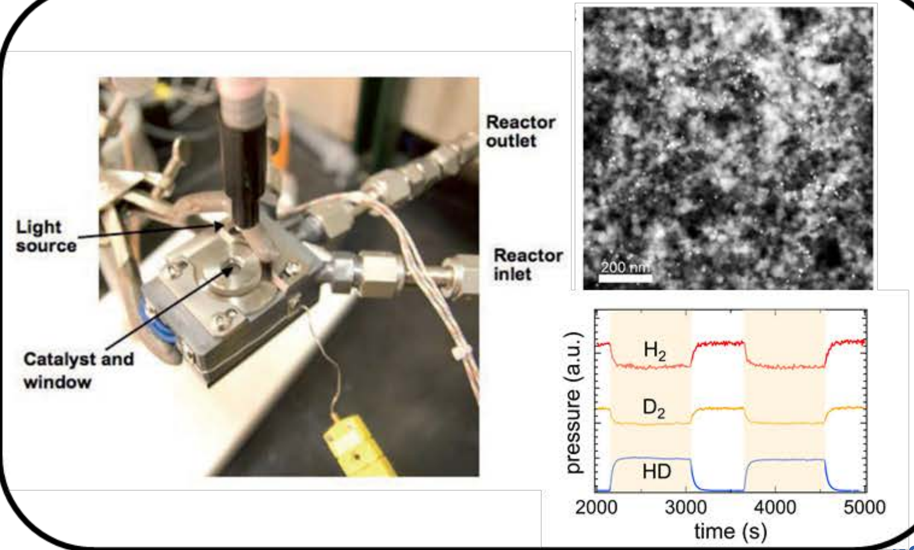
Efficient plasmon-mediated energy funneling to the surface of Au@Pt core-shell nanocrystals.
ACS Nano, **14**, 5061-5074 (2020).

Bulk Photocatalysts



Uniform supported metal nanocrystal catalysts prepared by slurry freeze-drying.
Yang, A. Y., Law, M. *Chem. Mater.*, **33**, 256-265 (2021).

Photocatalysis Studies



CaSTL CENTER
Chemistry at the Space-Time Limit
UCI
NSF

Sub-Theme 2: Nuclear Energy


Shen Dillon, MSE


Tim Rupert, MSE


Bill Evans, Chemistry


Athan Shaka, Chemistry


George Miller, Chemistry


John Keffer, TRIGA Reactor


Tro Babikian, TRIGA Reactor


Sarah Finkeldei, Chemistry

Nuclear Energy towards zero-Carbon Emission

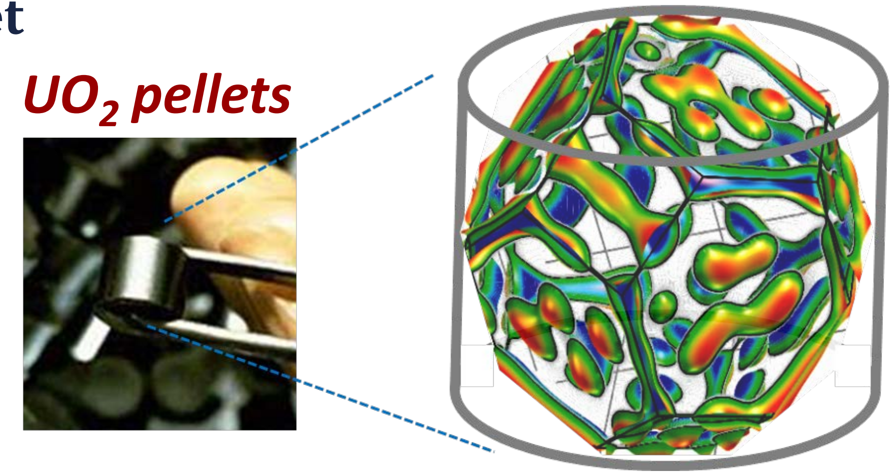
Sarah Finkeldei
Department of Chemistry

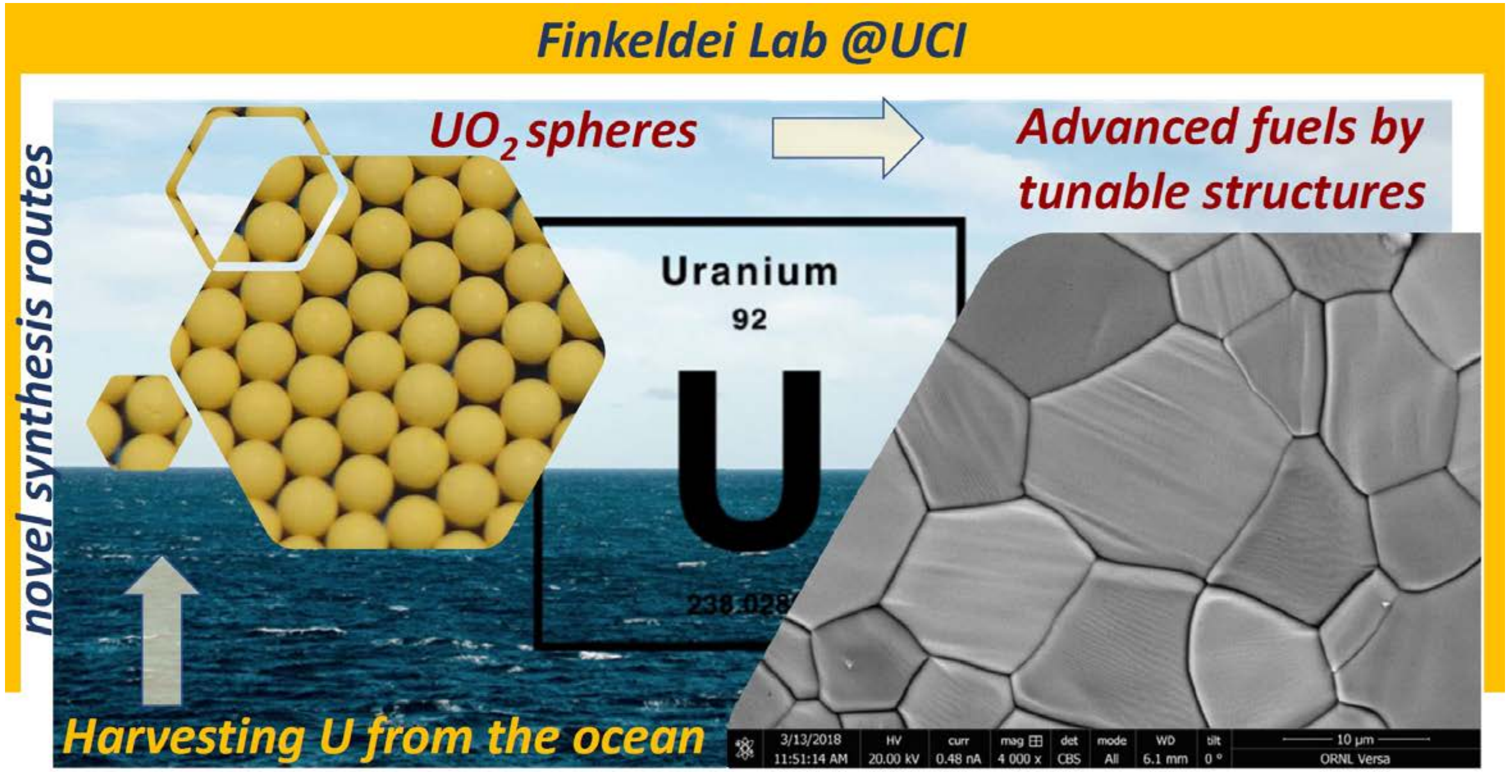
High energy density of nuclear fuel: 20% of U.S. electricity

Perpetual improvements of operating reactor fleet
(efficiency & safety)

Design of advanced reactor systems:
- **Small modular reactors**
- **Advanced fuel forms**

UO_2 pellets





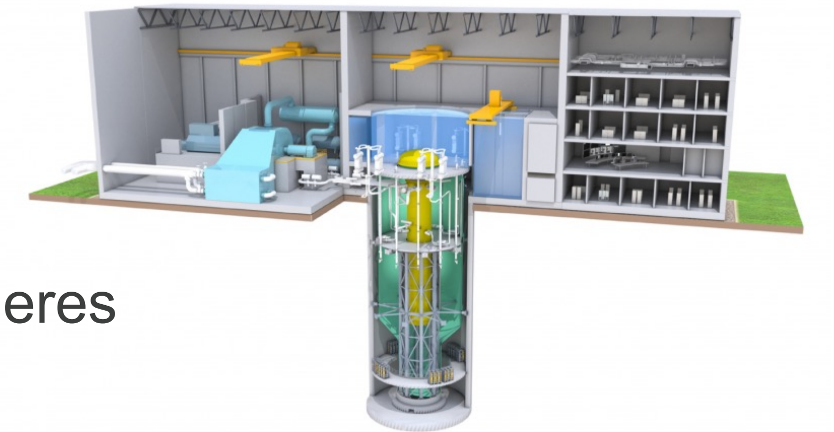
Impact:
- **Diminish reliance on fossil fuels/zero carbon emission**
- **Hydrogen production**
- **Advanced nuclear waste management**
- **Uranium extraction from seawater**

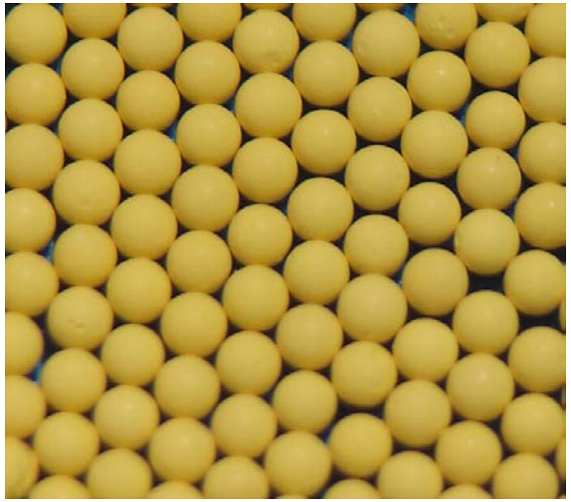
Revival of Nuclear Materials Labs @ UCI

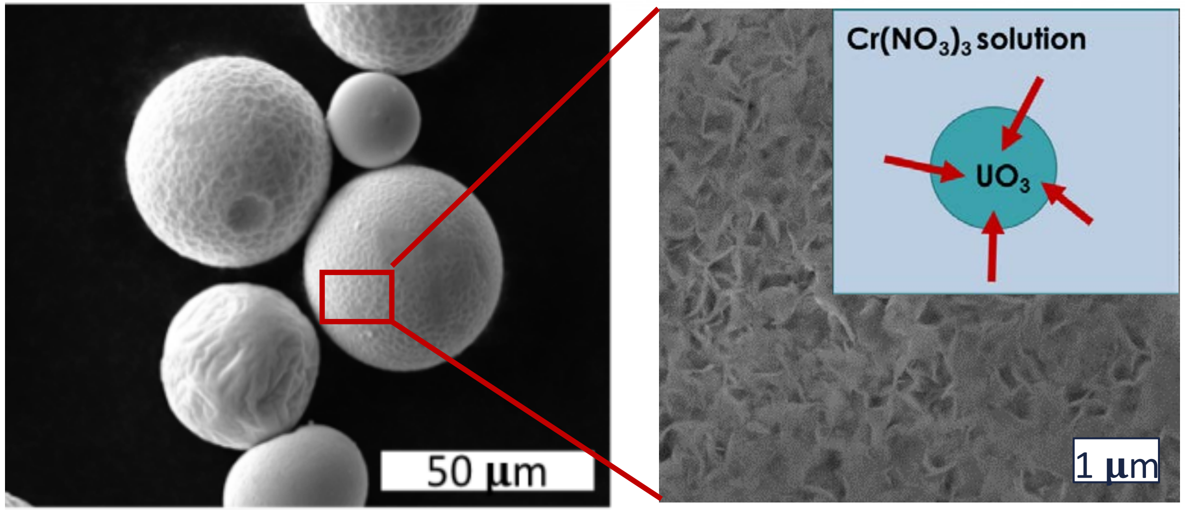
Tunable synthesis of advanced reactor fuels

- Fuel candidate development for MMRs & SMRs
- Highly versatile sol-gel fabrication line
- Adjustable microsphere size
- Control of uranium crystal morphology & porosity in gel-spheres

➢ tailor-made feedstock production







Materials chemistry for nuclear waste disposal

Aim:
safe disposal

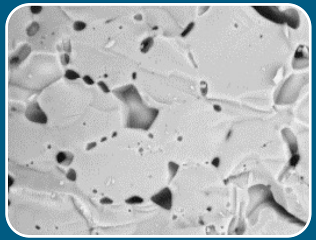
→ stable materials

Spent fuel

- UO_2 based

Glass

- Borosilicate glass



Ceramics

- Polyphase: Synroc
- Singlephase: tailor made **pyrochlore**

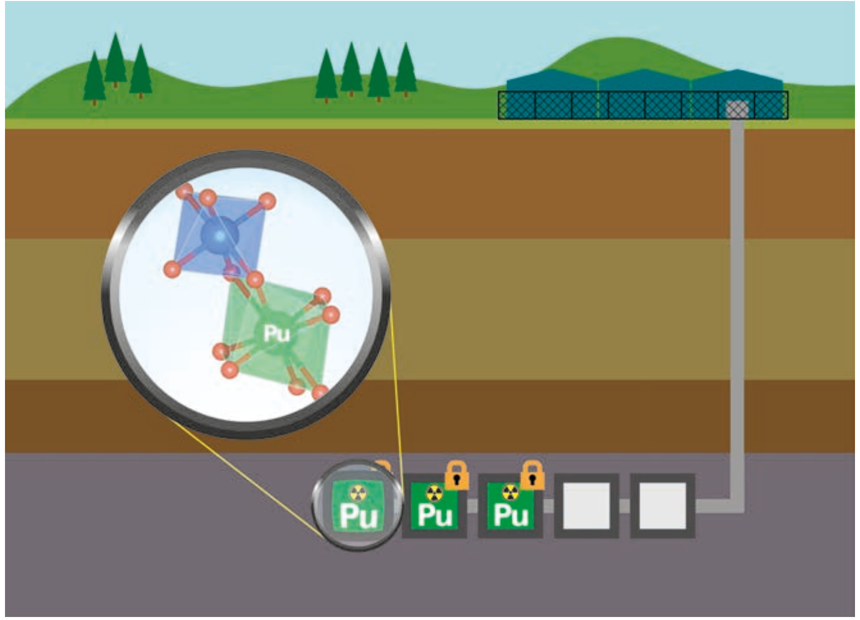
Pyrochlore: $A_2B_2O_7$, fluorite type structure

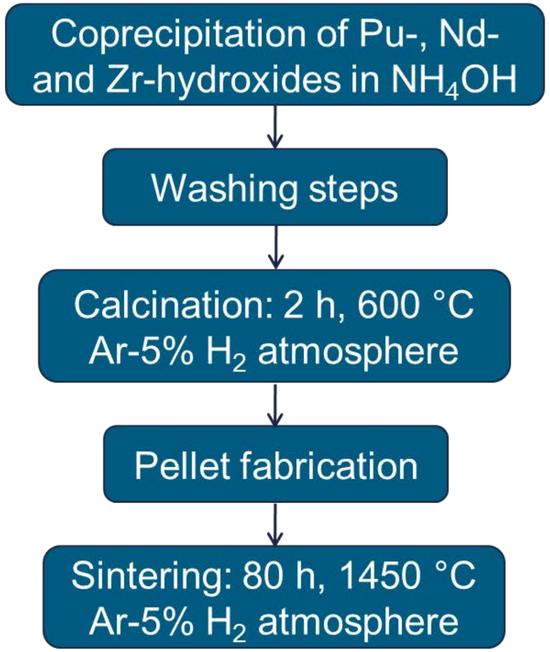
Waste form development:

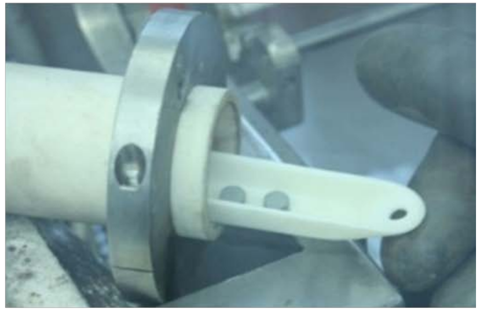
Waste form development:

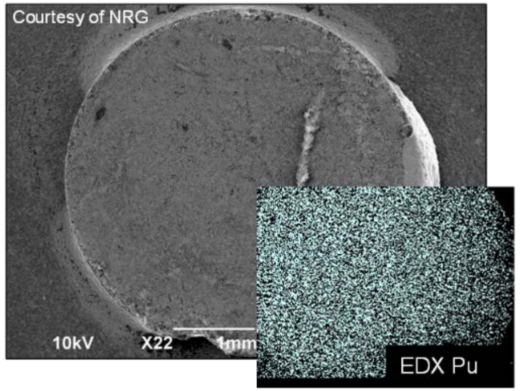
- Immobilization of Plutonium in stable ceramic waste forms: $Nd_{2-x}Pu_xZr_2O_7$
- Complementary experiemntal & computational approaches
➢ Structural uptake of Plutonium in pyrochlores

Site	Valence	ΔH_{soln} (eV) DFT (DFT + *U*)
Nd	Pu(III)	2.37 (-0.03)
Zr ($V_O^{\cdot\cdot}$)	Pu(III)	3.02 (+0.05)
Zr	Pu(IV)	1.33 (+0.11)
Nd (O_V'')	Pu(IV)	1.00 (-0.06)
Nd (V_{Nd}''')	Pu(IV)	3.83 (-0.06)









S. Finkeldei, et al. J. Mater. Chem. A. (**2020**), *8*, 2387–2403. https://doi.org/10.1039/C9TA05795A

Materials chemistry for nuclear waste disposal

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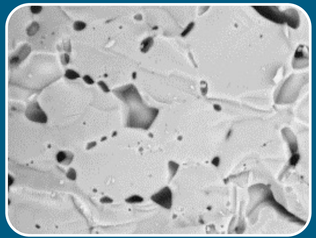


Ceramics

- Polyphase: Synroc
- Singlephase: tailor made **pyrochlore**

Pyrochlore: $A_2B_2O_7$, fluorite type structure

NEUP Nuclear Energy University Program
U.S. Department of Energy

In Collaboration with EES-14 @ LANL:

Dr. Caporuscio

Dr. Sauer

Dr. Migdissov

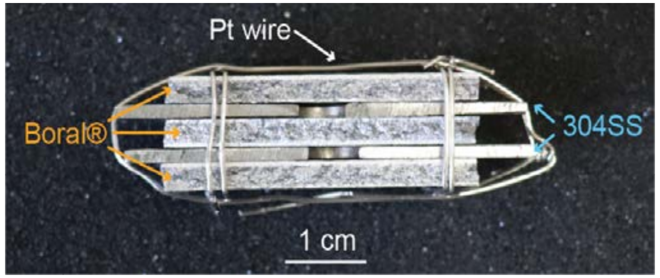
Redox Chemistry of UO_2 under Repository Relevant Conditions in the Presence of Zircaloy and Waste Canister Material

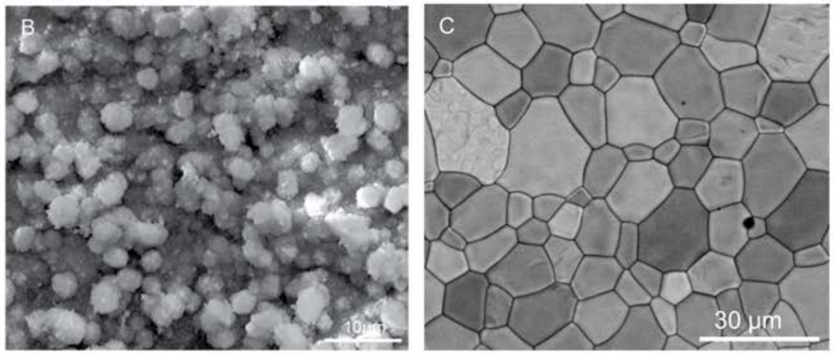
PI: Dr. Sarah C. Finkeldei, University of California, Irvine

Collaborators: Dr. Juliane Weber – Oak Ridge National Laboratory;
Dr. Kirsten Sauer, Dr. Florie Caporuscio, Dr. Artaches Migdissov – Los Alamos National Laboratory

Program: Fuel Cycle Technologies

ABSTRACT:
This project aims to gain a fundamental understanding of how the redox chemistry of UO_2 in contact with cladding and waste container material determines the matrix corrosion of spent nuclear fuel (SNF) in a deep geological repository (DGR). Currently, there is no clear understanding which processes control

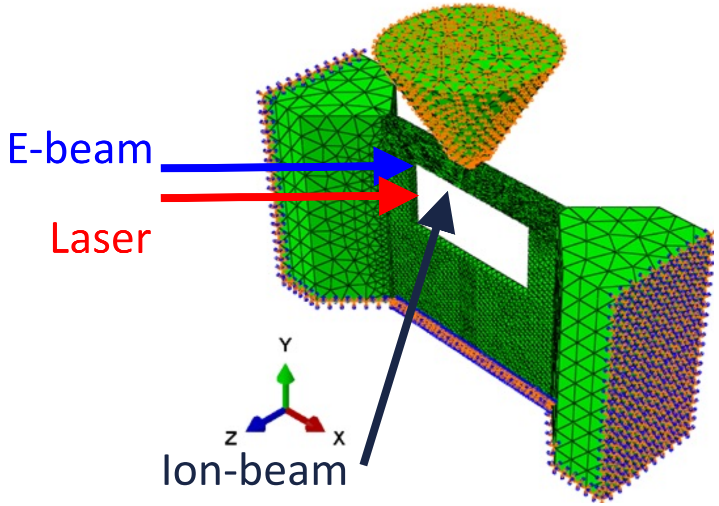




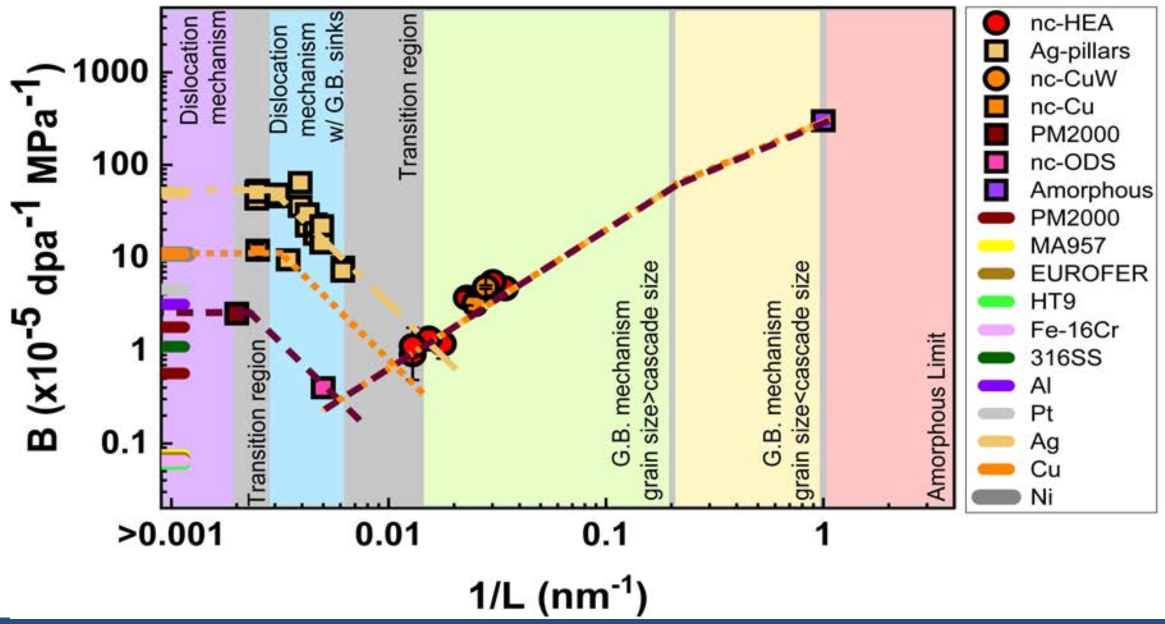
- Contribute to an **improved and predictive understanding** of long-term matrix dissolution of spent nuclear fuel in a deep geological repository

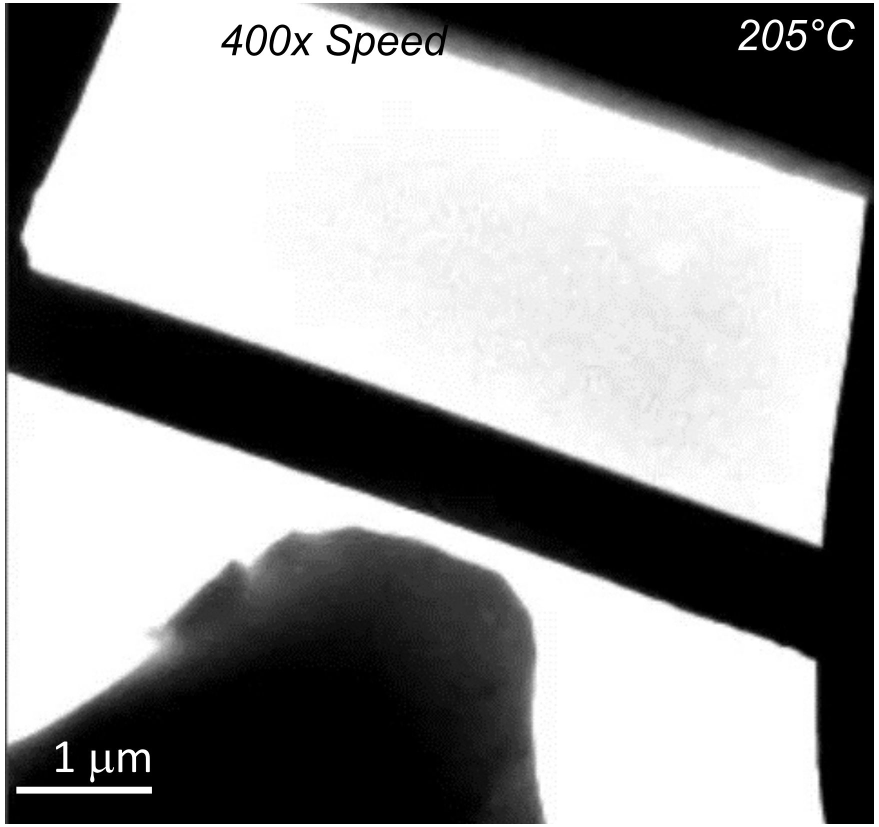
Irradiation Induced Creep

Shen Dillon, MSE



3 MeV Ag^{3+} 10^{-3}-10^{-2} dpa/s





$20M DOE Award for Hydrogen from Nuclear:

Light Water Reactor Integrated Energy Systems
Hydrogen End Use Demonstration

Jack Brouwer

Luca Mastropasqua

GOAL:

Support the advancement of integrated low temperature electrolysis (LTE) and high temperature electrolysis (HTE) at commercial NPPs, as well as increase the scale of integrated hydrogen generation at nuclear plants

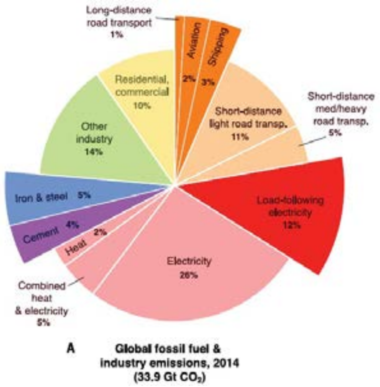
UCI-National Labs Connections

Sub-Theme 3: System Level Studies and Demonstration

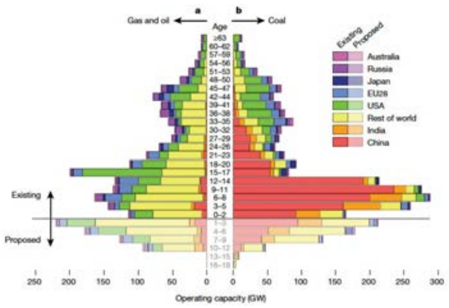
UCI

Steve Davis: Sources and Mitigation of GHGs

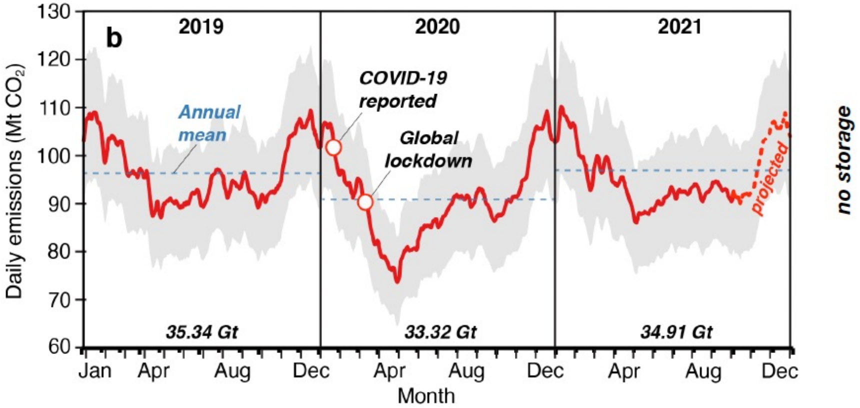
- Monitoring of global GHG emissions and energy infrastructure
- Energy systems modeling focused on fundamental challenges of net-zero emissions
- Energy—water — food — air pollution nexus
- Some recent work:



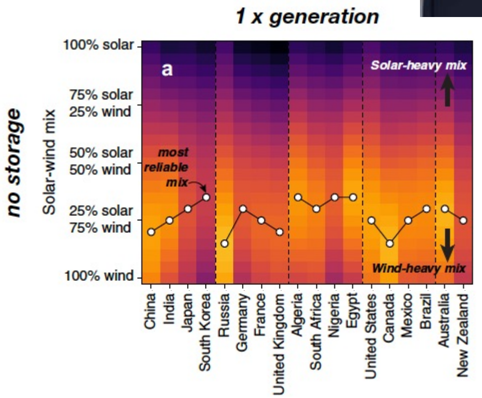
Review of net-zero emissions energy systems incl. difficult-to-abate sectors (*Science* 2018)



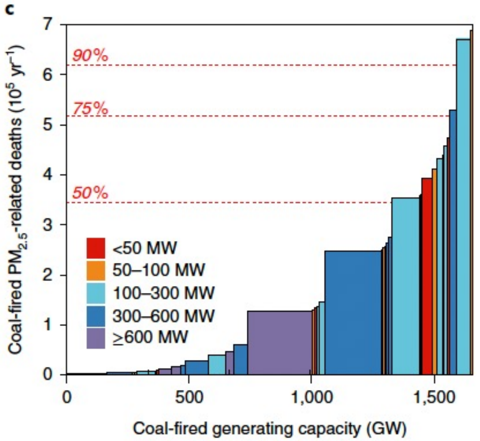
Committed emissions from existing energy infrastructure jeopardize 1.5°C target (*Nature* 2019)



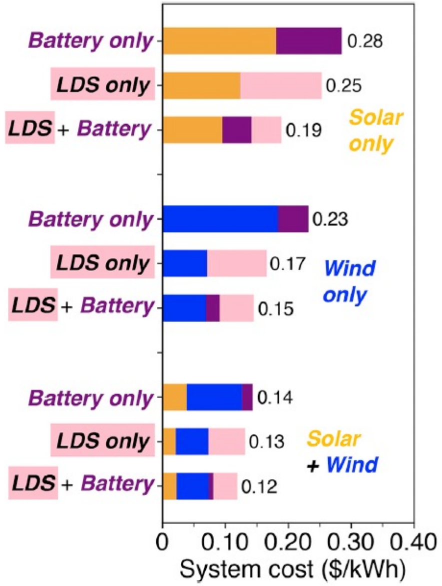
Near-real-time monitoring of daily global CO_2 emissions (*Nature Comm.* 2020)



Country-level differences in the reliability of solar and wind power systems (*Nature Comm.* 2021)



Strategic retirements of super-polluting power plants needed to maximize health co-benefits of climate mitigation (*Nature Climate Change* 2021)



Long-duration energy storage lowers system costs of all-VRE eve at current tech. costs. (*Joule* 2020)

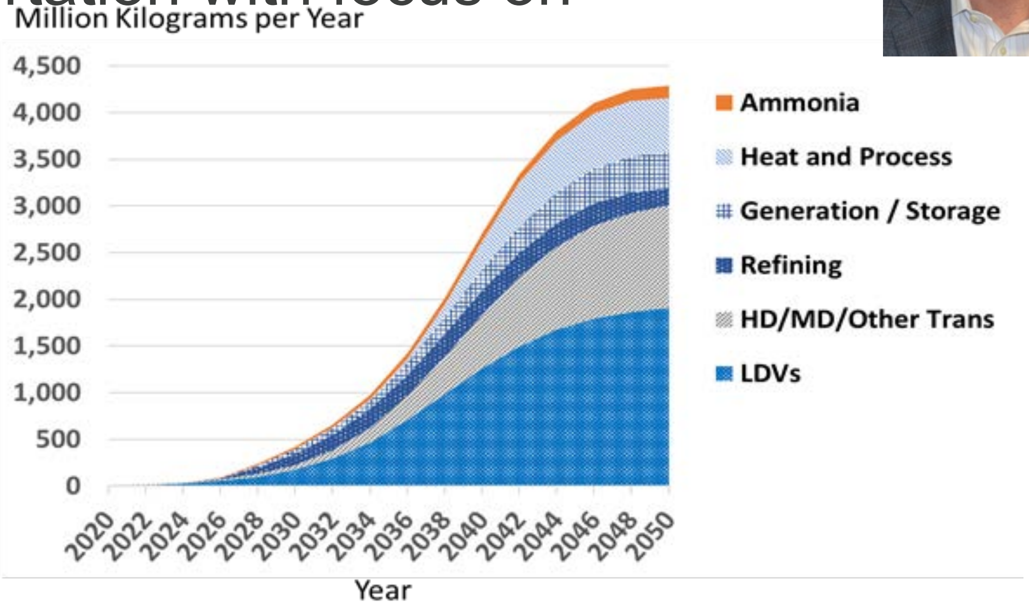
UCI

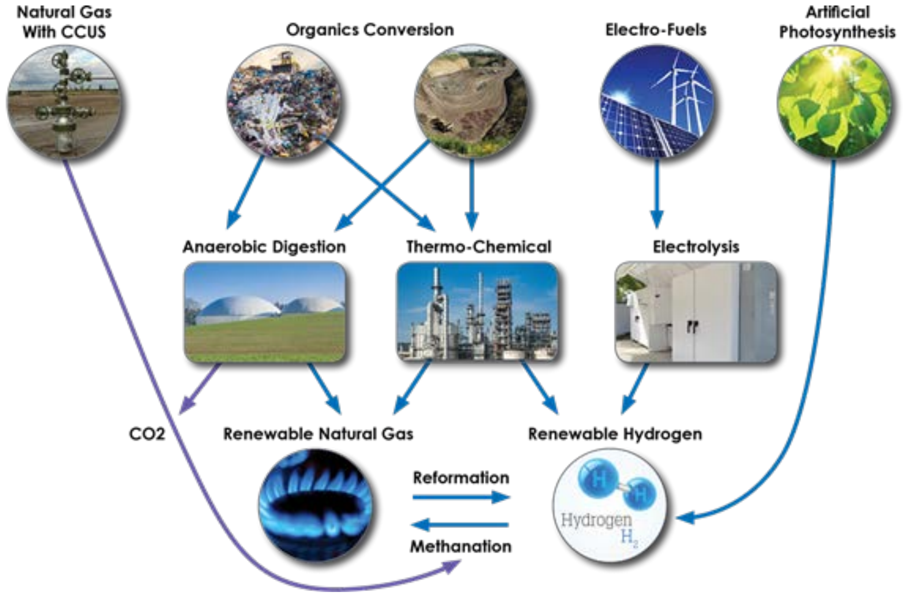
CARBON MONITOR

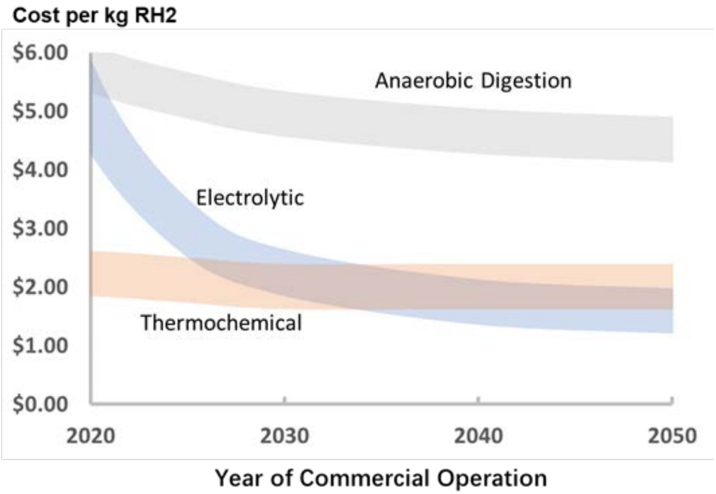
GLOBAL CARBON project

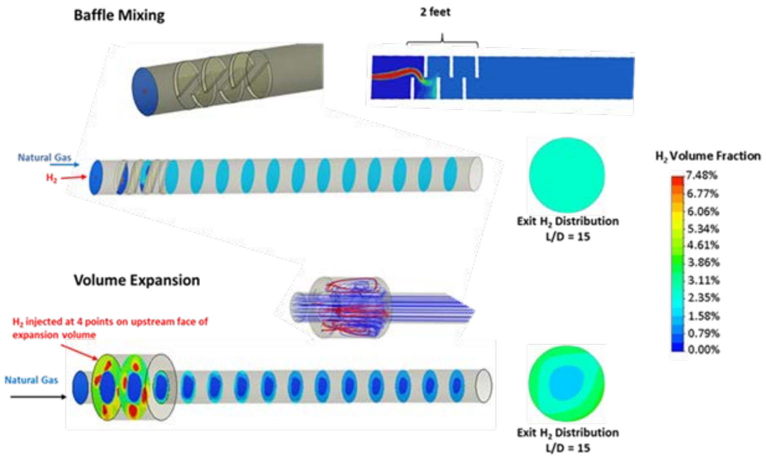
Jeff Reed: Renewable Fuels and Energy Storage

- Decarbonization strategies for energy & transportation with focus on hydrogen solutions
- Forecasting technology cost and performance
- System modeling and trade-off analysis
- Technology commercialization and deployment









UCI

Scott Samuelsen: Energy Systems

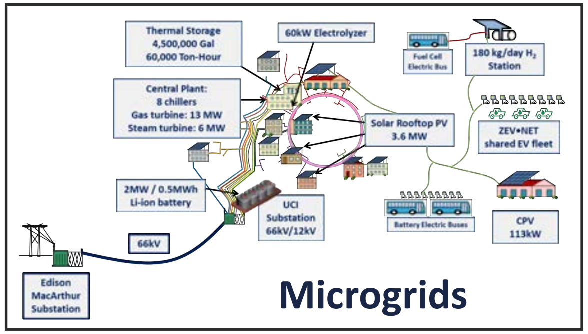
- Hydrogen fueling infrastructure
  - Strategic planning tool (“STREET”) for siting fueling/charging infrastructure
  - Launched FirstElement Fuel, owner/operator today of the majority of CA H_2 stations
- Renewable hydrogen generation
  - “Roadmap to the Generation of Renewable Hydrogen” published by CEC (April 2020)
  - Stationary fuel cell Tri-Generation of renewable hydrogen
  - Grid integration of electrolytic renewable hydrogen
- Microgrid evolution
  - Established the Generic Microgrid Controller (GMC) for US DOE (now IEEE 2030.7)
  - Islanded UCI campus (20MW class) and seamless re-connected
  - Building two connected 230 home community microgrids with KB Home and SunPower

U.S. first & most popular

World first tri-gen system

World first SOFC-GT system

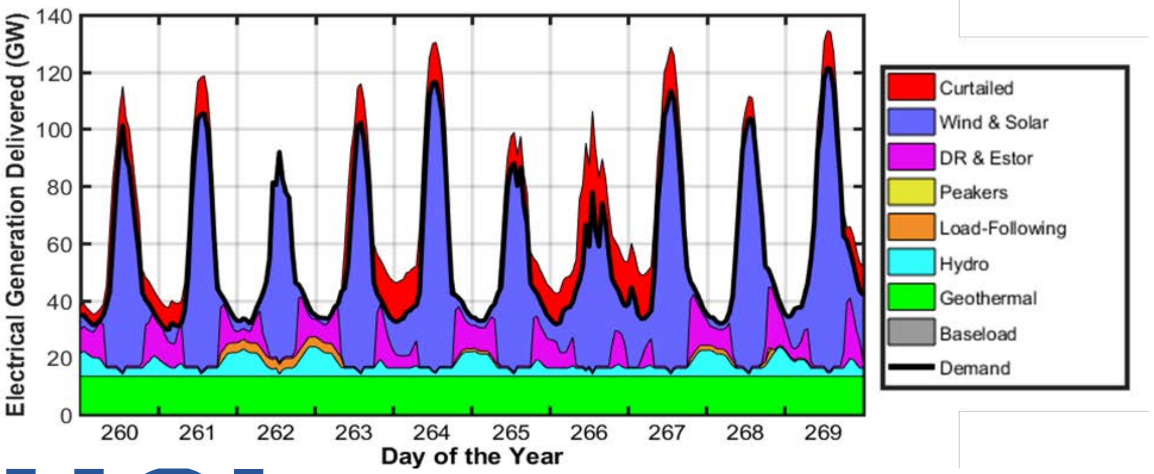
World-leading UCI Microgrid

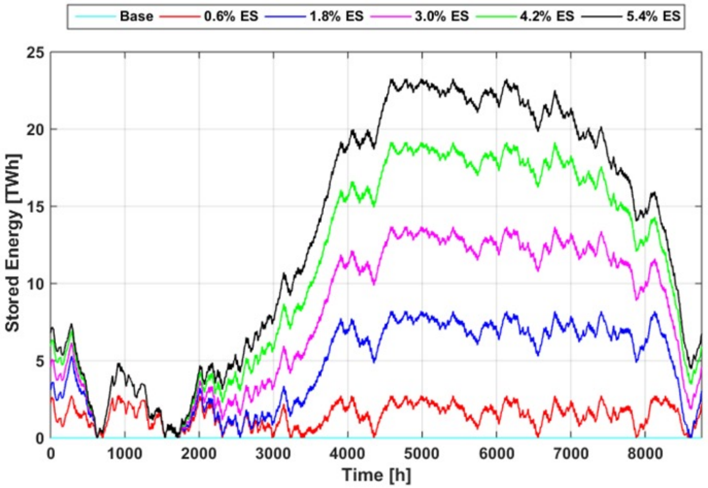


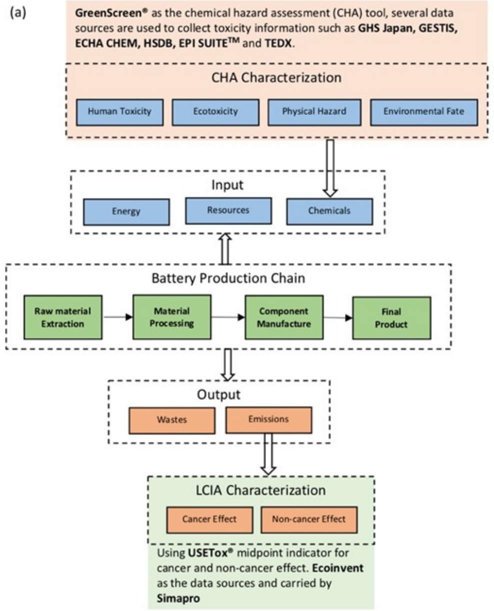
UCI

Brian Tarroja: Grid Dynamics; Life Cycle Analysis

- Dynamics & Dispatch Modeling of Highly Renewable Electric Grids and Supporting Resources
  - Characterizing the interaction of electrochemical energy storage with increasingly renewable electric grids with the Holistic Grid Resource Integration and Deployment (HiGRID) model
- Life Cycle Analysis of Electrochemical Energy Storage Technologies
  - Performing environmental life cycle assessment of current and emerging energy storage technologies
  - Assessing tradeoffs between life cycle environmental impacts and in-use environmental benefits of battery storage





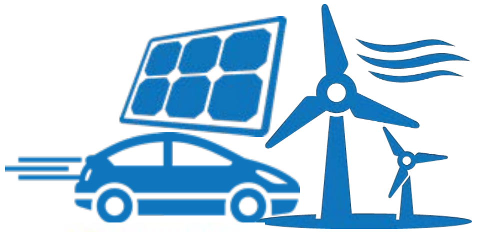


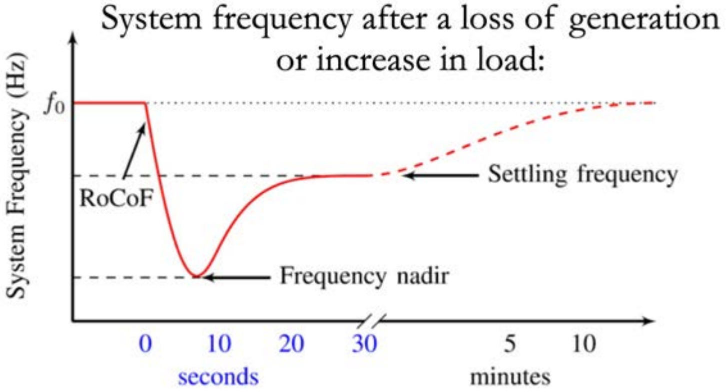
UCI

David Copp
Mechanical and Aerospace Engineering

Motivation

- Address grid stability challenges related to renewables and electrification
- Realize firm and dispatchable electricity
- Lower inertia → faster rate of change of freq. (RoCoF) and lower nadir
- Steep ramps (currently accommodated with, *e.g.*, natural gas "peaker" plants)



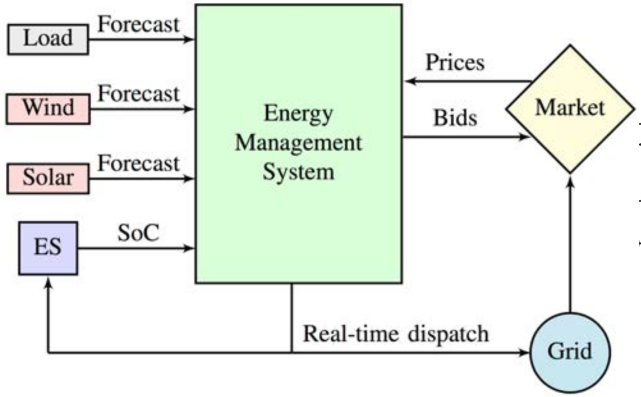


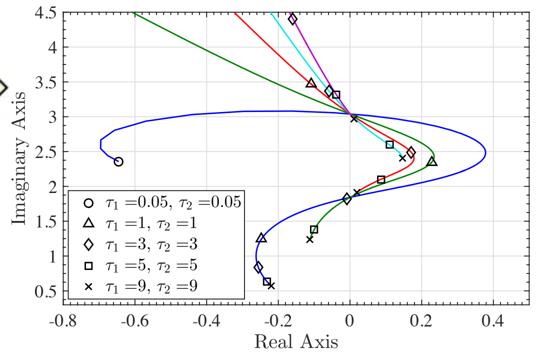
Tamrakar, <u>Copp</u>, Nguyen, Hansen, Tonkoski. *IEEE Trans. Energy Conversion* 2020
Headley, <u>Copp</u>. *Energy* 2020
<u>Copp</u>, Nguyen, Byrne. *American Control Conference* 2019
Nguyen, <u>Copp</u>, Byrne, Chalamala. *IEEE Trans. Power Systems* 2019
Rosewater, <u>Copp</u>, Nguyen, Byrne, Chalamala, Santoso. *IEEE Access* 2019
Byrne, Nguyen, <u>Copp</u>, Chalamala, Gyuk. *IEEE Access* 2018

UCI Sandia National Laboratories U.S. DEPARTMENT OF ENERGY SOUTH DAKOTA STATE UNIVERSITY

Technological Approach

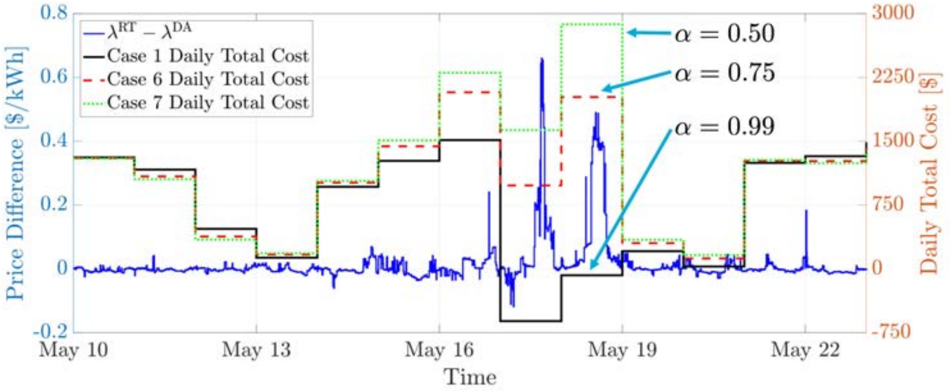
- Energy management algorithms
- Optimal estimation and control
- Utilization of real-time information and computation





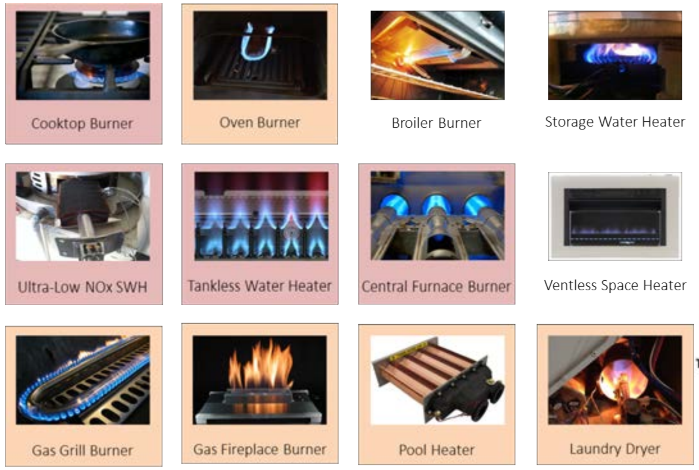
Potential Impact

- Integration of more intermittent renewable generation
- Reliable and resilient grid with real-time situational awareness
- Value streams for new technologies



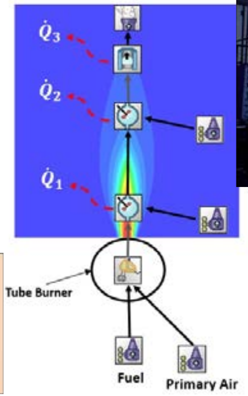
Vince McDonell: H2 & Renewable Low NOx Combustion

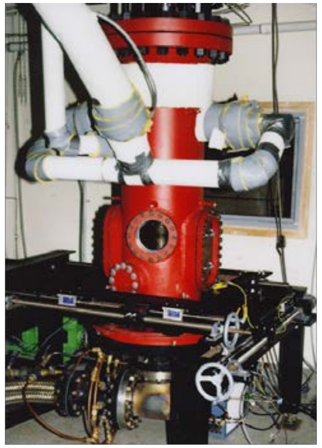
- UCI Co-PI Vince McDonell research capabilities & interests in:
  - Experimental and analytical evaluation of end use device performance as operated on various mixtures of renewable fuels and natural gas
  - Modification of end use devices to operate reliably on high hydrogen content fuels with low pollutant emissions
  - Development and integration of sensors to facilitate control and actuation of devices to accommodate variation in fuel composition
  - Consideration of codes and standards including test procedures for assessing performance



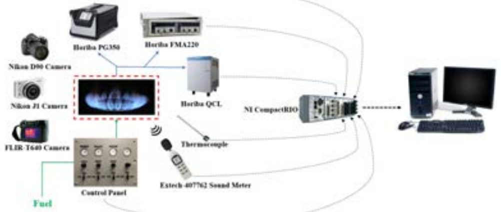
CFD
Experiment Test + CFD

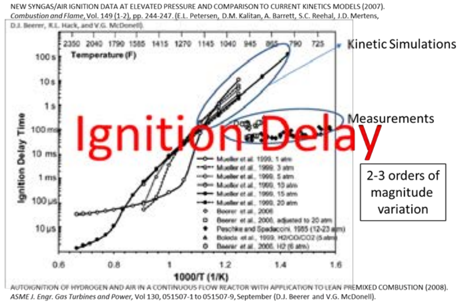
Burner Performance Reports Available for each—Appendices for Final Report

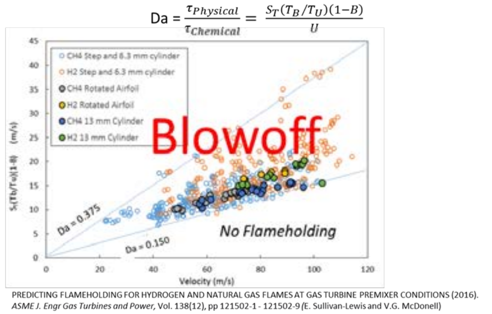


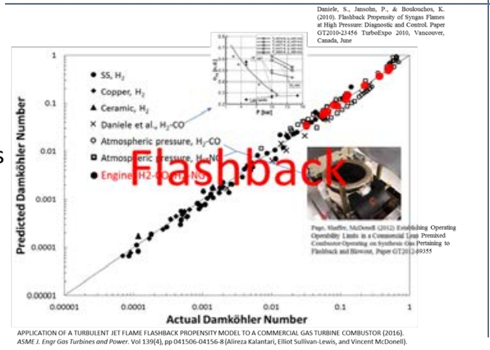


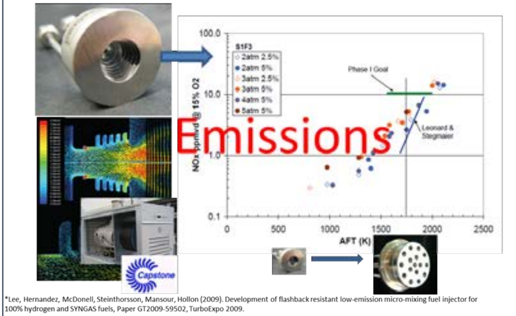
Simulation Of Practical Conditions
(1000 K, 15 atm, 2.2 kg/s)



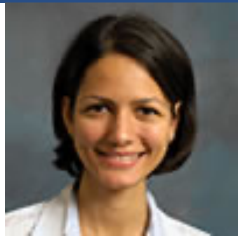








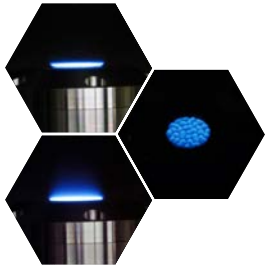
Bihter Padak: Carbon Capture & Management

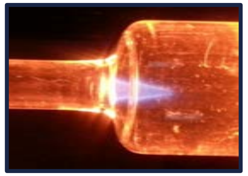


Utilization of Carbon-free Fuels in Combustion Processes:

Adding renewable H_2 and NH_3 to natural gas

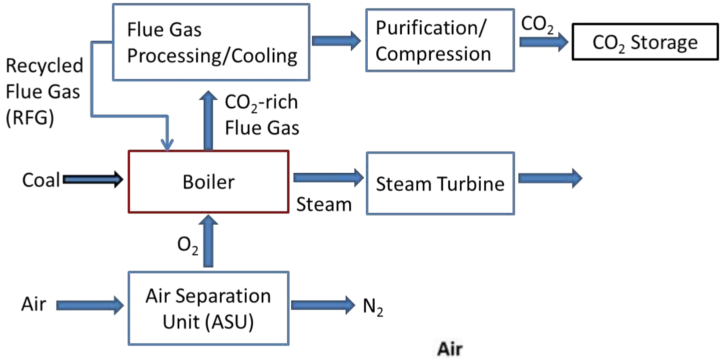
- Stationary power systems
  - Gas-fired utility boilers
  - Gas turbines
  - Process heaters
  - Gas-fired reciprocating engines
- Transportation
  - Medium/heavy-duty vehicles
  - Ocean going vessels
- Residential and commercial appliances



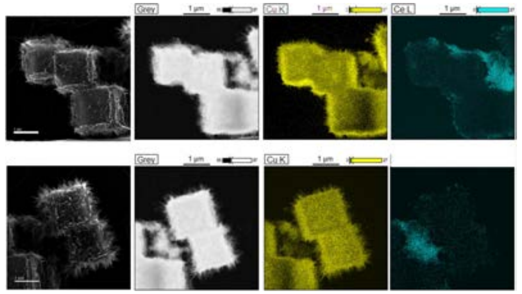


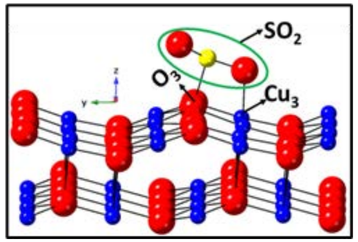
Carbon Capture and Storage Technologies:

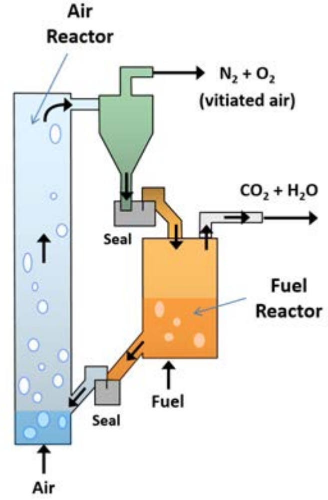
- **Oxy-combustion**
  - Combustion in O_2 rather than air
  - Results in reduction of NO_x and SO_x emissions



- **Chemical looping combustion**
  - Combustion of fuel by metal oxide reduction instead of direct oxidation with air



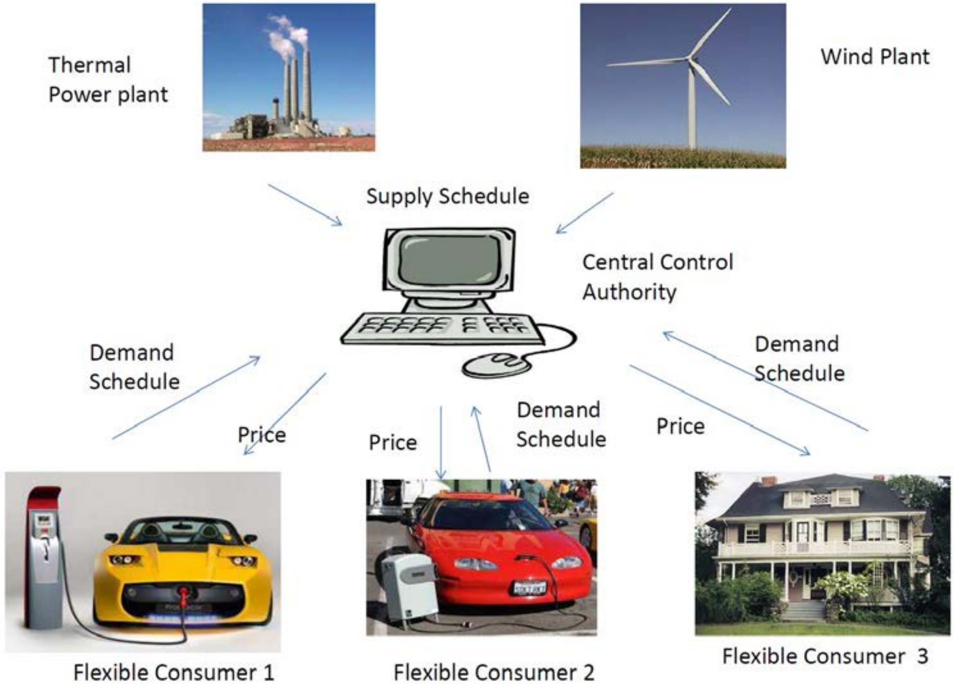


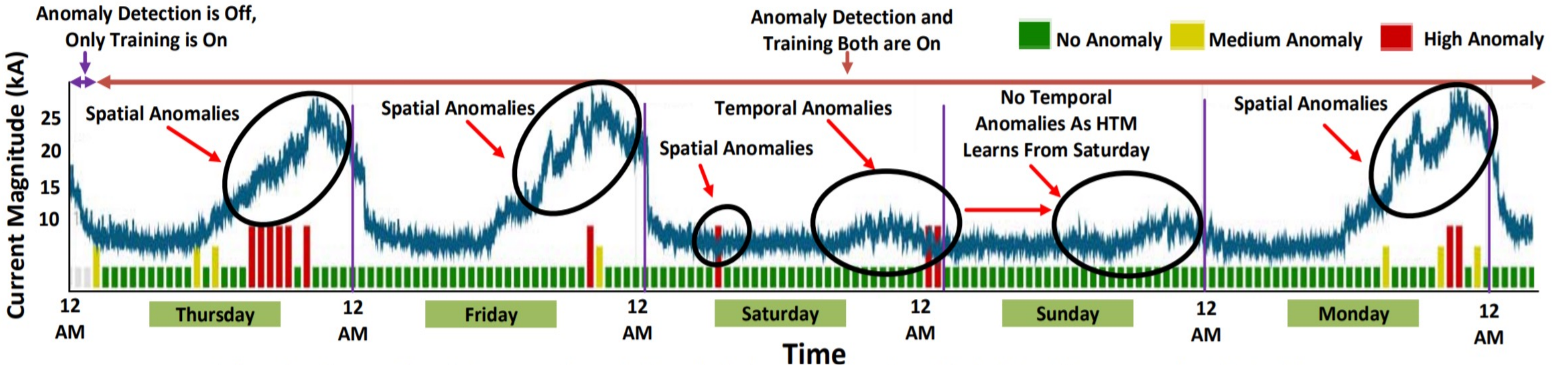


UCI

Pramod Khargonekar: Integration of Renewables and Distributed Energy Resources in Smart Grids

- Renewable producers and storage in electricity markets and operations
- Control and management of load flexibility for renewable integration
- Causation based cost allocation principles and algorithms
- Distributed control for integration of renewable sources
- Matching markets for distributed energy resources
- Stochastic optimization for residential energy management
- Machine learning for grid control
- Cybersecurity and smart grid

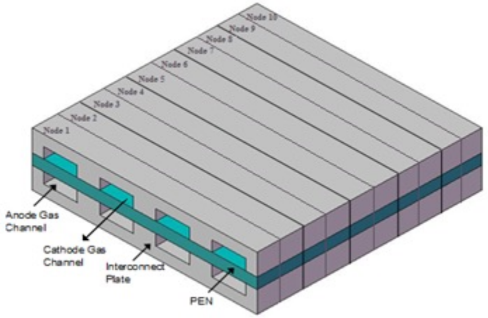


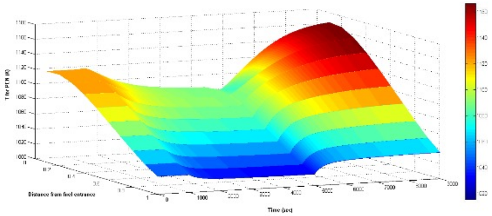


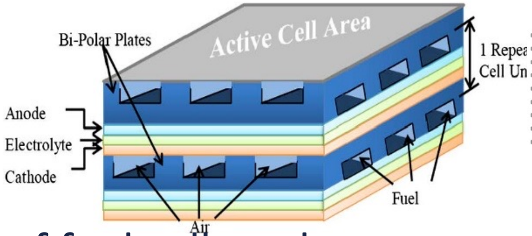
A. Barua, D. Muthirayan, P. P. Khargonekar and M. A. Al Faruque, *2020 ACM/IEEE 11th International Conference on Cyber-Physical Systems (ICCPS)*, 2020, pp. 188-189, doi: 10.1109/ICCPS48487.2020.00027.

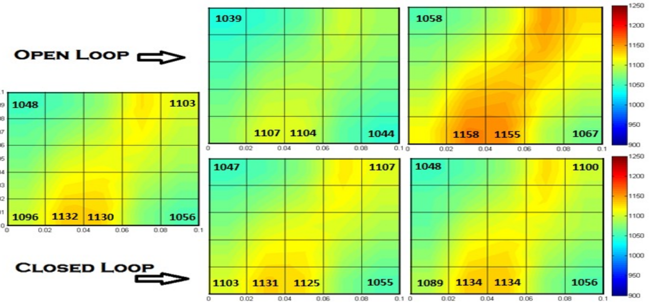
Faryar Jabbari: Dynamics and Controls

- Dynamic models, for control, for fuel cell and electrolyzer stacks;
- System level modeling for reversible FC and EC for complementing renewables;
- Optimization techniques for district cooling/heating and unit commitment problems;
- Dynamic programing for economic dispatch;
- Distributed decision for smart BEV charging algorithms in residential/commercial applications.

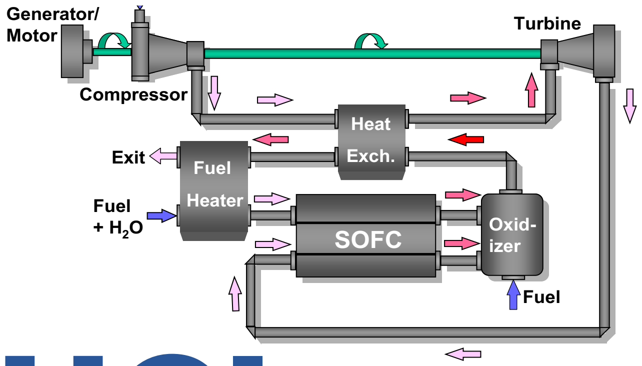


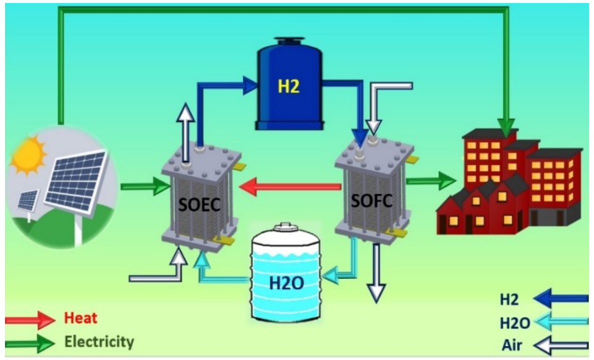




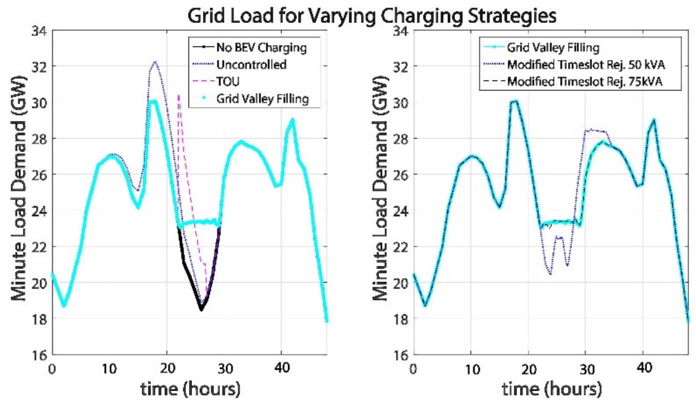


Modeling and thermal control of fuel cell stacks





System level modeling



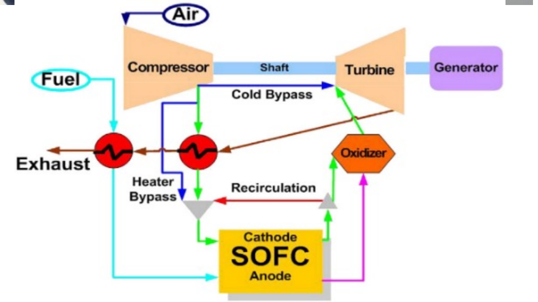
Smart BEV Charging

UCI

Jack Brouwer: Fuel Cell and Electrolysis Systems

- Conceptualization & physical dynamic modeling of fuel cell, electrolysis & energy connv.
- Dynamic modeling of high renewable use & electrochemical system dynamics
- Integration of fuel cells, electrolyzers & hydrogen storage with solar and wind
- Experimental & theoretical study of power-to-gas incl. U.S.-first plant in UCI microgrid
- Integration, theoretical & experimental investigation of fuel cells for data centers incl. world-first direct DC-powering of a server rack with a PEM fuel cell

US first renewable H_2 P2G2P



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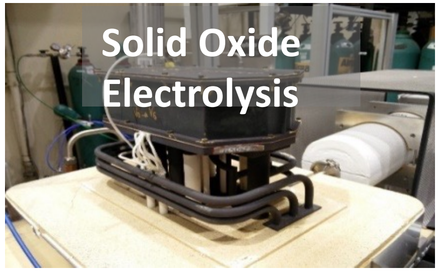
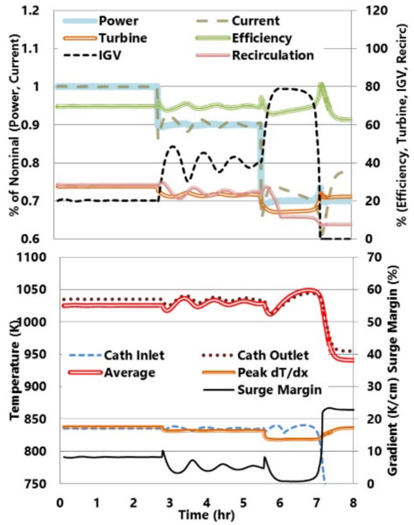
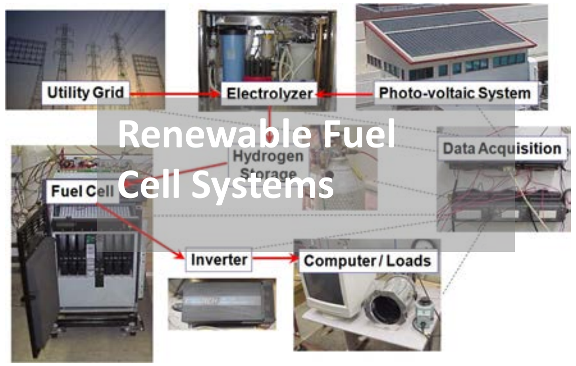
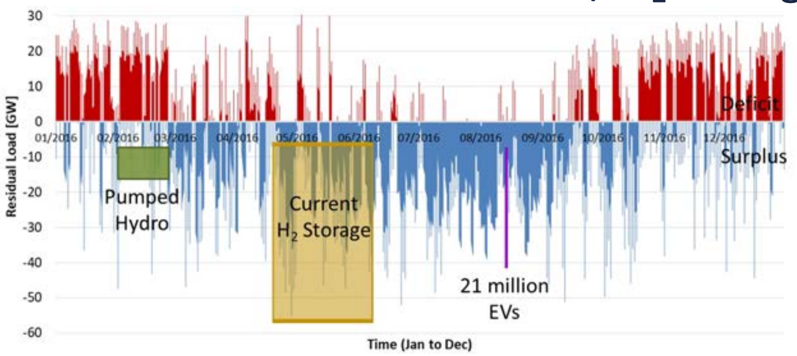


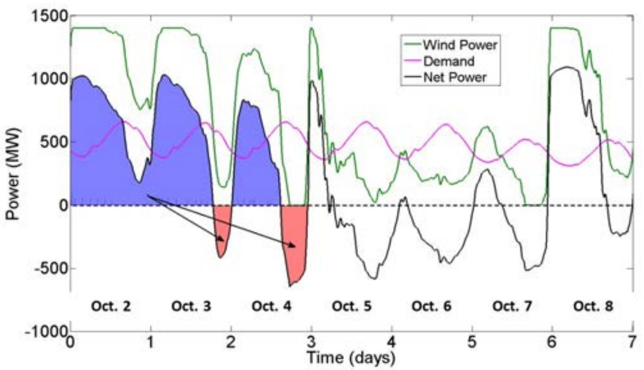




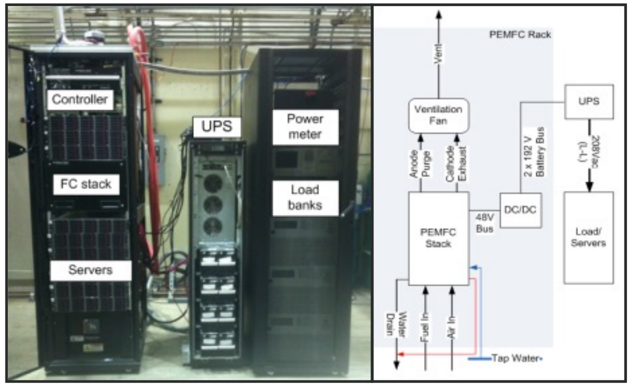
100% Renewable CA Grid w/ H_2 Storage



H_2 storage w/ Texas Wind



World first fuel cell powered server rack



Potential Discussion Topics

- Novel material solutions for energy conversion and storage
- New generation scientists' pipeline
- Partnerships in fundamentals of electrochemical engineering (electrocatalysis, fuel cells, batteries, solar fuels, nuclear)
- Future energy conversion scenario development and techno-economic analysis to support investment in electrochemical and hydrogen technologies (some political & environmental opposition)
- Grid simulation (renewable dynamics, distribution system infrastructure, waveform level dynamics)
- Transformation of the gas system for renewable hydrogen
- Fuel cell systems (esp. SOFC, PEMFC) development and control
- Bridging climate change and materials/electrochemical technologies

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