

BASIC ENERGY SCIENCES ADVISORY COMMITTEE (BESAC)

DECEMBER 6TH, 2021

# ACCELERATING CLIMATE AND CLEAN ENERGY INNOVATION: ROLE OF THE DOE NANOSCALE SCIENCE RESEARCH CENTERS (NSRCs)

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Sandia National Laboratories





BERKELEY LAB  
**MOLECULAR  
FOUNDRY**



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**CENTER FOR INTEGRATED  
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Sandia National Laboratories*

**ADAM RONDINONE**



**CENTER FOR  
NANOSCALE  
MATERIALS (CNM)**

*Argonne National  
Laboratory*

**ILKE ARSLAN**



**BROOKHAVEN** | Center for Functional  
Nanomaterials

**CENTER FOR  
FUNCTIONAL  
NANOMATERIALS (CFN)**

*Brookhaven National  
Laboratory*

**CHARLES BLACK**

**THE MOLECULAR  
FOUNDRY (TMF)**

*Berkeley Lab*

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SCIENCES (CNMS)**

*Oakridge National Laboratory*



Office of  
Science

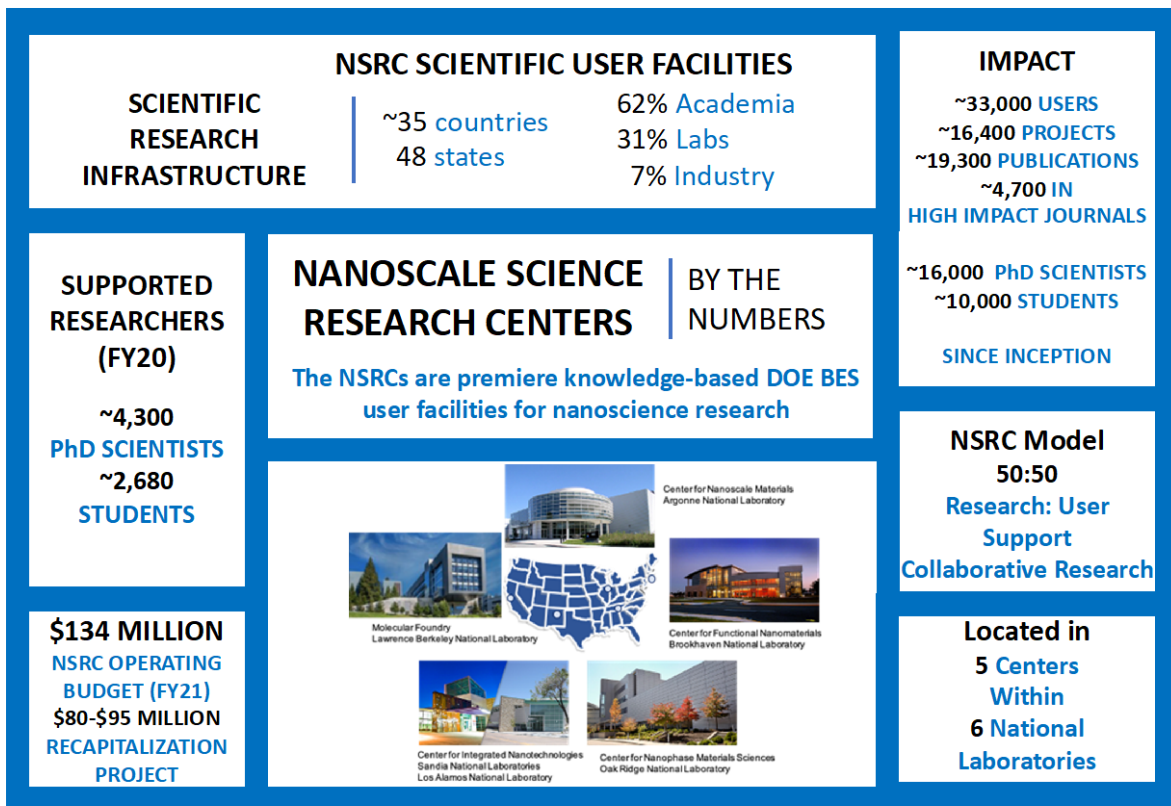
**NANOSCALE SCIENCE  
RESEARCH CENTERS**

5 NSRCs operated at  
6 national labs

**KARREN MORE**



# NSRC User Facilities – Collaboration & Innovation Ecosystem



**Unique** expertise and research equipment in nanoscale synthesis, characterization, modeling, and fabrication

**Merit-review** access process – 2-3 page innovative nanoscience research proposal

**FREE** access to staff expertise and equipment for open science – publish in open literature



Center for Functional Nanomaterials



Los Alamos National Laboratory

Argonne National Laboratory



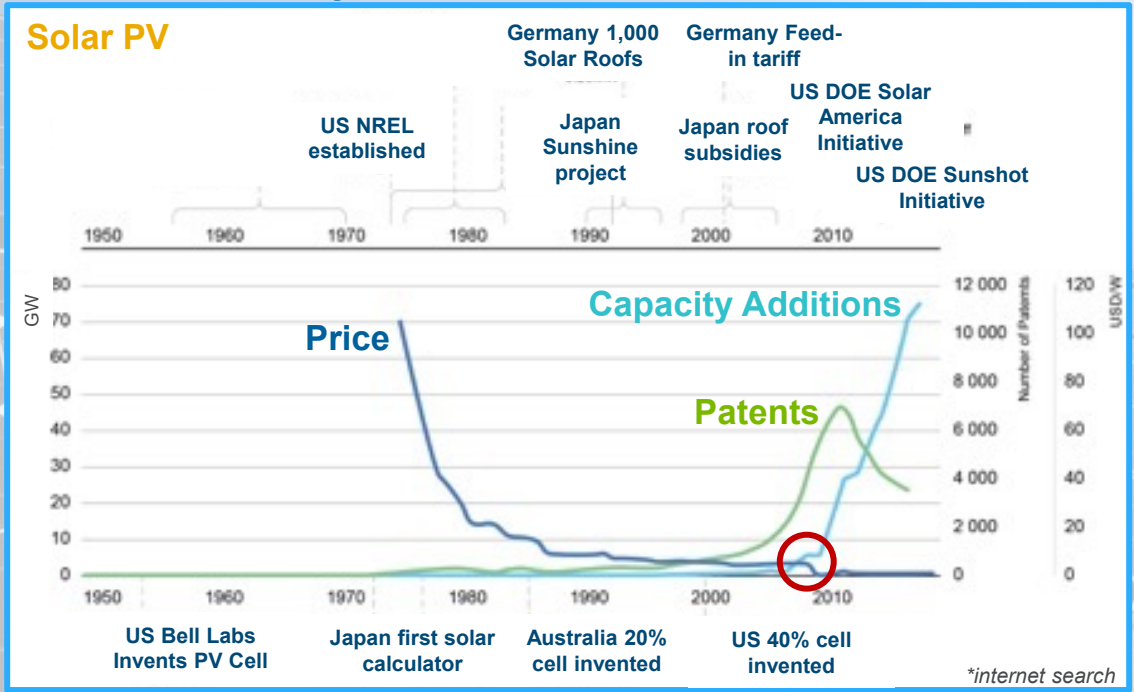
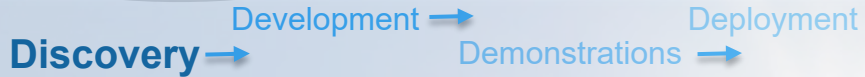
Molecular Foundry



# Discovery to Deployment of Future Decarbonization Technologies

We don't have 70 years !

NSRCs



# NSRC Collaboration Highlights

Accelerating climate and clean energy innovation

## COLLABORATION HIGHLIGHTS

-  Energy Storage
-  Carbon Neutral Hydrogen
-  Sustainable Fuels
-  Solar Energy & Solid-State Lighting
-  CO<sub>2</sub> Separations
-  Clean Water

- We recognize the vast amount of amazing research going on around the world
- Highlights shared today –
  - Emphasis on collaborative teams and resources (exp + theory) brought together by the NSRC scientists
  - Atomic, nanoscale understanding the NSRCs can bring to the climate and clean energy innovation community

# Energy Storage: Improving Performance



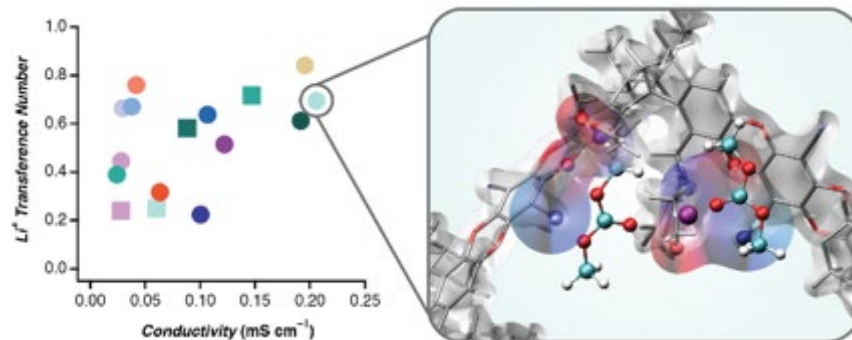
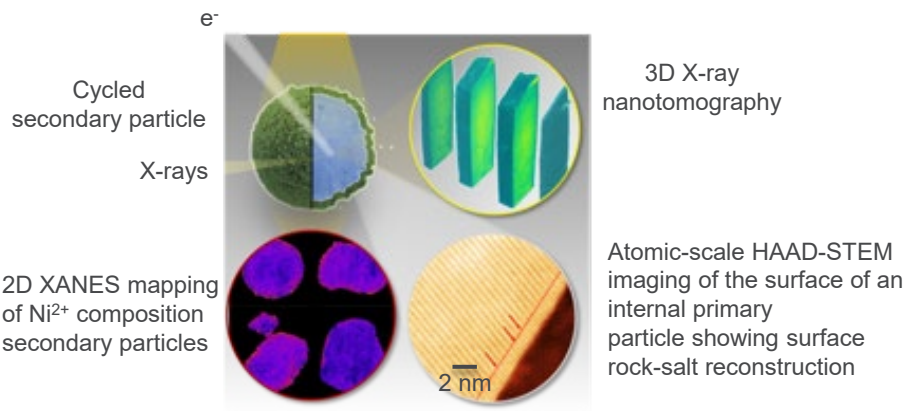
## High Energy Density, High-Nickel-Content Cathodes

**Impact:** Nickel valence gradients from the surface to the interior improves cyclability.



## Designing Selective Membranes for Batteries using a Drug Discovery Toolbox

**Impact:** Polymers containing solvation cages bind lithium ions and enable rapid transport through the membrane.



**PARTNERS:**

*Nature Communications*  
12, 2350 (2021)

*Nature*, 592, 225 (2021)



Center for Functional Nanomaterials

National Synchrotron Light Source II



Berkeley UNIVERSITY OF CALIFORNIA



Advanced Photon Source



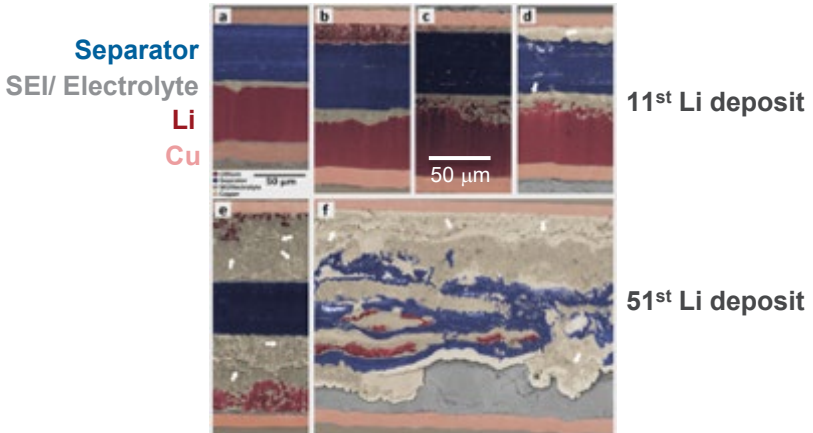
BINGHAMTON UNIVERSITY

# Energy Storage: Understanding Degradation

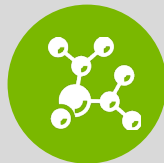


## Cryogenic Laser Ablation Reveals Short Circuit Mechanism in Li Metal Batteries

**Impact:** Separator penetration is enabled by SEI formation to connect bridging Li grains forming soft short circuits.



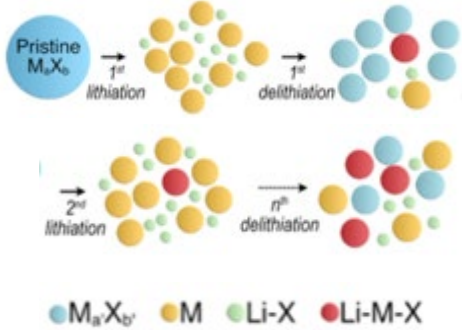
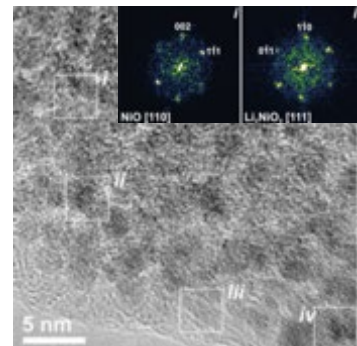
ACS Energy Letters. 2021, 6, 2138 (2021)



## X-Rays & TEM Monitor Structural Changes in Conversion-Type Electrodes

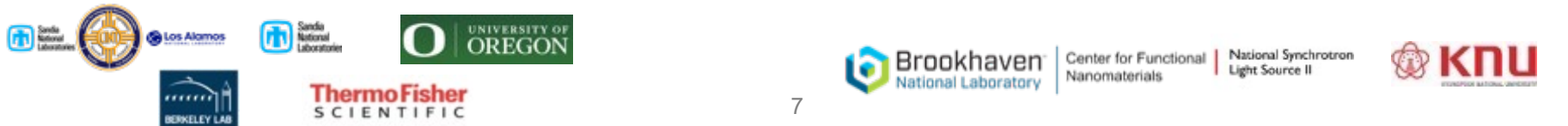
**Impact:** Asymmetric reaction pathways for lithium insertion and extraction accelerates electrode degradation.

### HRTEM from NiO after 2<sup>nd</sup> charge



Chem. Mater. 33, 3515 (2021)

**PARTNERS:**



# Carbon-Neutral Hydrogen: Novel Catalysts



## Platinum Group Metal (PGM)-Free Catalyst for Polymer Electrolyte Fuel Cells

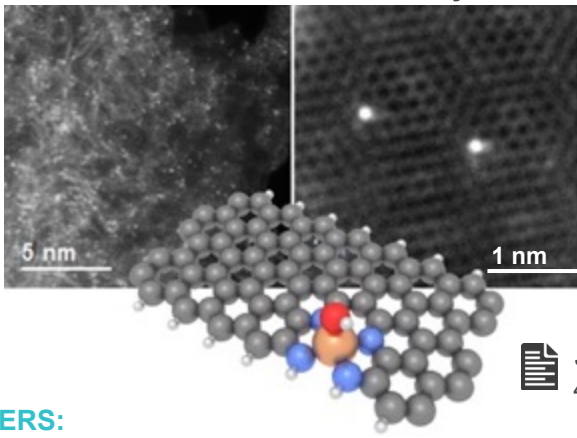
**Impact:** Zigzag edge-hosted  $\text{FeN}_4$  spontaneously ligated with OH leads to highly ORR-active structures.



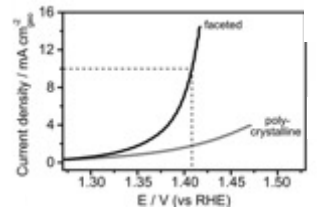
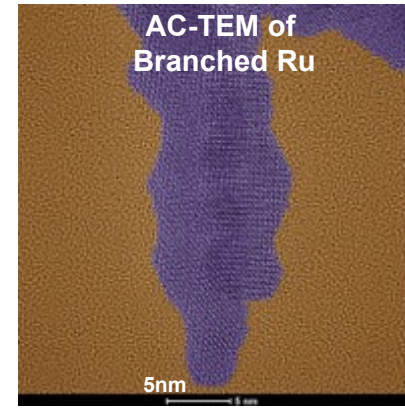
## Branched Ruthenium Nanoparticle Catalyst for Water Splitting

**Impact:** Controlling the ruthenium's crystal structure enables improvement in how well ruthenium performs in electrolysis systems.

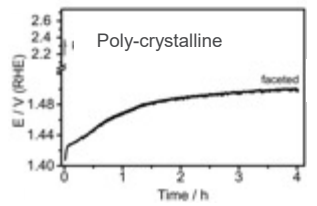
ADF-STEM of Fe-N-C Catalyst



*Science* 357, 479 (2017)



branched  
Poly-crystalline



branched  
*Small* 15 (17), 1804577 (2019)

PARTNERS:



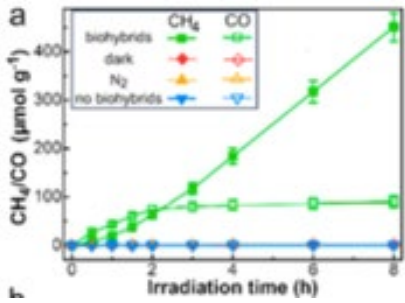
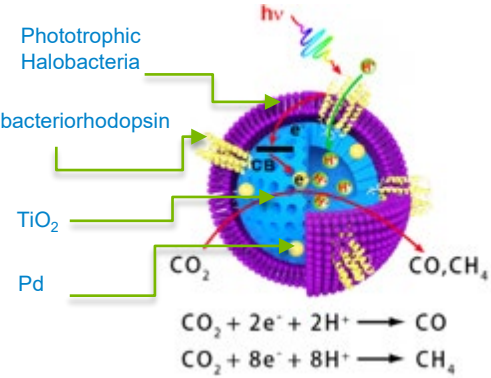


# Sustainable Fuels: CO<sub>2</sub> Conversion Catalyst



## Semi-artificial Photosynthetic Biohybrid Inspires Sustainable Fuel Production

**Impact:** Cell-mimic assembly could facilitates CO<sub>2</sub> conversion to CO and methane under visible light irradiation.



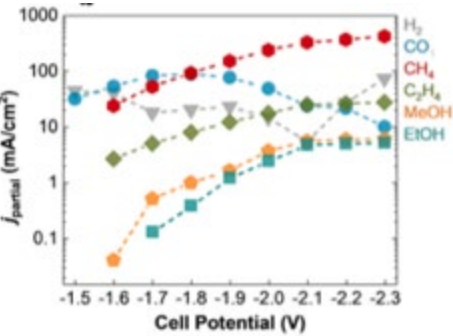
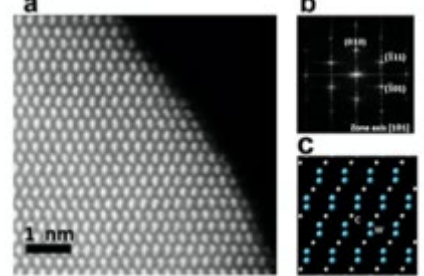
*J. Am. Chem. Soc.* 2019, 141, 11811–11815.



## Di-Tungsten Carbide Driven Catalysis of CO<sub>2</sub> Reduction

**Impact:** Earth-abundant, highly active catalyst that selectively produces hydrocarbons opens the door to low-cost, sustainable large-scale production of fuels from CO<sub>2</sub>.

### HAADF-TEM of W<sub>2</sub>C Nanoflakes



Nature Communications 12, 5067 (2021).

**PARTNERS:**



# Solar Energy and SSL: Stabilizing Perovskites



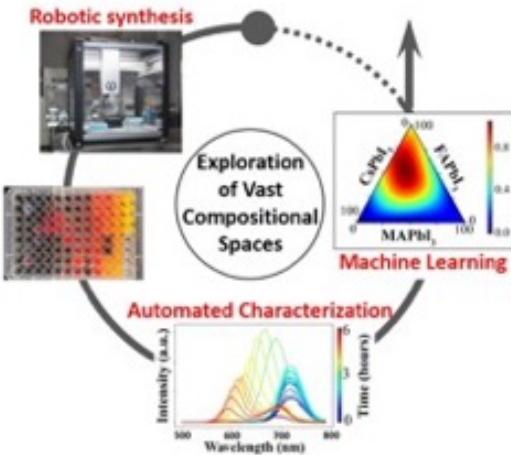
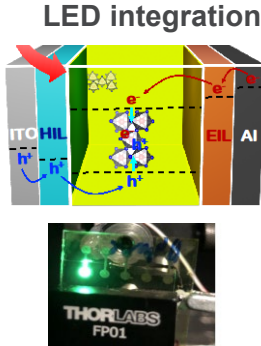
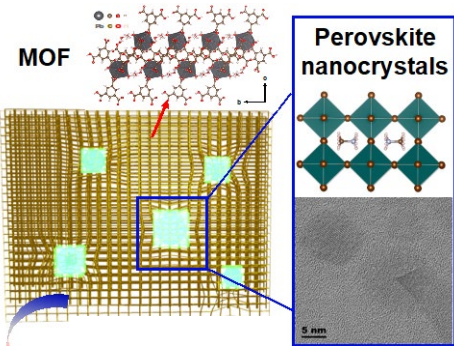
## Metal Halide Perovskite Nanocrystals Stabilized in MOF

**Impact:** Optical and x-ray spectroscopy shows localized carrier recombination leads to 15% efficient LEDs.



## Chemical Robotics for Discovery Stability of Metal Halide Perovskites

**Impact:** Workflow provides an opportunity to accelerate the production of MHP materials with vast compositional spaces by several orders of magnitude.



Nature Photonics. (2021), doi.org/10.1038/s41566-021-00857-0



ACS Energy Lett. 2020, 5, 11, 3426–3436

**PARTNERS:**

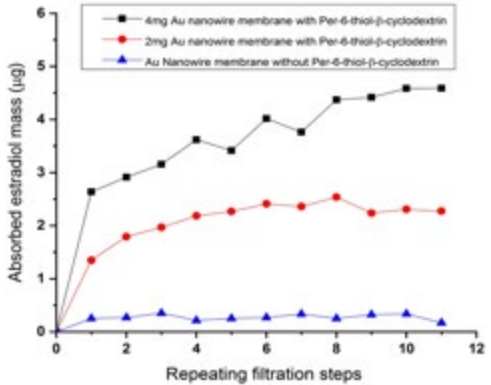
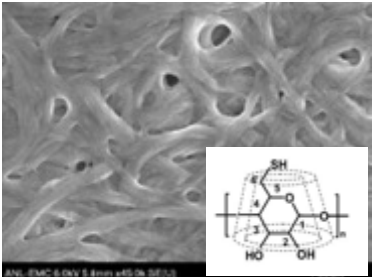


# Water Purification: Enhancing Membrane Selectivity



## Ultrathin Nanoparticle Membranes Remove Trace Organic Compounds from the water supply

**Impact:** Engineered nanowire-based membrane, functionalized with molecular buckets (hydrophobic interior hydrophilic exteriors) traps *Endocrine Disrupting Compounds*.



Lin, Wu and Sankaranarayanan, US patent 11,020,711, 2021

**PARTNERS:**

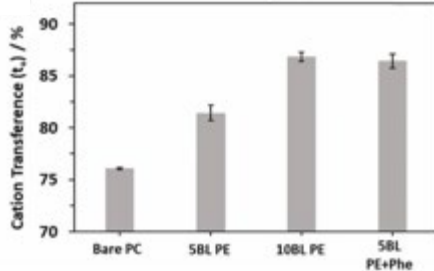
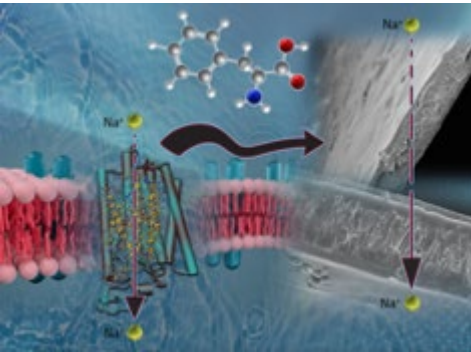


- DOE Technology Commercialization Fund
- Metropolitan Water Reclamation of Chicago (MWRD)
- Illinois Sustainable Technology Center (ISTC)



## Bio-Inspired electro dialysis membrane provides fresh water from impaired water supplies

**Impact:** Incorporation of the amino acid phenylalanine enhances ionic selectivity in layer-by-layer deposited polyelectrolyte films, reducing energy consumption



• Sandia membrane competitive with commercial state-of-art ion exchange membranes



Soft Matter, 2021, 17, 6315



Membranes, 2021, 11, 217



Small, Percival and Spoerke, US Patent 10, 766,005, 2020



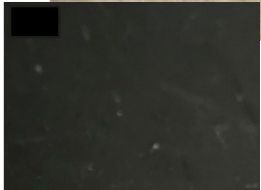
# COVID-19 Research

## NSRCs supported research to:

- understand the virus and develop novel detection methods including fast, nanotechnology-based portable diagnostics sensors
- synthesize custom nanoparticles for vaccine encapsulation and delivery
- improve effectiveness of personal protective equipment including masks, and nanoparticle-based antiviral coatings
- develop epidemiological models to predict virus spread

## Characterization of Exhaled Breath

Hydrogel bed housed in a 3D printed “whistle” allows capture of cells, bacteria, fungi, and live virus from breath. Modeling and testing determined impact of surface topography, composition, and airflow on pathogen capture. **(CNMS)**



Hydrogel lattice

## Mask Fabrics Combining Mechanical & Electrostatic Filtration

Developed a layer of high thread count cotton followed by a layer of silk, performed best. **(CNM)**

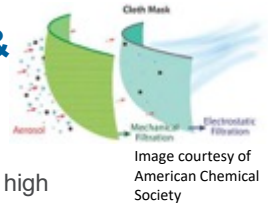
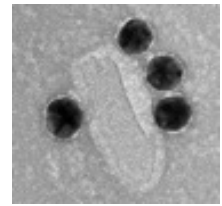


Image courtesy of American Chemical Society

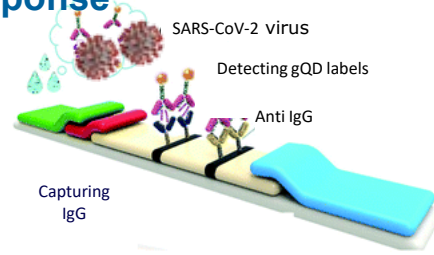


## Virus Tagging For Optical Detection

rVSV virus expressing SARS-CoV-2 spike is tagged with anti-spike antibody functionalized 50 nm Au nanoparticles for optical detection. **(CFN)**

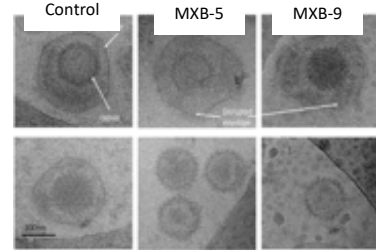
## Lateral Flow Assays (Lfas) for Immune Response

Demonstration of a LFA platform for inexpensive yet high-sensitivity/high-reliability rapid diagnostics for COVID virus and antibodies. **(CINT)**



## Cryo-EM Imaging Identified Antimicrobial Peptoids Disrupt the Viral Envelope

Samples treated with peptoids disrupted envelopes (top panels) and naked capsids (bottom panels – no envelopes). **(Foundry)**





We are ready to work with you to accelerate climate and clean energy innovation

