H2NEW Hydrogen from Next-generation Electrolyzers of Water
U.S. DEPARTMENT OF ENERGY

AMERICAN SOLAR ENERGY SOCIETY

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NREL Transforming ENERGY

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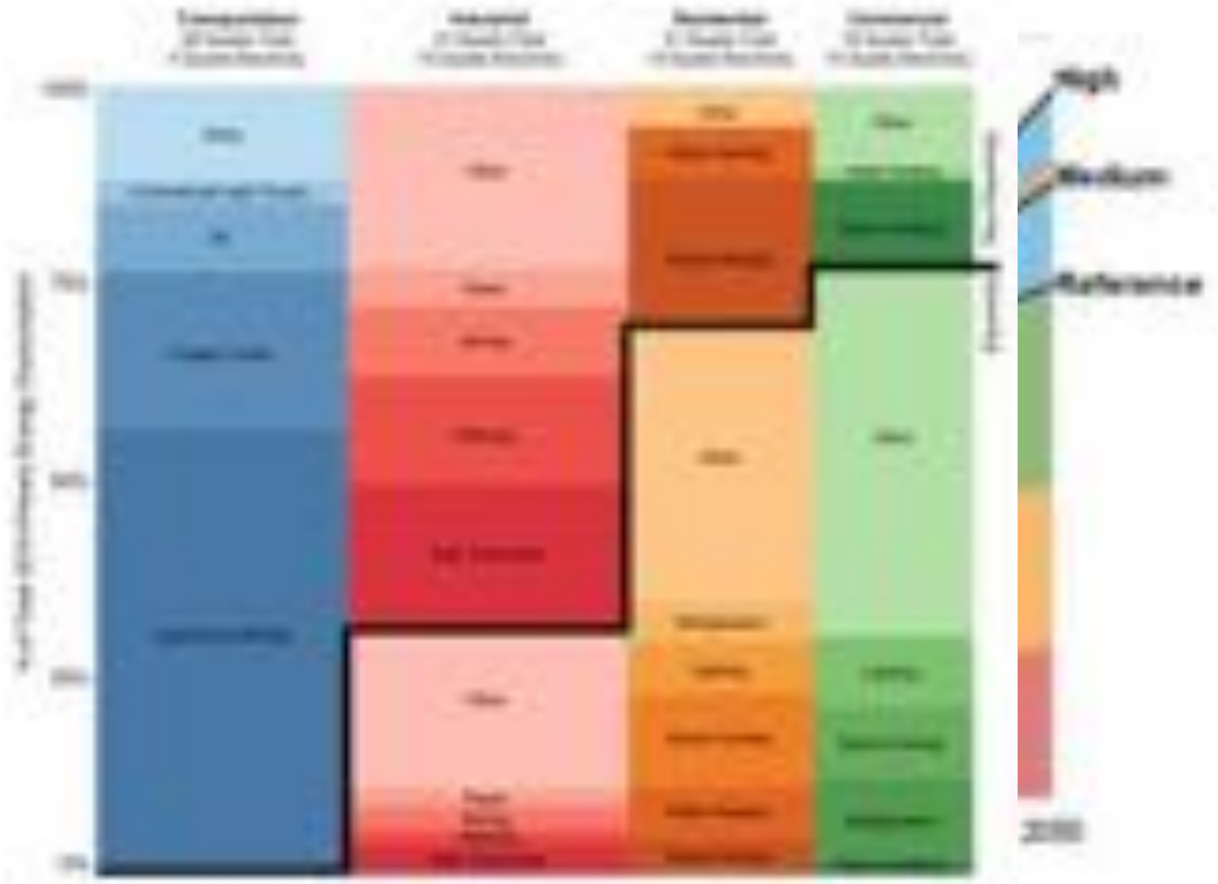
NY Times

- The United States still gets most of its energy by setting millions of tiny fires everywhere. Cars, trucks, homes and factories all burn fossil fuels in countless engines, furnaces and boilers, creating pollution that heats the planet.
- To tackle climate change, those machines will need to stop polluting. And the best way to do that, experts increasingly say, is to replace them with electric versions — cars, heating systems and factories that run on clean sources of electricity like wind, solar or nuclear power.
- **But electrifying almost everything is a formidable task and will require substantial amounts of green hydrogen.**

Electrification Key Sectors



[illegible]

These key sectors need to be the target for electrification based on the fossil energy consumed, the CO2 footprint and societal impact.

Electrification Not Just for Well-off Nations

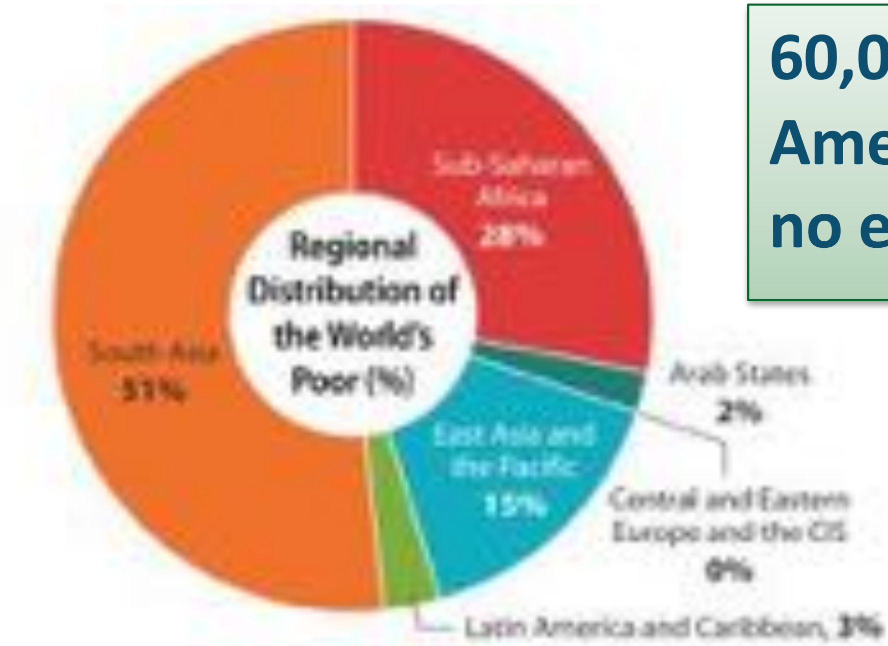
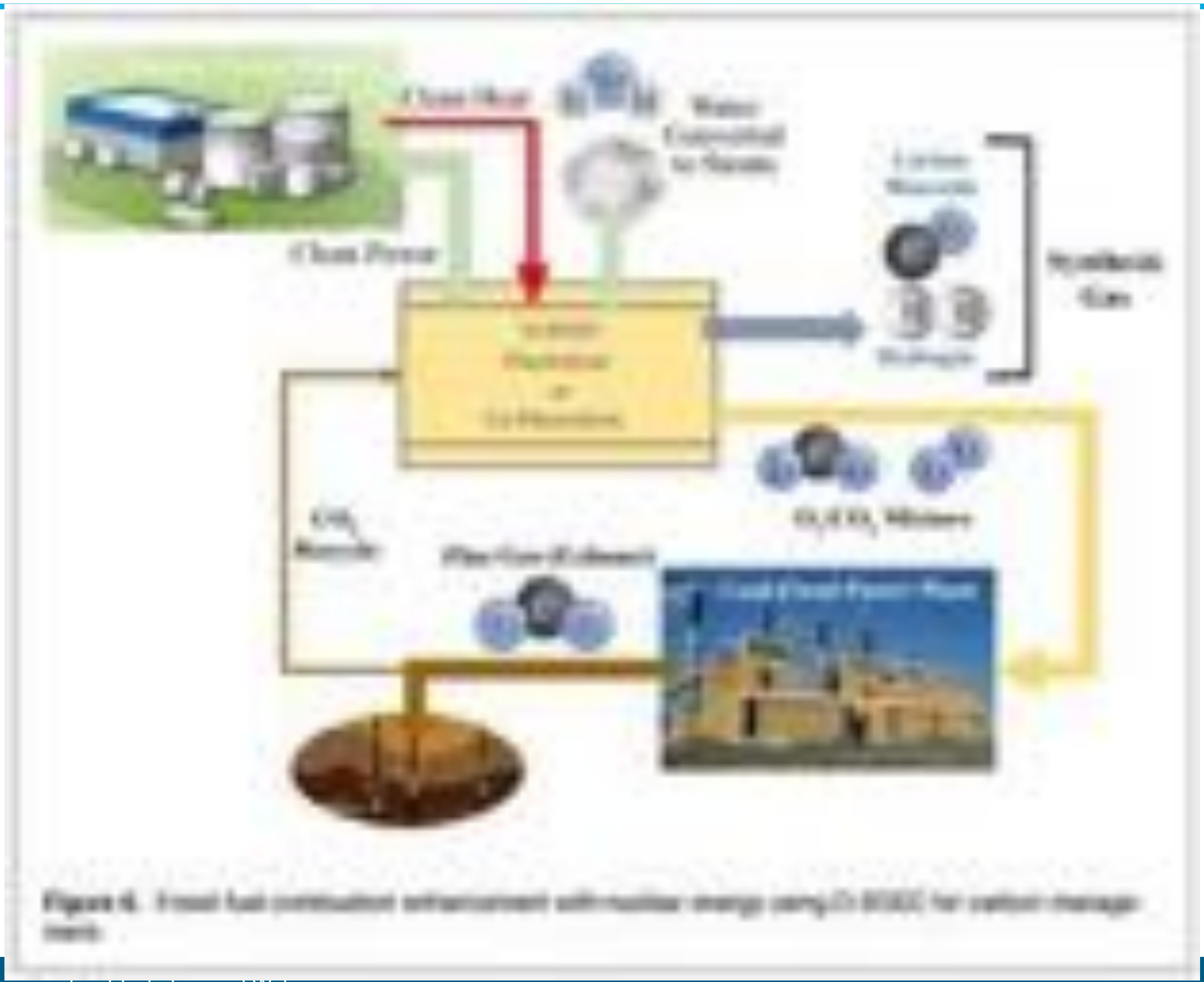


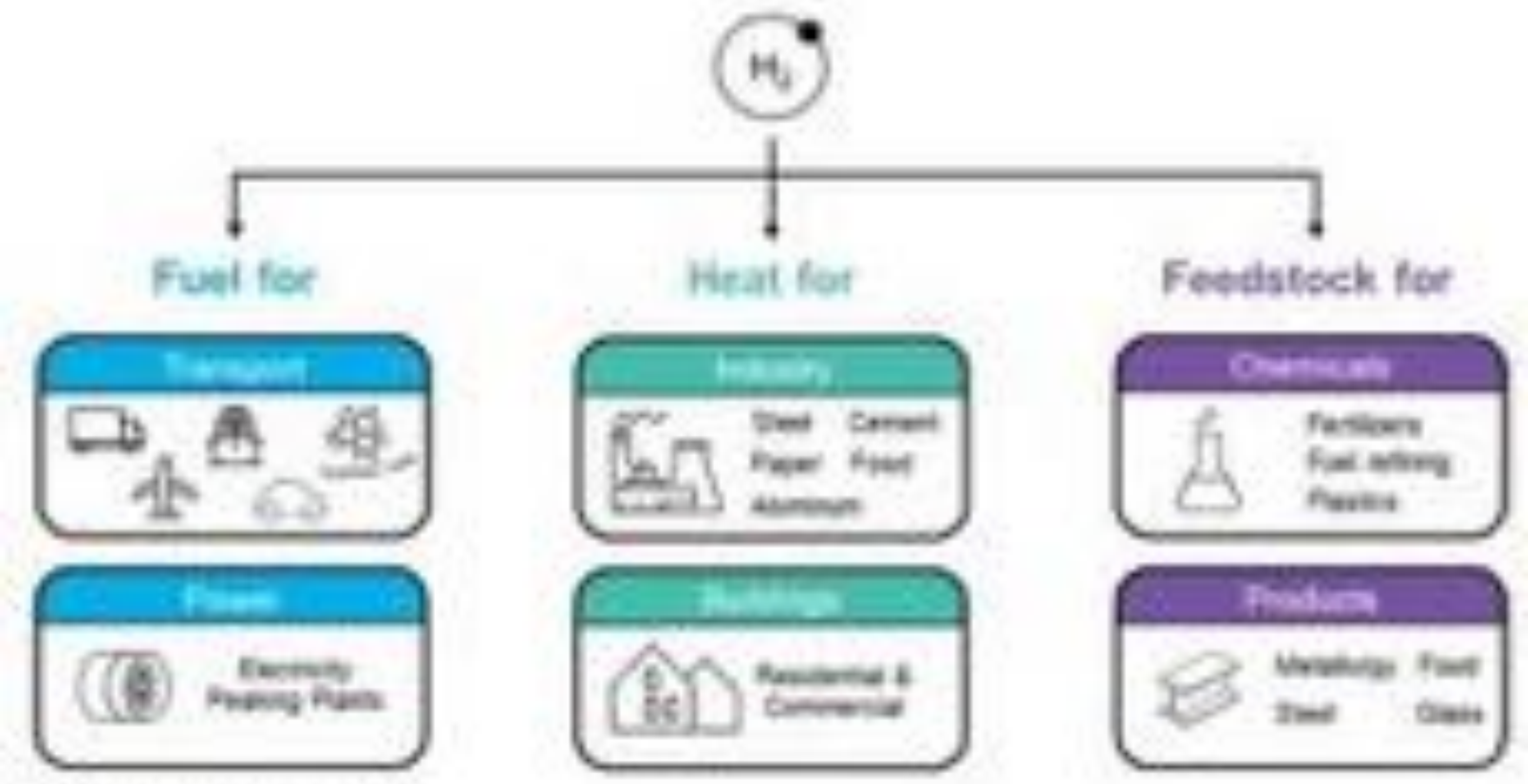
Figure 10 shows a recent compilation of the the worlds poor based on the Multidimensional Poverty Index (MPI) as used by the UN. [23]

60,000 Americans have no electricity

Green Hydrogen the Enabler but requires massive system change

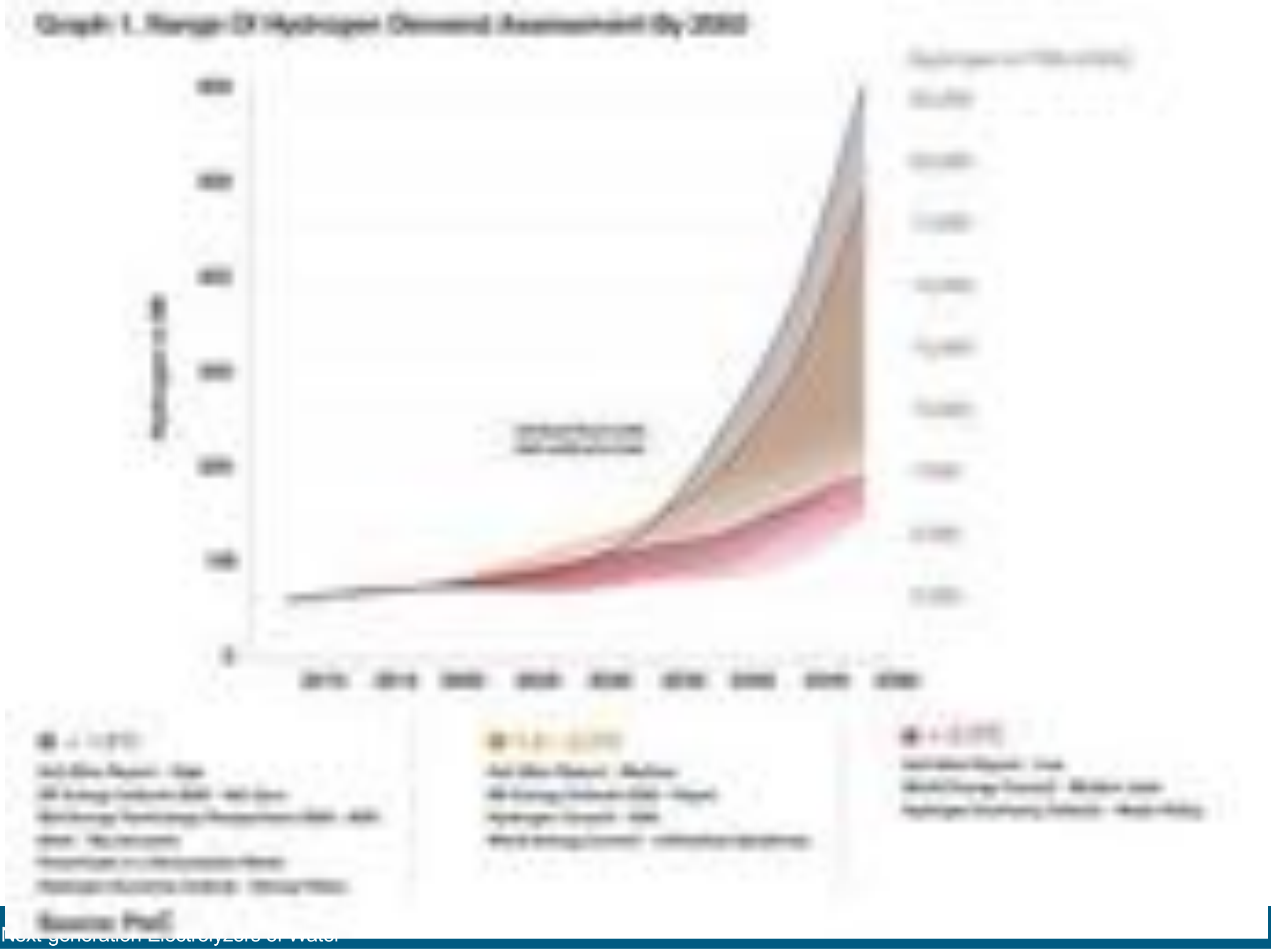


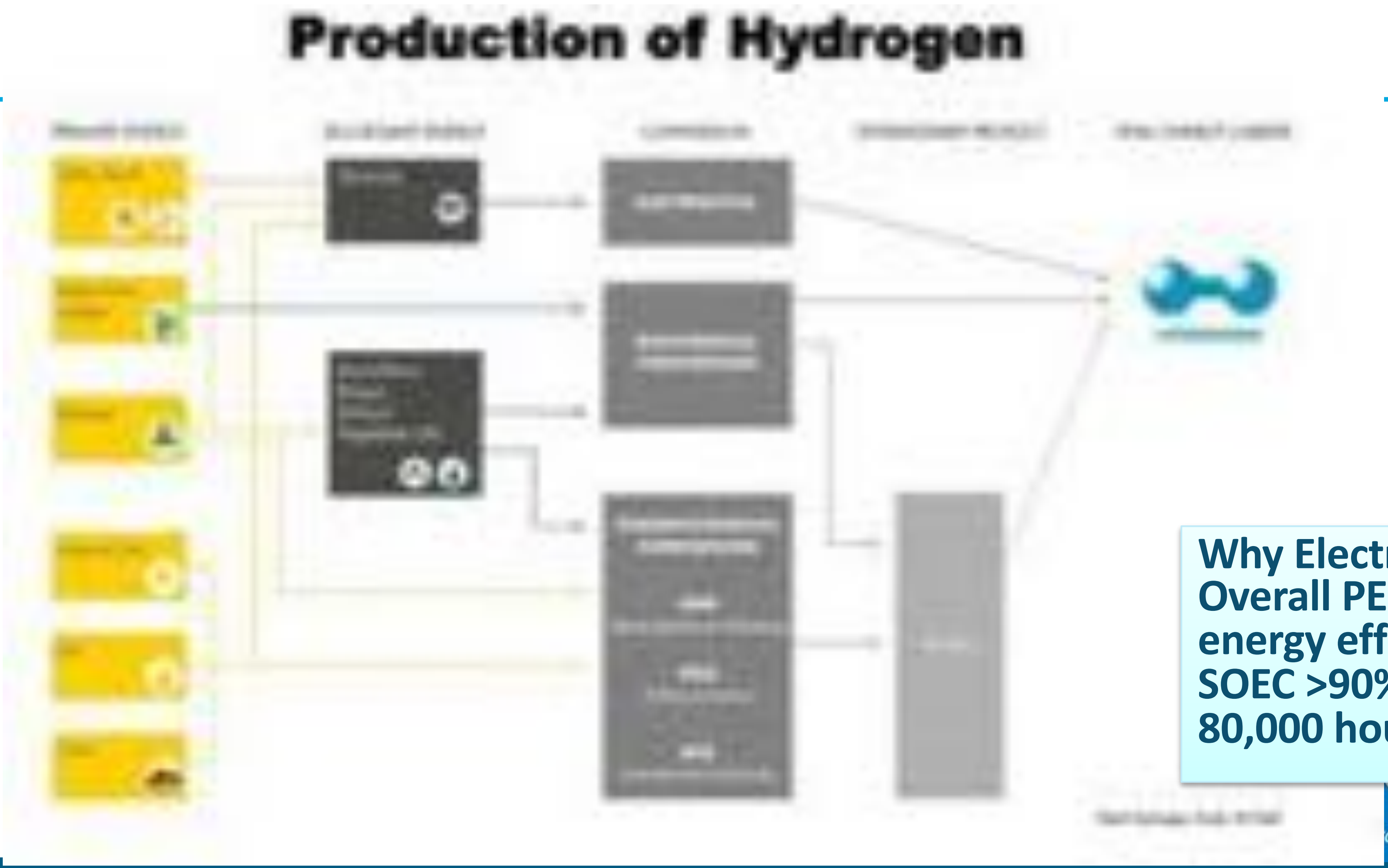
H2 Is broadly applicable and can replace many existing systems



Source: BloombergNEF

How Much is Needed





Why Electrolysis?
Overall PEM 60% energy efficiency
SOEC >90% need 80,000 hour lifetime

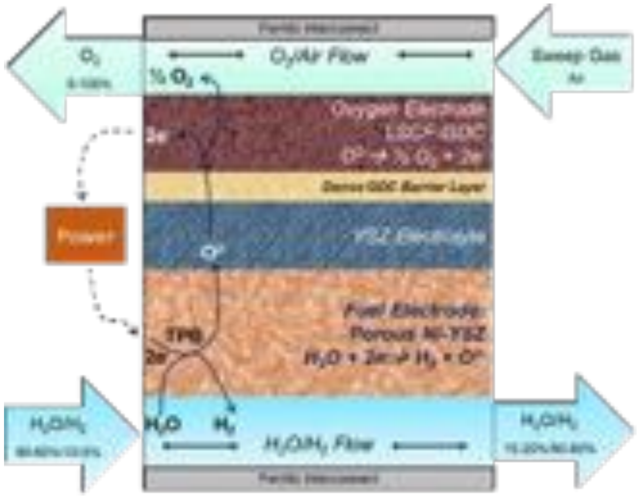
Relevance – H2NEW connection to H2@Scale

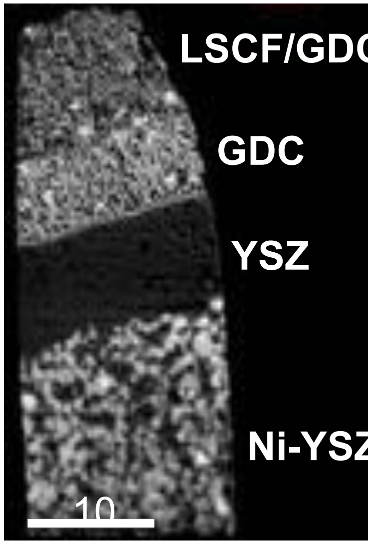
Illustrative example, not comprehensive

https://www.energy.gov/eere/fuelcells/h2-scale

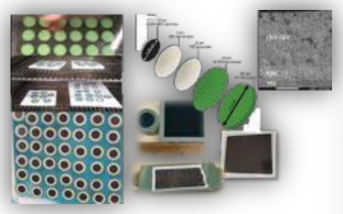
- Making, storing, moving and using H2 more efficiently are the main H2@Scale pillars and all are needed.
- Making H2 is the inherently obvious, first step to spur the wide-ranging benefits of the H2@Scale vision.
- Electrolysis has most competitive economics and balances increasing renewable generation challenges.

Overall Research Strategy

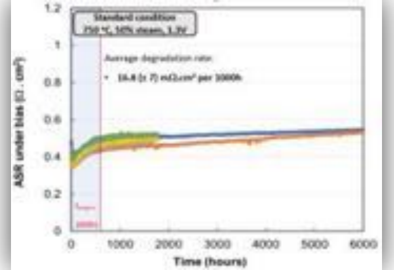


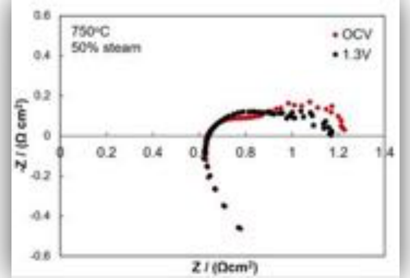


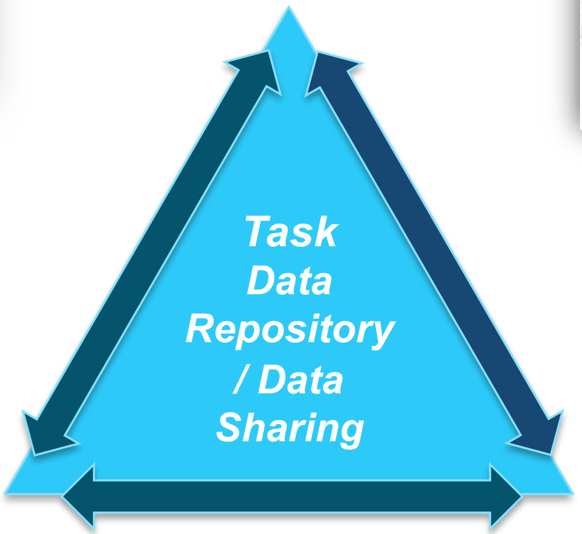
Approach: High Temperature [Steam] Electrolysis: o-SOEC



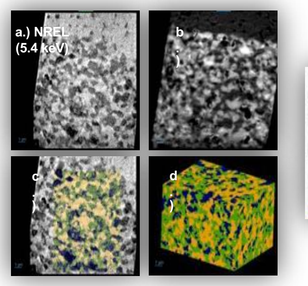
Cell Accelerated Stress Testing and Measurements

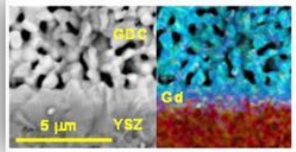


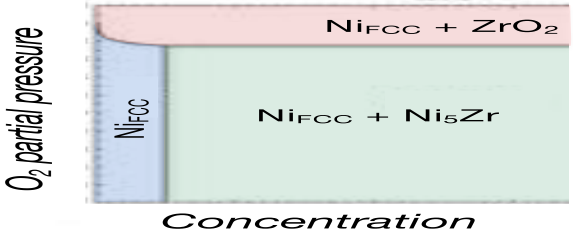




Task Data Repository / Data Sharing







Characterization: Cell and Materials Analysis

Multi-Scale Degradation Modeling

Relevance: HTE Path to DOE hydrogen cost goals.

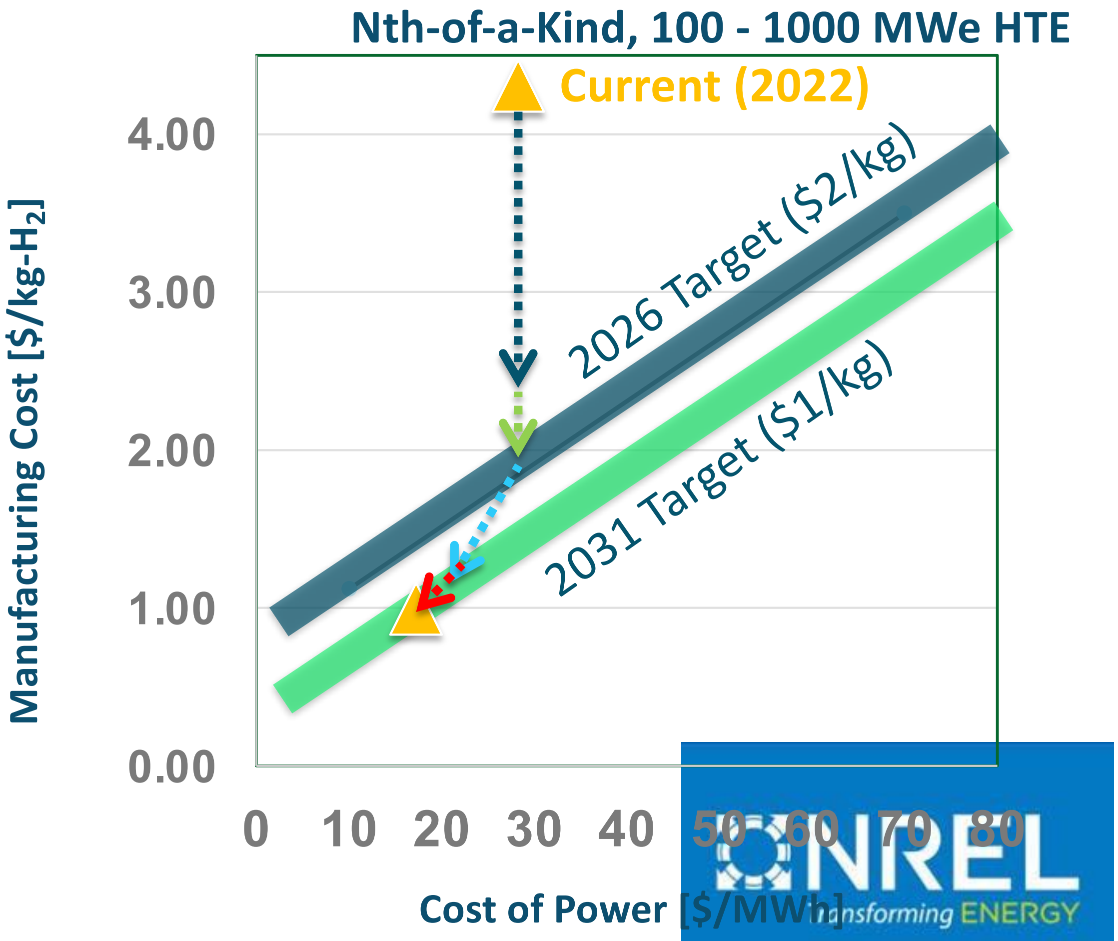
☐ **Reduce systems/balance of plant costs**
  - Lower operating temperature
  - Reduce oxygen-sweep
  - Increase external heating source
  - Optimize systems design and operations
  - Maximize plant scale

☐ **Reduce stack manufacturing costs**

☐ **Increase stack efficiency**
  - Increase steam conversion efficiency
  - Reduce ohmic heating by reducing area-specific resistance
  - Increase area-specific Faradaic efficiency by increasing current density

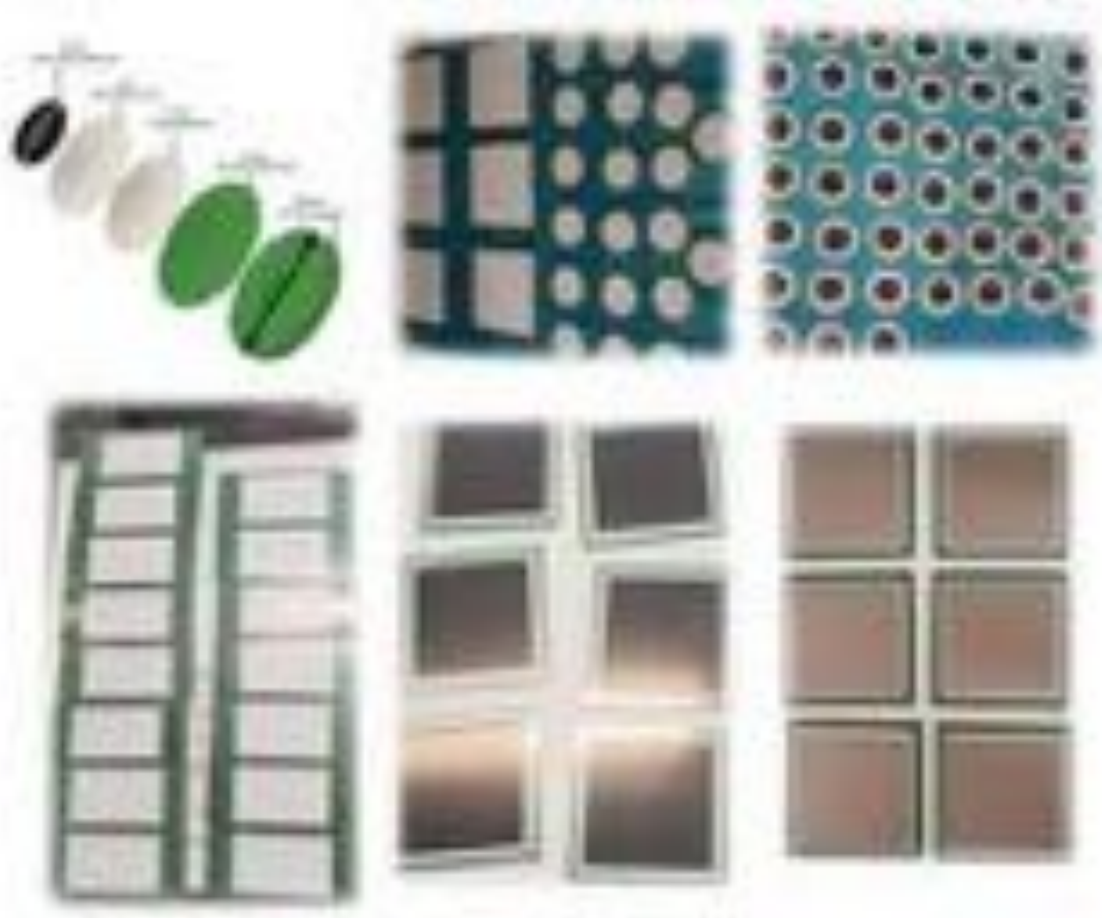
☐ **Increase stack endurance (>80,000 hr)**

☐ **Couple with industrial process**
  - Heat source (e.g., ammonia or fuels synthesis
  - Replacement of air-separation unit for O_2



Established Multiple Size Cell Production for H2NEW Partners

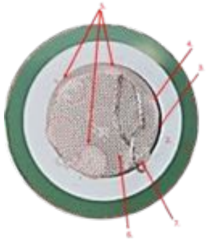
- Consortium labs use identical cells for testing, performance validation, and characterization
- Ni-YSZ electrode-supported cells in 4 different formats:
  - 2.5 cm diameter (1-5 cm^2 active area) cells
  - 1-5 cm^2 symmetric cells
  - 4 x 9 cm cells (13 cm^2 active area)
  - 5 x 5 cm cells (16 cm^2 active area)
- A batch fabrication process was developed to minimize the variance between separate cells



Established Inter-Lab Standardized Testing Protocol and Operating Procedures

LSCF electrode paste used to mount platinum mesh current collectors on the oxygen electrode.

Steam/Hydrogen electrode uses nickel paste to mount nickel mesh.



Cell preparation standardization

- Current collectors & attachment
- Precious metal reduction

Cell testing standardization:

- Heat-up
- Reduction
- Compositions

Button-Cell
2-4 cm^2
active area

Enlarged Planar Cell
10-25 cm^2
active area

Text Parameters

- Temperature
- Voltage & Current Density
- Steam/H2 mixture flow and contact with cell

Characterization of oxygen electrode and barrier layer – Potential Impact

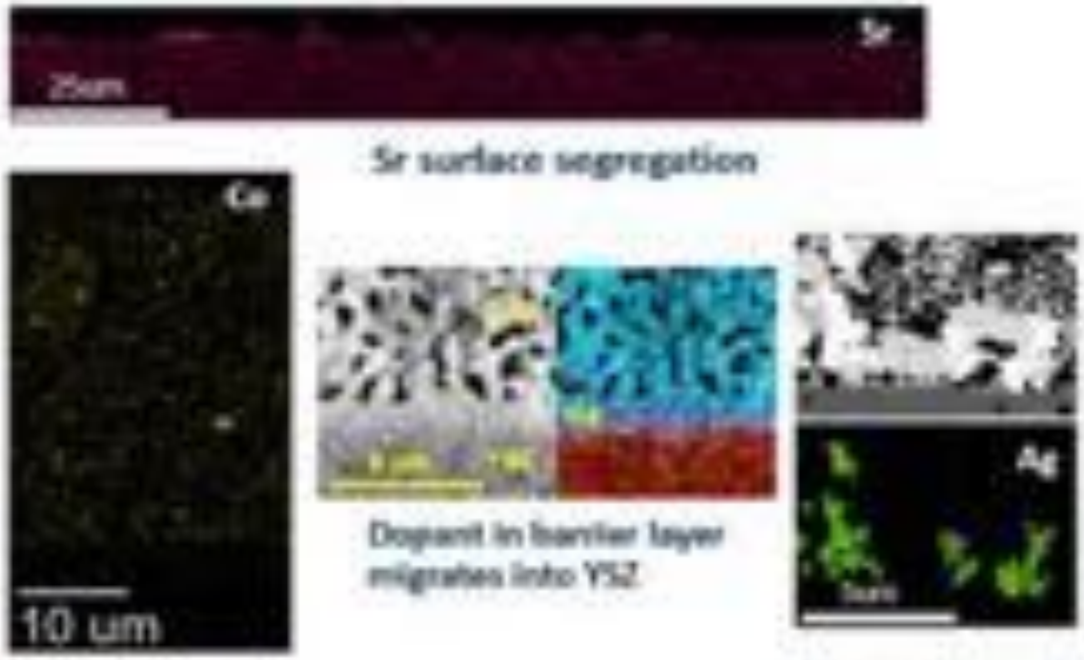
Highly integrated synchrotron XRD and electron microscopy approach.

STEM/EDX	Synchrotron XRD
Identifies frequently occurring cation correlations and locations at 1 nm-scale resolution. *XRD results inform TEM what phases are present	Identifies & quantifies all phases present at 1-µm resolution within minutes. *EDX results critical to differentiating between candidate phases w/ identical scattering patterns
Local phase concentrations	Bulk phase concentrations
Cation location within nm-resolution and migration pathways	Phase location with µm-resolution
Sub-nm resolution technique requiring significant sample prep	No sample prep/high throughput/µm-scale technique valuable for statistically relevant results & down selecting cells for further analysis

Results are integrated directly into the modeling effort.

Technical Accomplishments: Performed SEM/EDS Post-Test Cell Charterization to Elucidate Degradation Mechanisms

Oxygen Electrode Characterization



Sr surface segregation

Spinel formation increases during testing

Dopant in barrier layer migrates into YSZ

Ag migration into barrier layer and YSZ

Elemental maps of Hydrogen Electrode

- No obvious Ni migration
- Ni coarsening and Ni – YSZ particle detachment observed in 90-100% steam at 750°C

Accomplishments and progress: Characterization of oxygen electrode and barrier layer

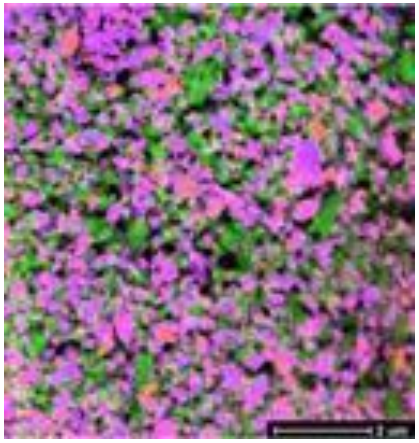
STEM-EDS – Pre Ni Reduction and Testing

- EDS of the oxygen electrode layer reveals initial cation exsolution (predominantly Sr) at the interface and in the barrier layer
- Formation of $CoFeO_x$, SrO, and other phases occur before testing

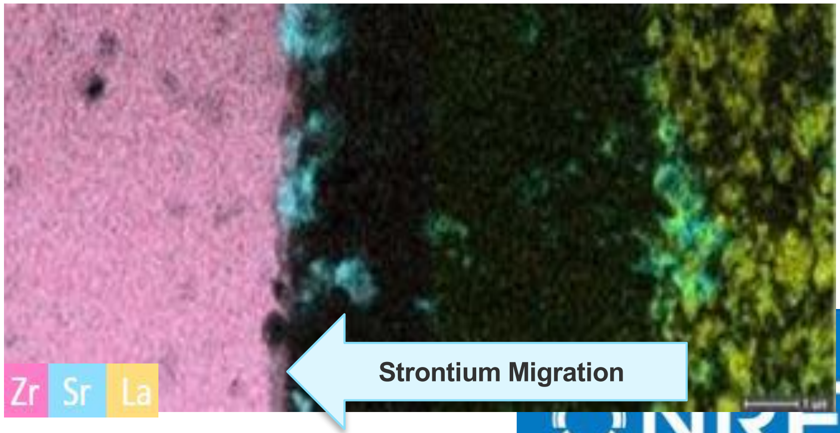
STEM-EDS – Tested for 1k hrs

- Sr migration through the GDC and accumulation at the YSZ interface occurs
- Increase in $CoFeO_x$ spinel concentration
- GDC breakdown resulation into $CeCoFeO_x$ spinelting in Gd accumulation at the YSZ interface

The oxygen electrode has undesired phases present prior to any ageing; cation migration and degradation increase in severity with cell ageing

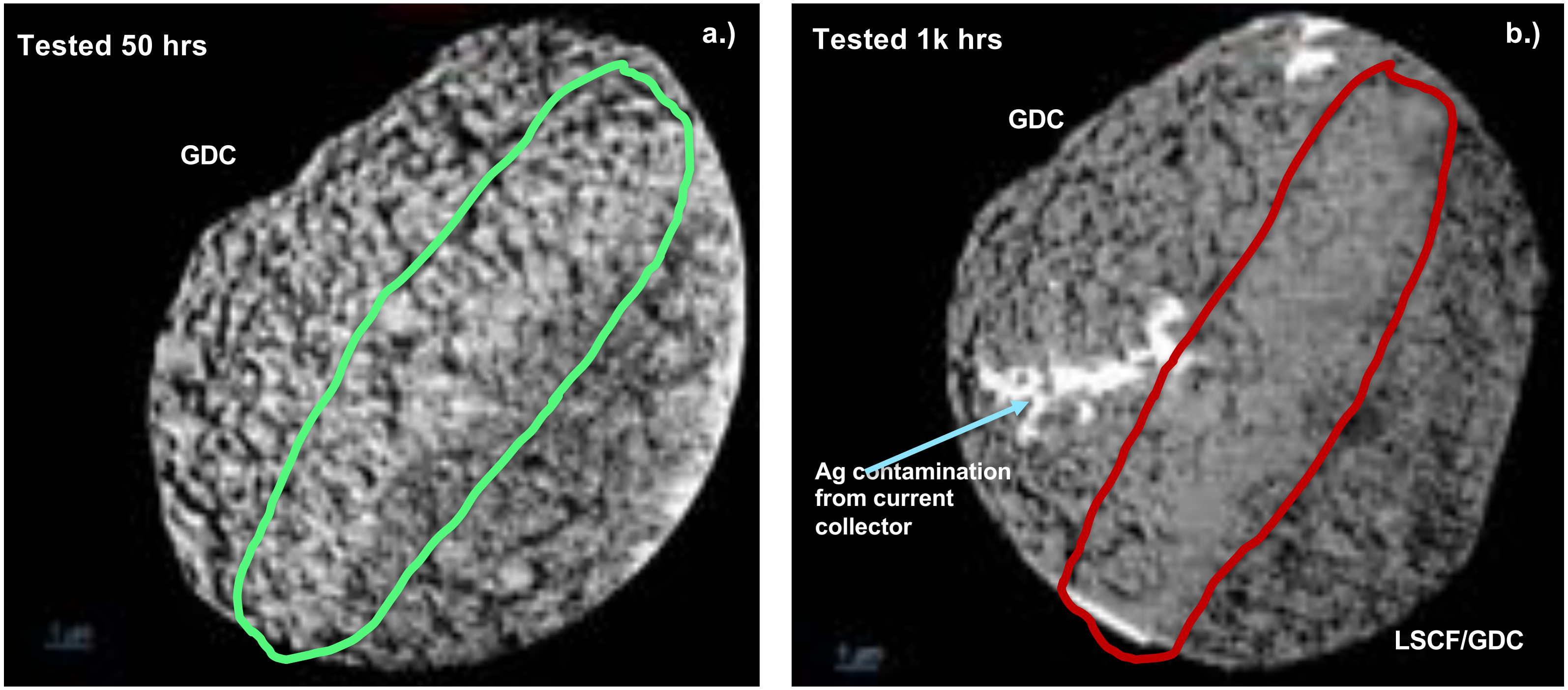


*EDS map of **Co**, **Fe**, and **Ce** in the oxygen electrode where $CoFeO_x$ spinel appears pink*



Zr, Sr, and La EDS map of the electrolyte, barrier layer, and oxygen electrode illustrating the migration of Sr

Accomplishments and progress:
Characterization of oxygen electrode and barrier layer



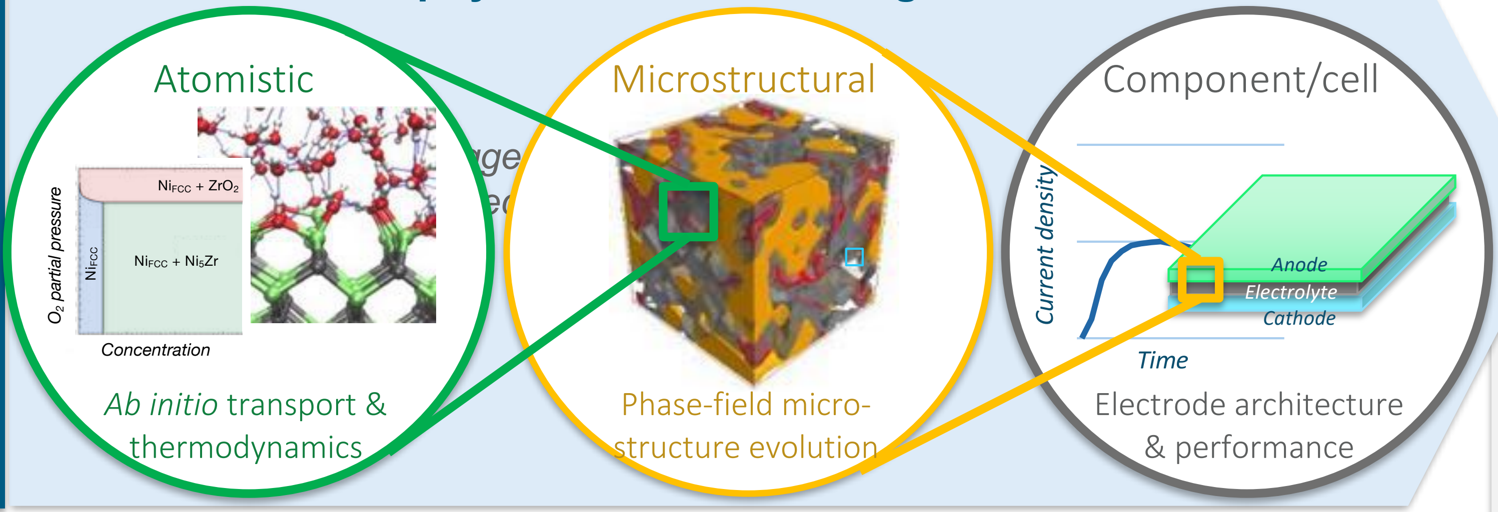
2D Nano-CT projections capturing the oxygen electrode and barrier layer interface in cells tested for a.) 50 and b.) 1k hours

Nano-CT images reveal interface densification occurring after extended cell operation, which may result in performance loss due to restricted mass and ionic transport

Multi-Scale Degradation Modeling- Approach

“Bottom-up”

Multiscale physics-based modeling of mechanisms



Atomistic

Ab initio transport & thermodynamics

Microstructural

Phase-field micro-structure evolution

Component/cell

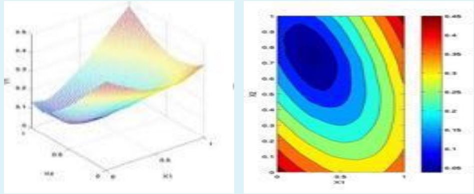
Electrode architecture & performance

Models are linked across scales, correlated to testing data, and accelerated with ML/AI

“Top-down”

Performance analysis

test matrix → correlations → inferences



Relevant degradation modes

Materials/ components/ cells

Operating conditions

Accomplishment: Computationally assessed impact of Ni/YSZ ratio, operating conditions, and microstructure on Ni redistribution

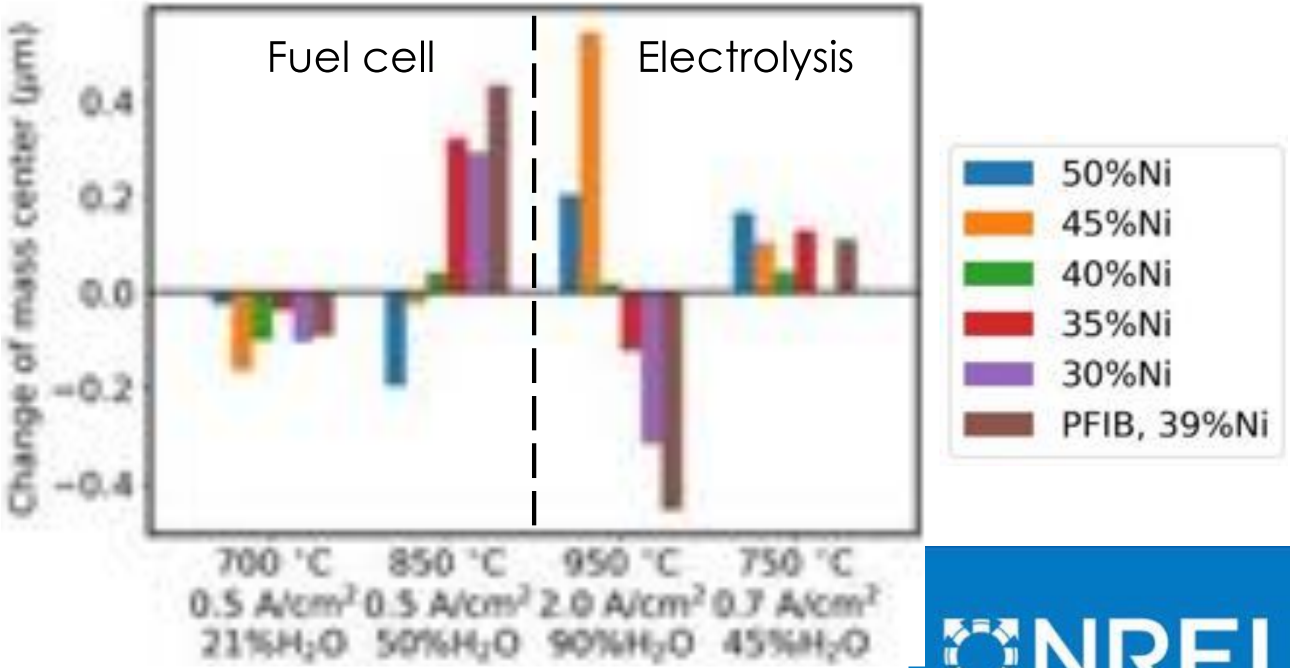
*Models suggest that not just **operating conditions**, but also **microstructural features** and **Ni loading** can impact the direction and magnitude of Ni redistribution*

Synthetic

Ni	YSZ	Pore
49.6%	30.0%	20.3%
44.5%	35.3%	20.2%
39.9%	40.0%	20.1%
34.5%	45.8%	19.7%
30.0%	50.1%	19.9%

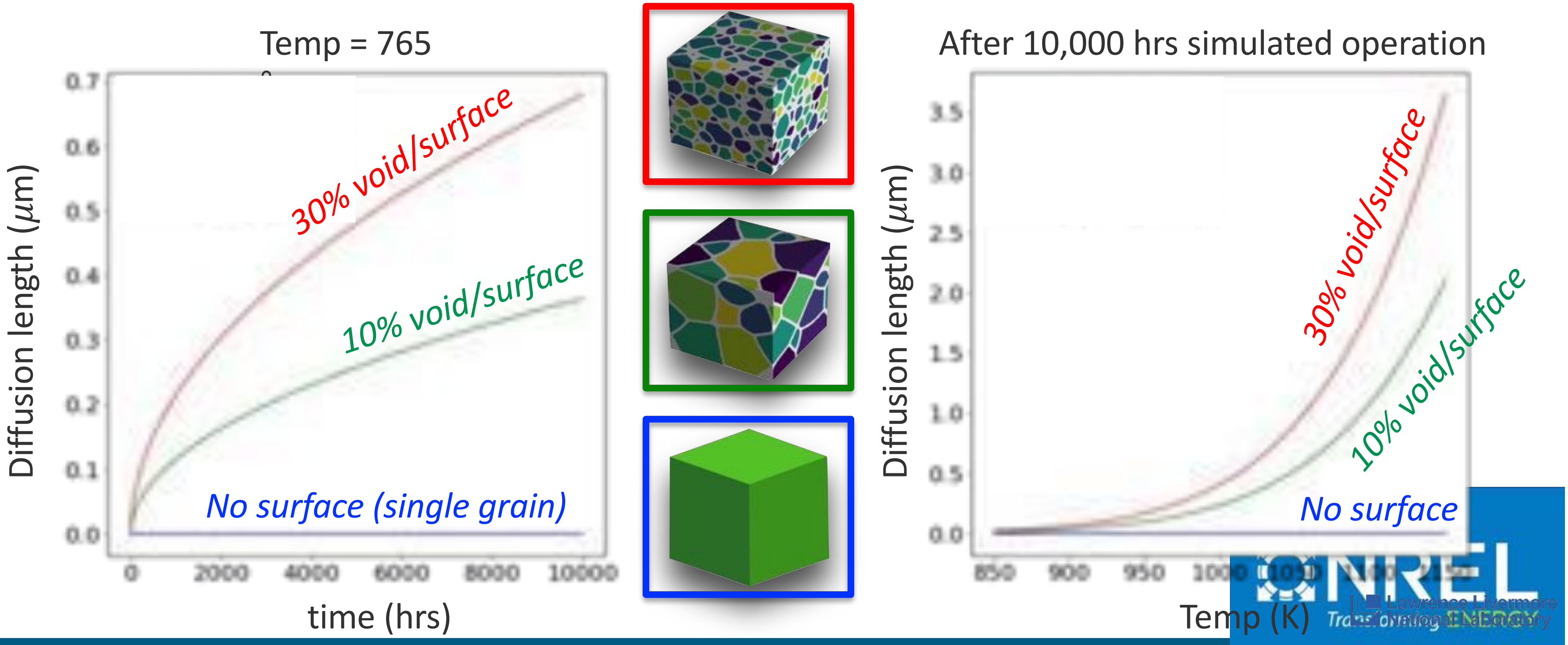
PFIB Reconstructed

Ni	YSZ	Pore
39.4%	43.2%	17.4%



Accomplishment: Demonstrated multiscale framework for predicting Sr penetration into packed GDC as a possible failure mode

Porosity and loose particle packing create surface-dominated diffusion pathway for Sr and other cation impurities, with full permeation of GDC interlayer predicted as possible under operation



Summary

- Green hydrogen is an enabler for moving away from petroleum to a more sustainable energy system
- It will be required in all sectors at scale
- Renewable electrons are key to all electrolysis approaches
- If lifetimes can be achieved (80,000 hours) current efficiencies are scalable
- If hydrogen can be made at scale then other areas are enabled
  - Solar fuels
  - Ammonia
- The development of new analysis and modeling is leading to an understanding of degradation mechanisms and and the validity of accelerated aging.