SOC Research and Development at NETL

Harry Abernathy

Team Lead, NETL SOC Research
Research & Innovation Center

OFCHC Solid Oxide Forum

11/19/2024

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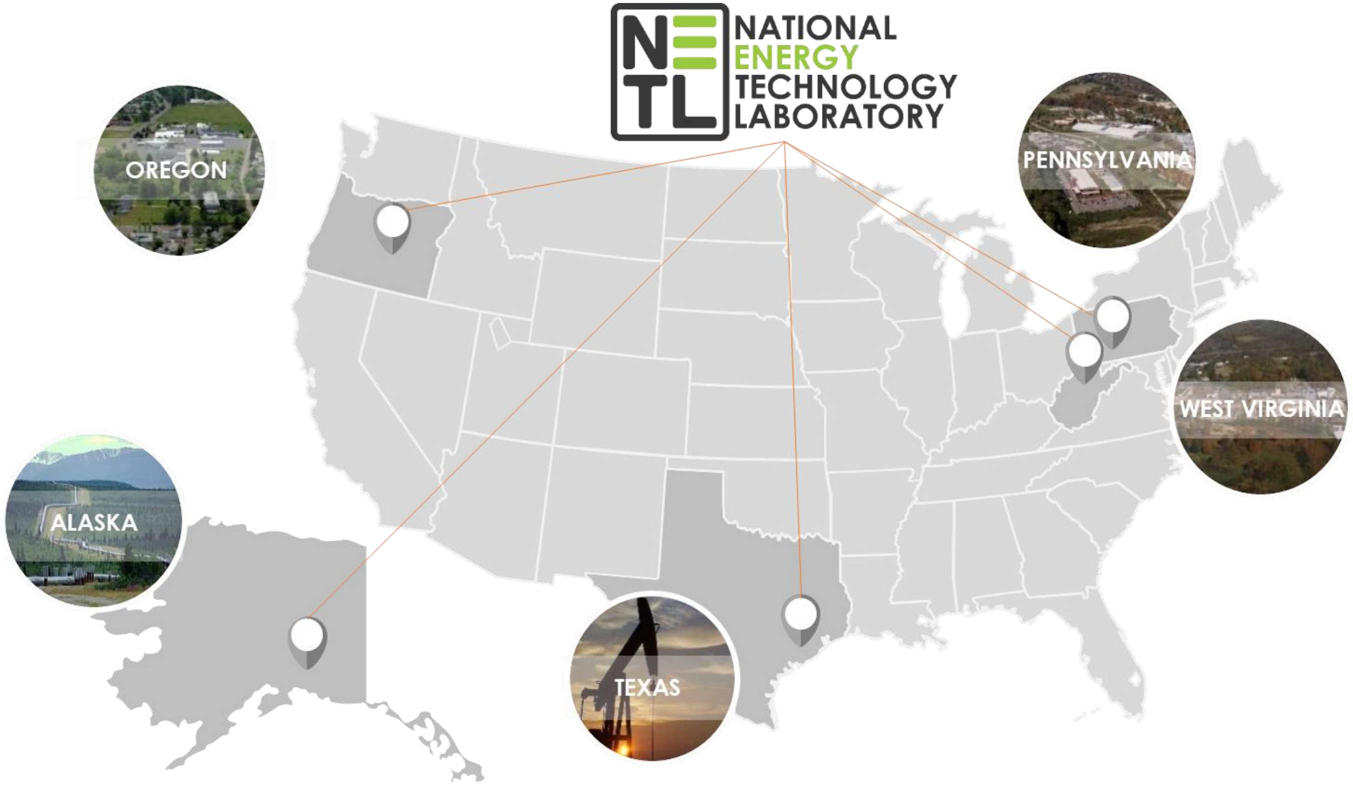
Outline

- **R-SOFC Program/NETL Overview**

- **Case Studies**
  - SOC systems analysis
  - Designing new materials
  - Engineering better electrodes
  - Optimizing lifetime performance



NETL SOC FY25 Personnel

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- **Harry Abernathy (TPL, MGN)**
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- **Kyle Buchheit (SOFC Task PI, PGH)**
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- William Kent (PhD student)
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- Rochan Bajpal (PhD student)

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- Arun Iyengar (KeyLogic/PGH)
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- Fei Xue (LRST/ALB)
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- Pattiya Pibulchinda (MSE PhD Student)

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- Ryan Jacobs (MSE)
- Chiyoung Kim (MSE PhD student)

West Virginia University
- Harry Finklea (Chemistry)
- Ed Sabolsky (MAE)
- Davis Warmuth (PhD student)
- Xueyan Song (MAE)
- Xingbo Liu (MAE)
- Yun Chen (WV Research Corp.)

FECM R-SOFC Program R&D Goals

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Enable:

- Highest efficiency and lowest cost electric power generation from hydrogen and natural gas with CCS
- Efficient and cost-effective distributed/utility scale hydrogen production
- Flexible modular hybrid SOFC/SOEC system design
- Hybrid R-SOFC systems for power production or hydrogen production as energy storage

KEY TECHNOLOGIES

Cell Development

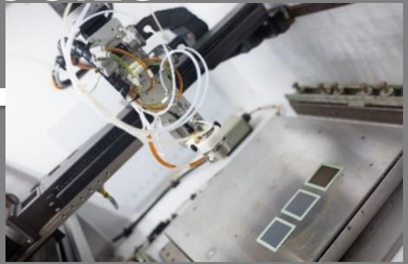


Figure courtesy NETL

Core Technology

Figure courtesy LG Fuel Cell Systems

Systems Development for SOFC and Reversible Systems

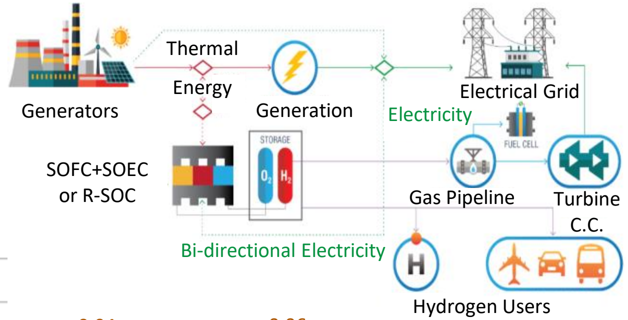
Figure courtesy FuelCell Energy

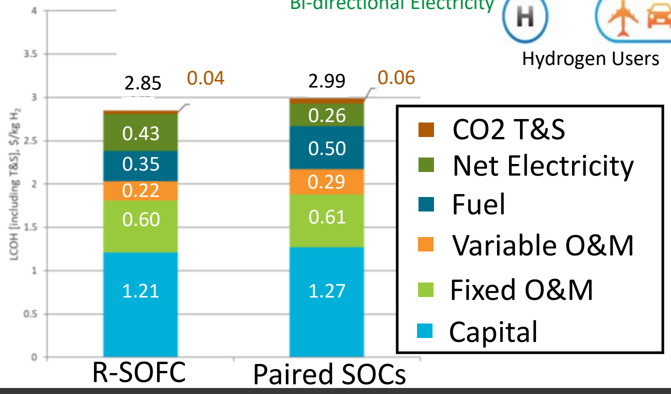
NETL SOC Capability Overview

CHALLENGE: SOC technology is cost prohibitive due to long-term performance degradation
APPROACH: Develop degradation modeling and mitigation tools to improve performance / longevity

Systems Engineering and Analysis

- Techno-Economic Analysis
- R&D Goals Evaluation

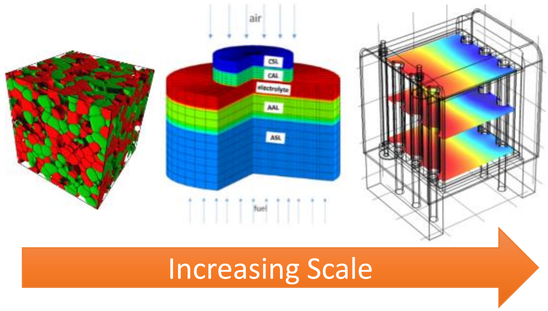


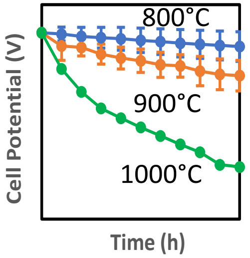


Levelized Cost of H_2 at $20/MWh Electricity

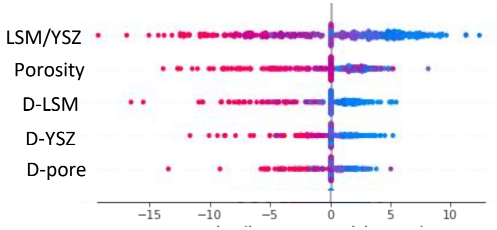
Performance Degradation Modeling

- Degradation prediction tools
- Atoms-to-System scale bridging
- Cell design optimization





Machine learning-informed design tools

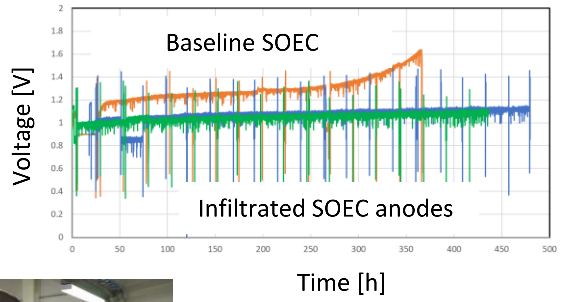


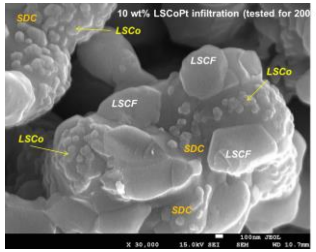
Impact of microstructural features on lifetime performance

Electrode Engineering

- Degradation mitigation
- Advanced manufacturing
- Technology scale-up and transfer

Infiltrated Cells from **6** Partners





Enabling R-SOC Technology

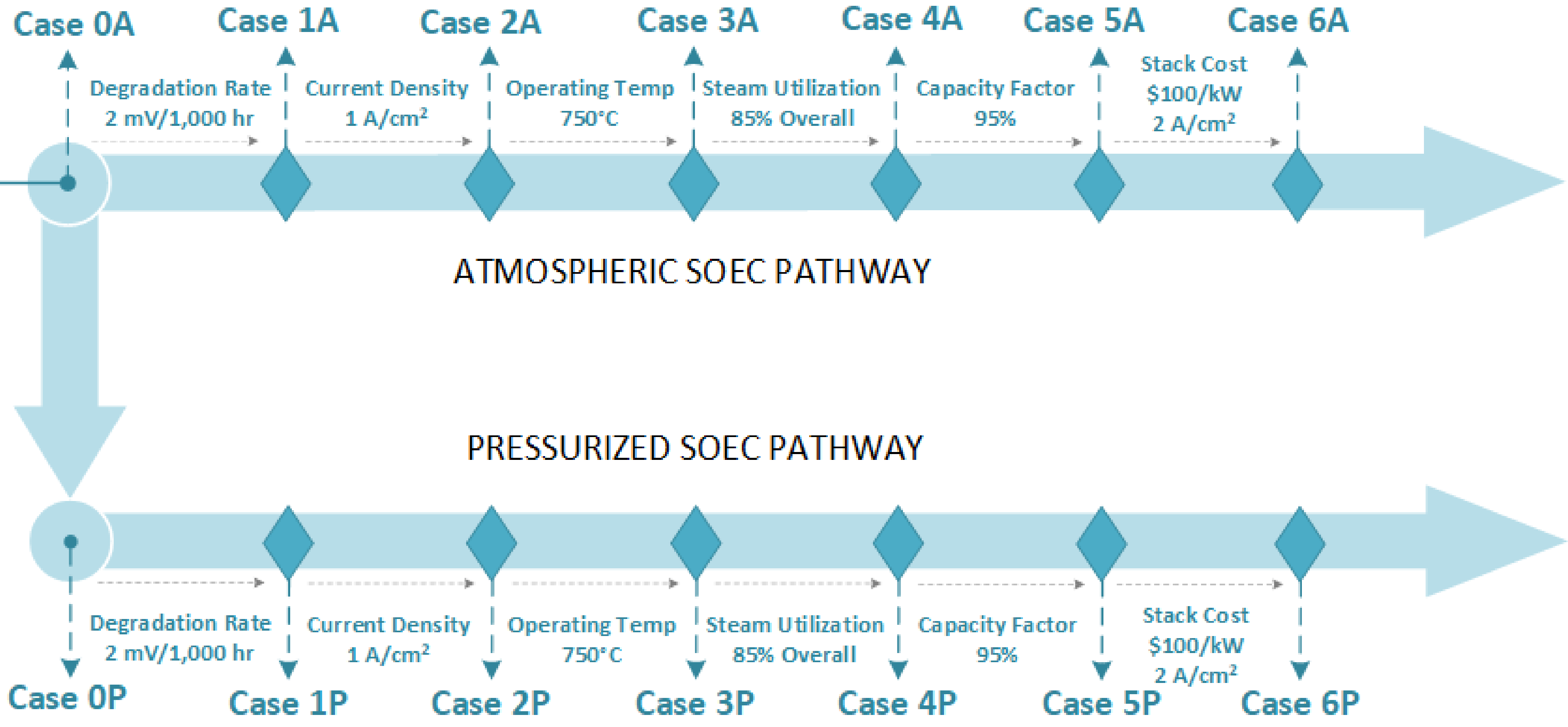
Systems Analysis

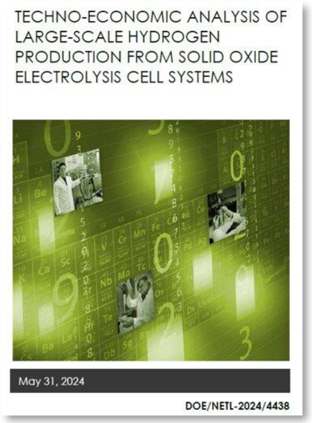
NETL SOEC Technology Pathway Study

Atmospheric Operation

SOEC State of the Art

Current Density: 0.5 A/cm²
Operating Temperature: 850°C
Degradation Rate: 8 mV/1,000 hr
Overall Steam Utilization: 80%
Capacity Factor: 90%
Stack Cost: $300/kW
Operating Pressure: 1 bar




TECHNO-ECONOMIC ANALYSIS OF LARGE-SCALE HYDROGEN PRODUCTION FROM SOLID OXIDE ELECTROLYSIS CELL SYSTEMS

May 31, 2024

DOE/NETL-2024/4438

Pressurized Operation (8 bar)

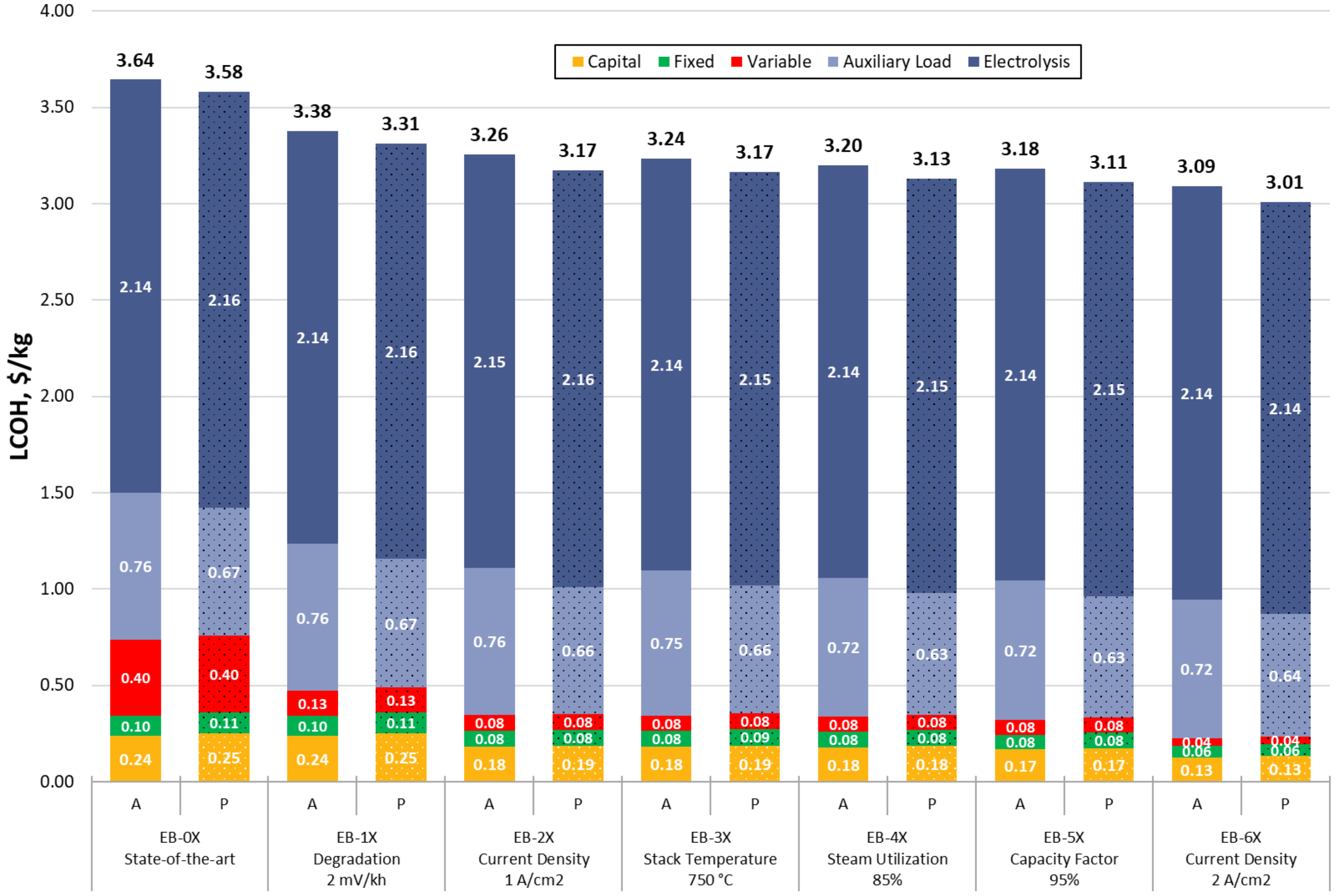
Note: Current density and degradation rate not changed between two pathways

Source: NETL

A. Noring, et al., "Techno-Economic Analysis of Large-Scale Hydrogen Production from Solid Oxide Electrolysis Cell Systems," NETL, Pittsburgh, May 31, 2024. ***doi.org/10.2172/2370402***

Breakdown of Costs for H_2 Production

- Integrating ***waste heat*** can save up to an additional $0.50/kg (for $60/MWh COE)



Electricity makes up majority of H_2 costs

SOEC improvements are critical to reach $1/kg H_2

* Costs based on electricity costs of $60/MWh in 2018$

Pathway Waterfall Plot (without electricity costs)

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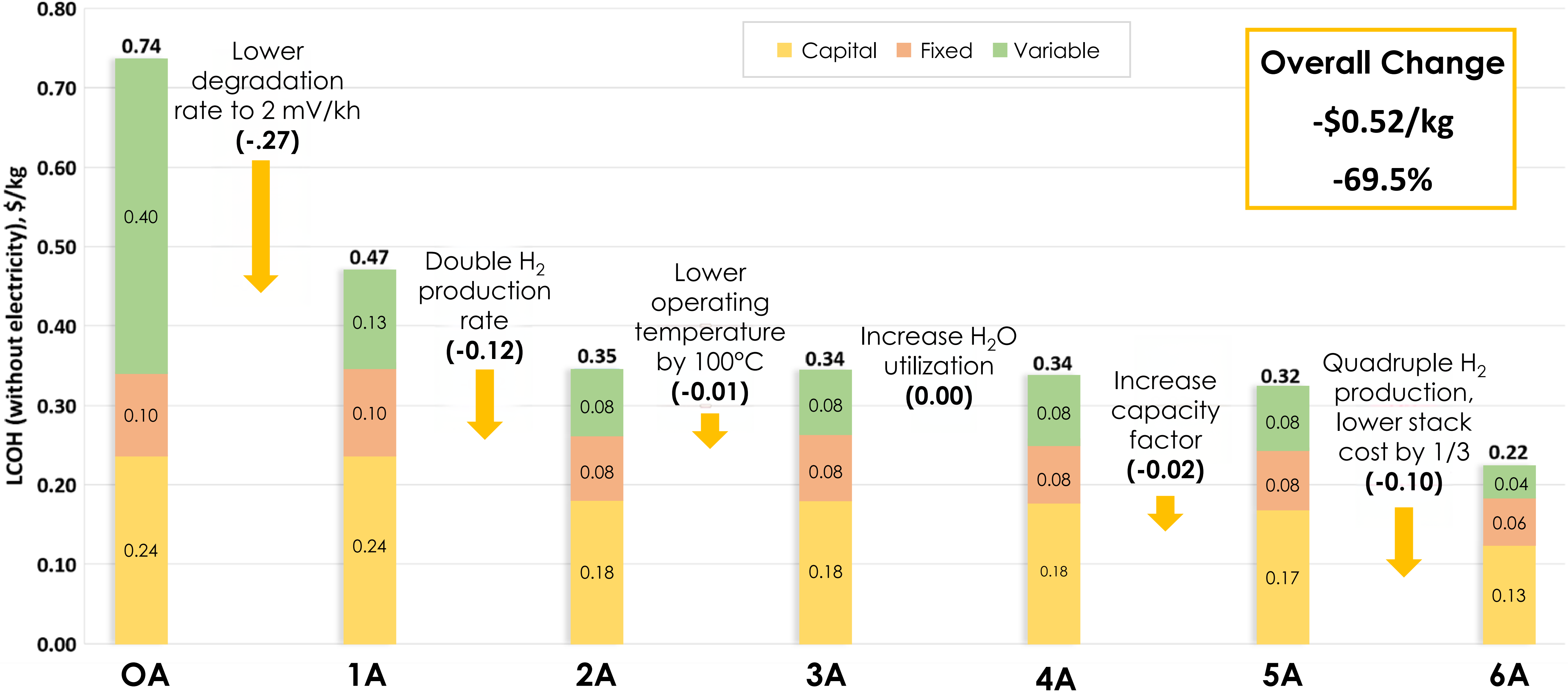

U.S. Department of ENERGY

Maximum Electricity Price Needed for $1/kg

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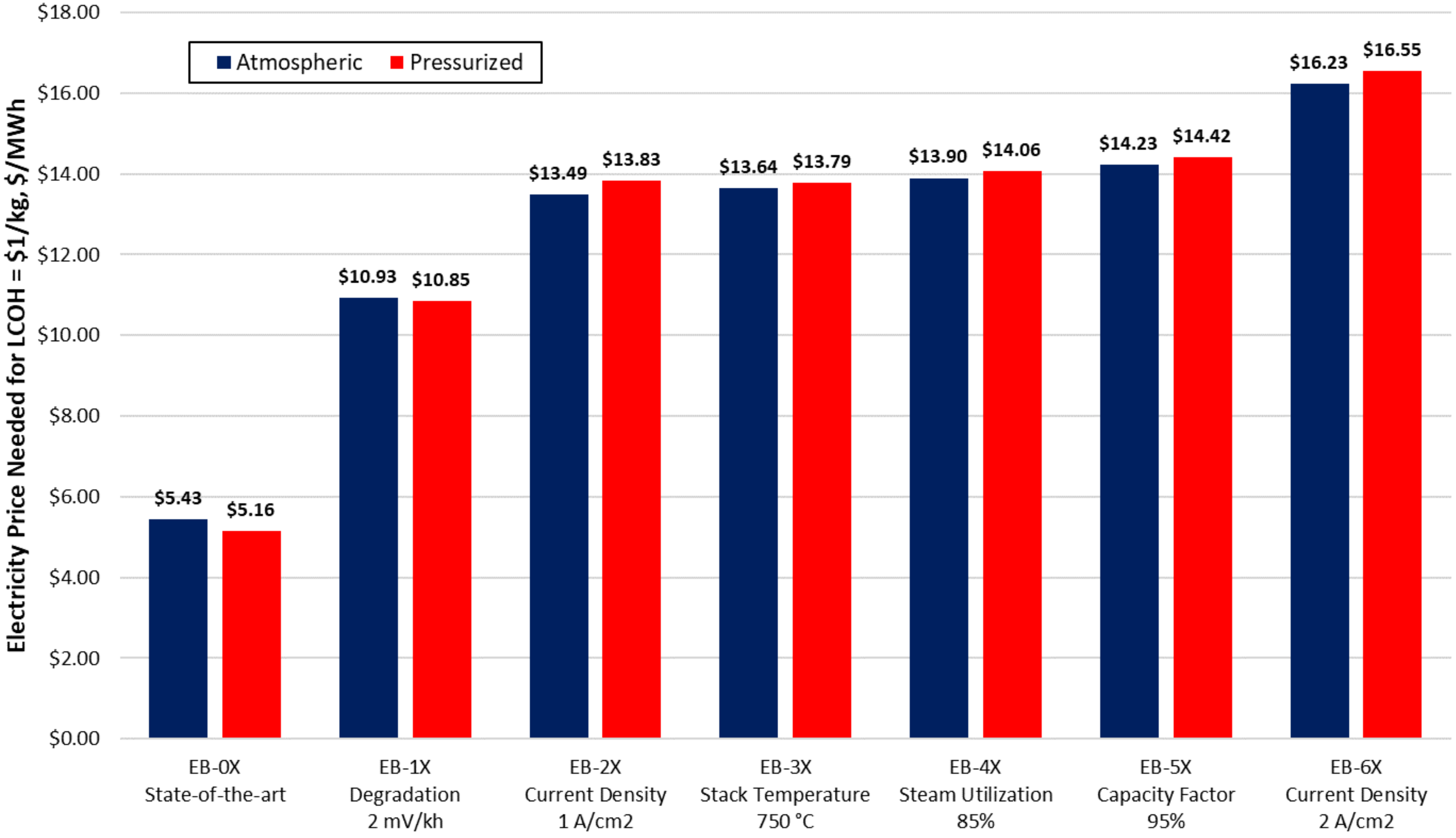
Providing perspective for Hydrogen Shot goal

H2 can be made for $1/kg only if COE is *BELOW* indicated price



Reversible Solid Oxide Cell Systems Analysis

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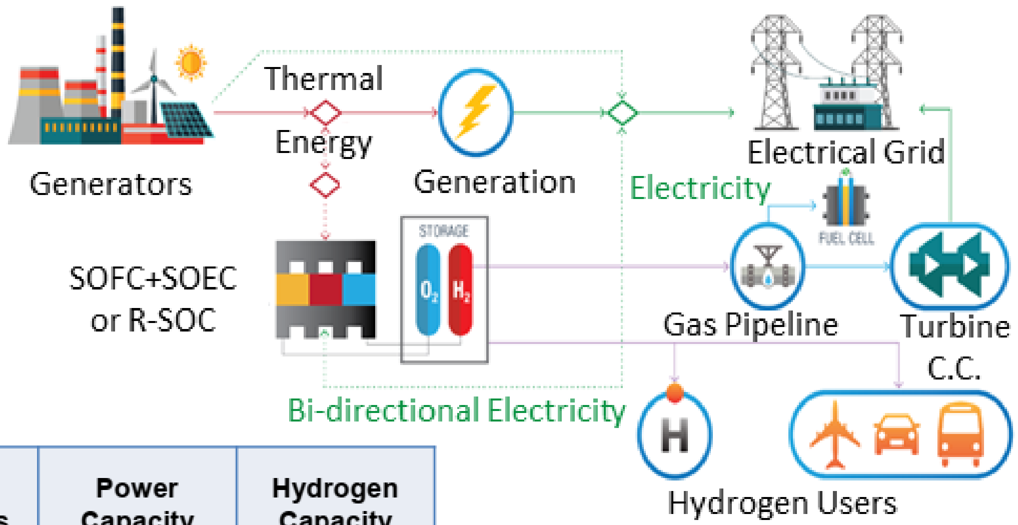
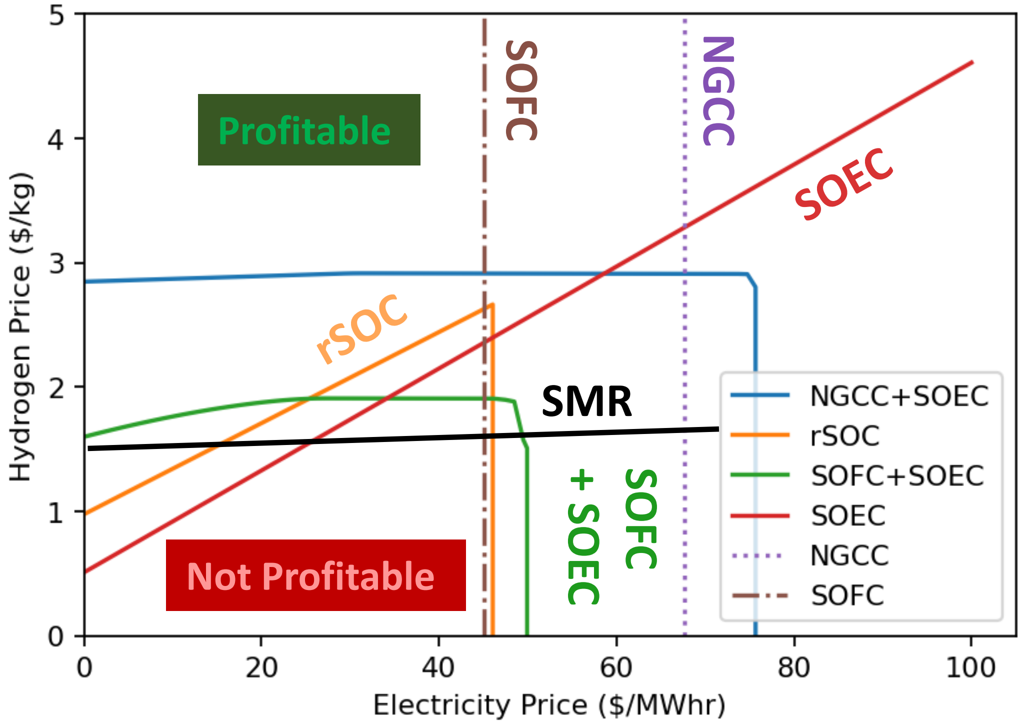
NETL is exploring whether coupled integrated energy systems with the flexibility to produce both power and hydrogen should play a role in decarbonizing the US power sector by 2035 and broader economy by 2050.



Process Concepts	Power Capacity ($MW_{e,net}$)	Hydrogen Capacity (kg/s)
NGCC	650	-
SOFC	650	-
NGCC + SOEC	650	5
rSOC	650	5
SOFC + SOEC	710	5
SOEC	-	5



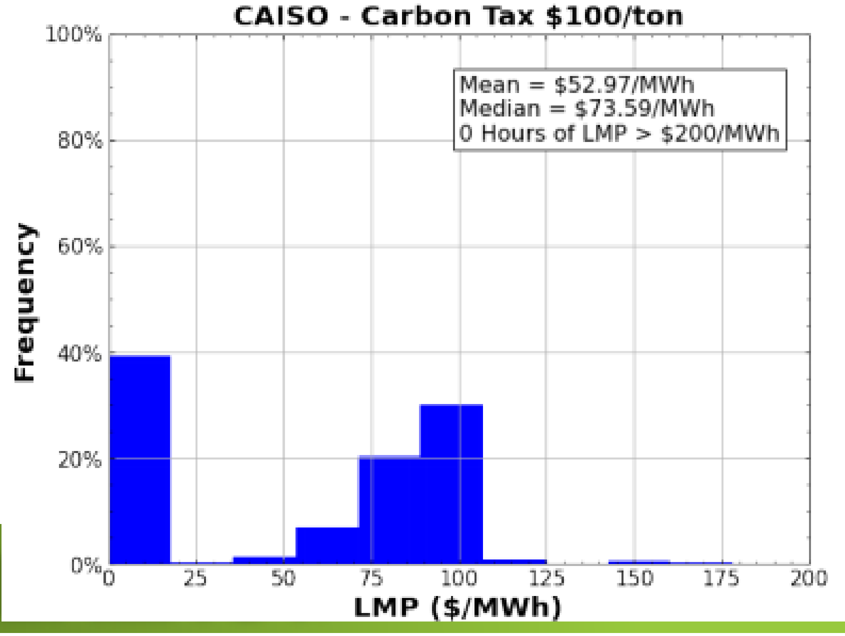
Breakeven curves for H_2/Power Production

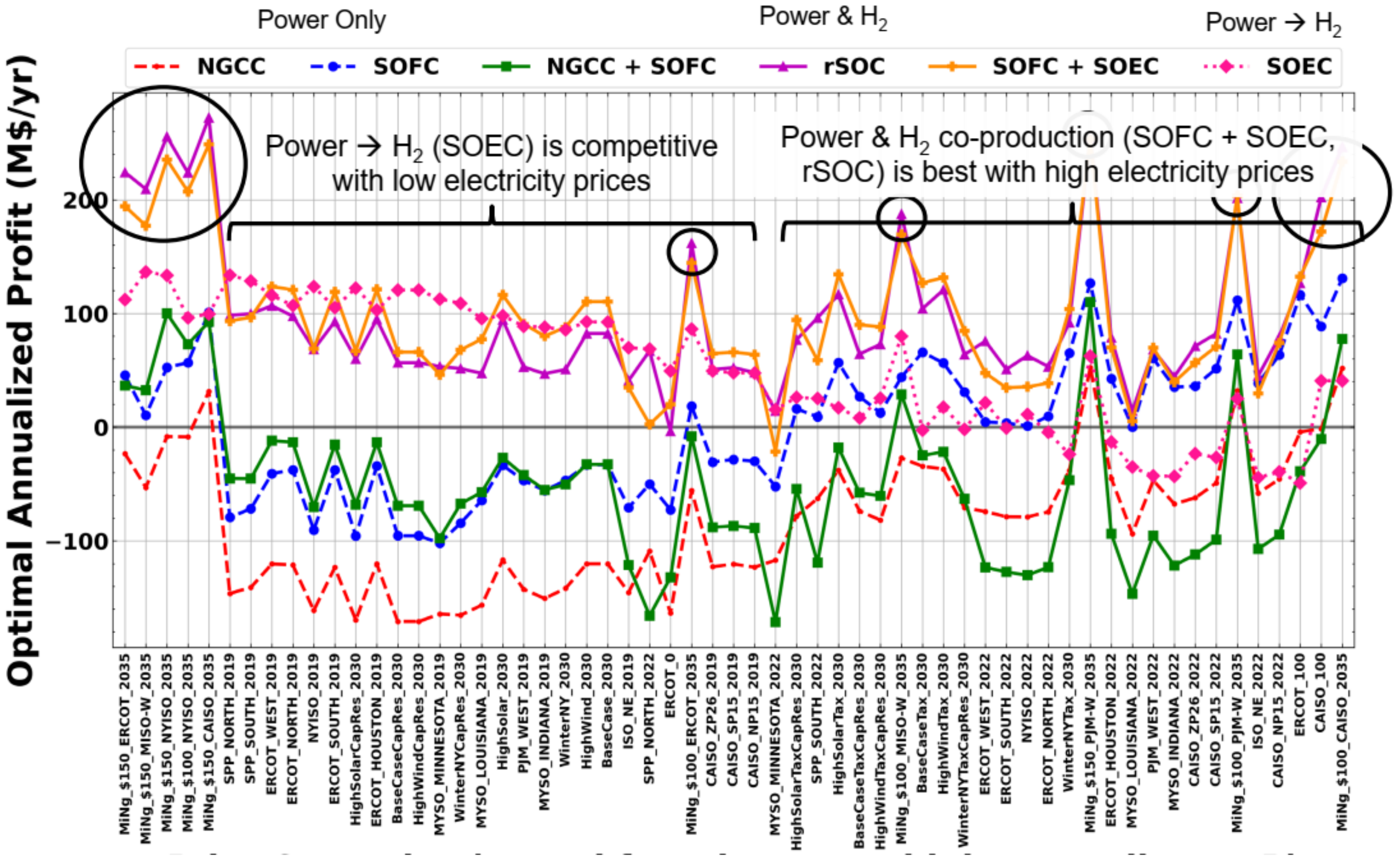
See “Technoeconomic Evaluation of SOFC Hydrogen/Electricity Co-Generation Concepts” https://www.osti.gov/servlets/purl/1960782

Market-based Technoeconomic Optimization

Reversible systems offer profitability across the greatest number of scenarios

https://www.ferc.gov/electric-power-markets





Price Scenarios (from lowest to highest median Locational Marginal Pricing)

NG Prices: 1.14 to 10.47 $/MMBTU, H_2 Price: $2/kg

Designing better electrodes

Electrode Materials

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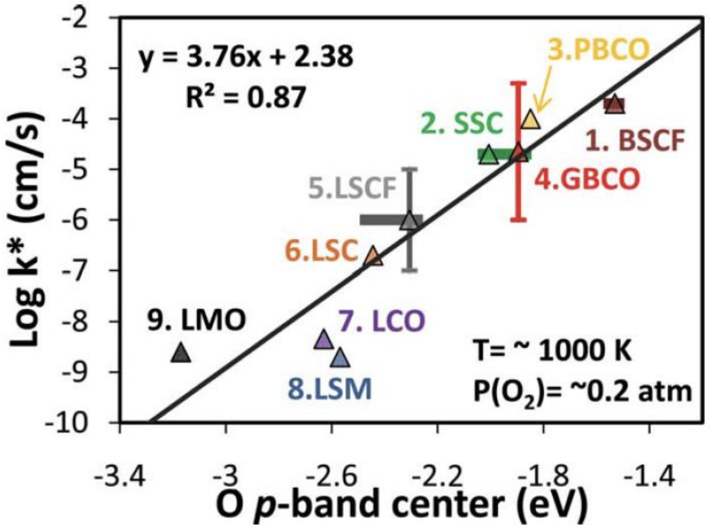
U.S. Department of ENERGY

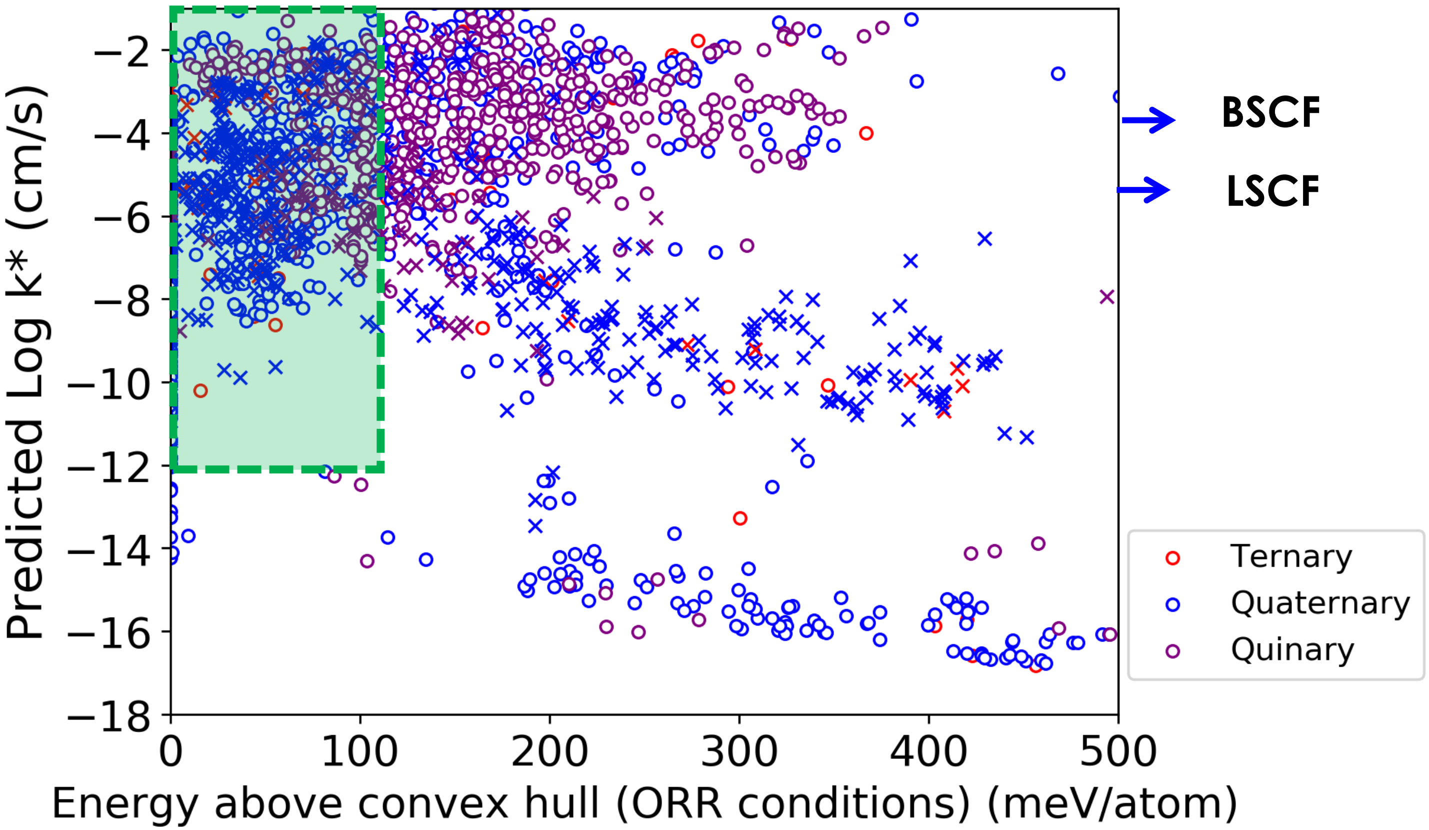
Developing materials through DFT

O p-band correlates well with air electrode material properties

ORR surface exchange [1]



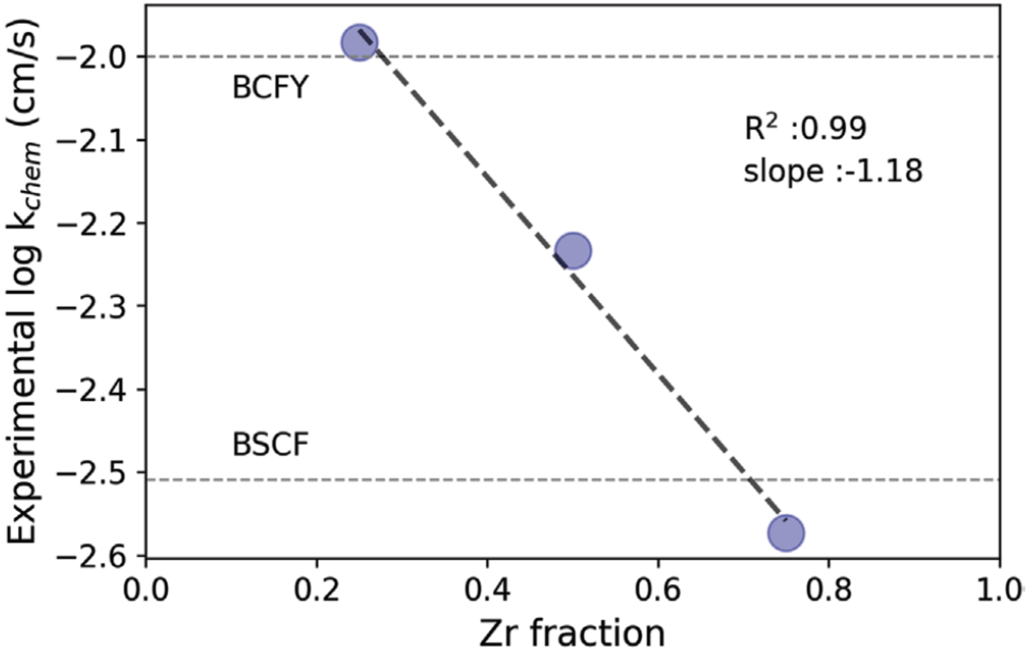
From predicted k* using DFT-calculated O p-band center of >2100 perovskites, NETL examined Ba(Fe, Co, Zr)O_3 (BFCZ) materials



[1] Lee, et al., Eng Env Sci (2011)
[2] Jacobs, et al., Adv. Eng. Mat. (2018)
[3] Jacobs, et al., Chem. Mat. (2019)

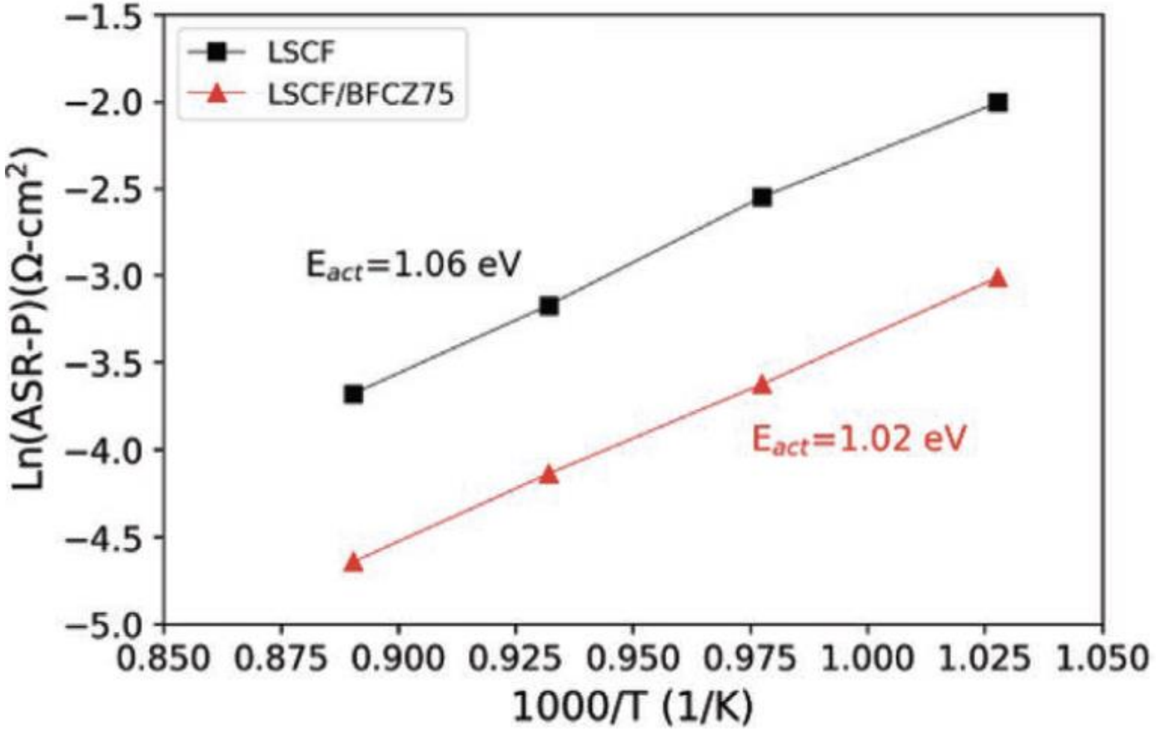
BFCZ (Zr = 25, 50, 75%) Performance

Higher k_{chem}, improved stability, not enough σ_{el}



All BFCZ compositions highly active, on par with BSCF, with only 0.5 log k_{chem} difference over entire Zr range

LSCF/BFCZ75 composite

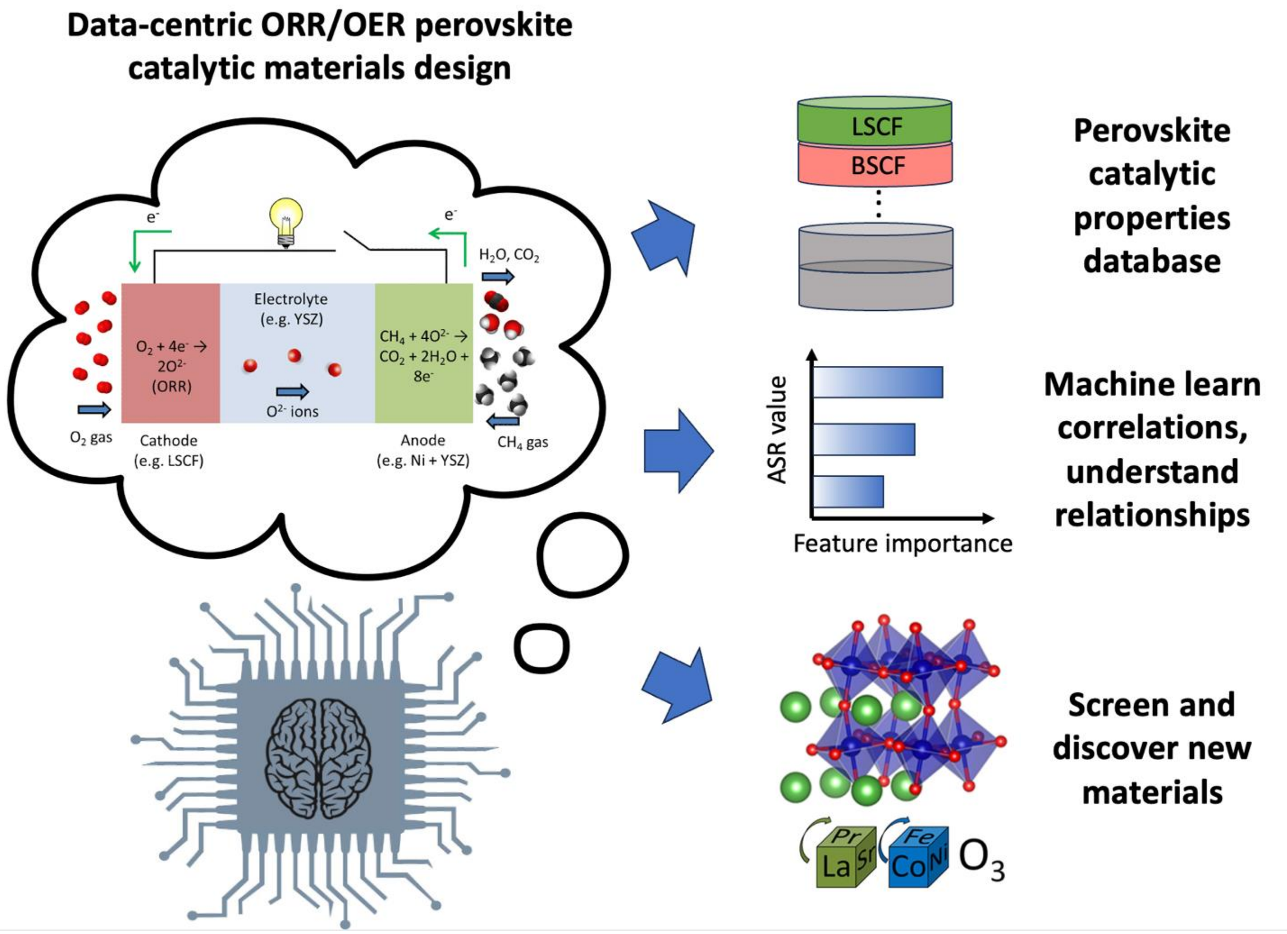


LSCF/BFCZ75 composite shows about 9x reduction in ASR at 800 °C, 65% less performance degradation vs. LSCF

[1] Jacobs, R., et al. Adv. Eng. Mat. (2022)

Machine learning prediction of properties

Using machine learning for faster calculations, larger sampling space



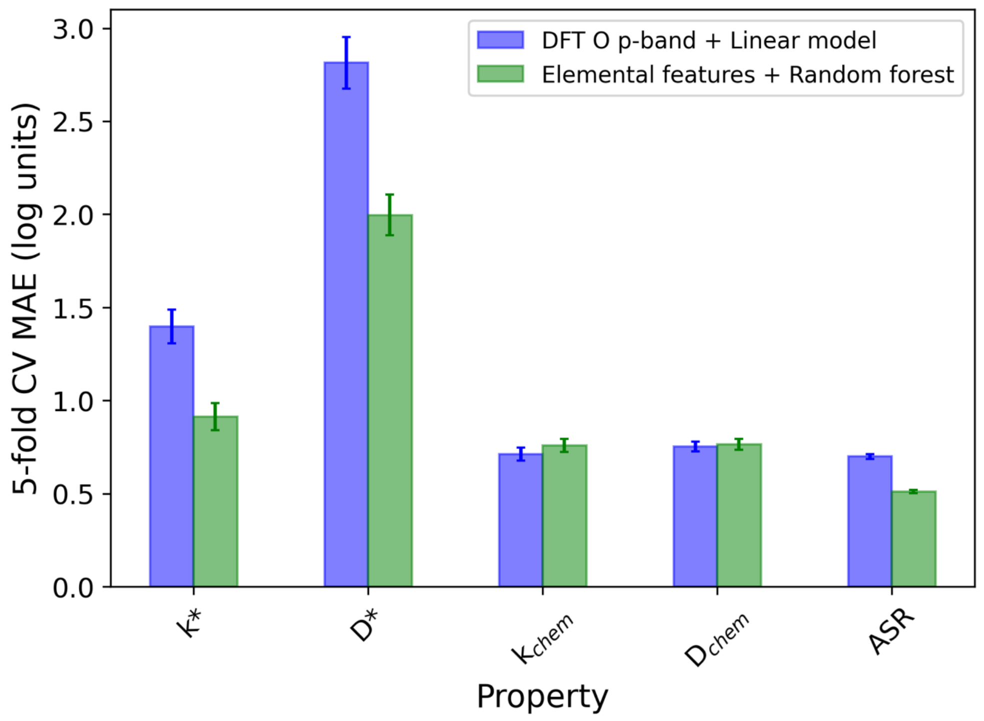
- 749 data points from 313 studies for 299 unique perovskite compositions
- Elemental features calculated using MAST-ML (UW-M) instead of using DFT
- **19 million perovskite oxides** were examined using ML model

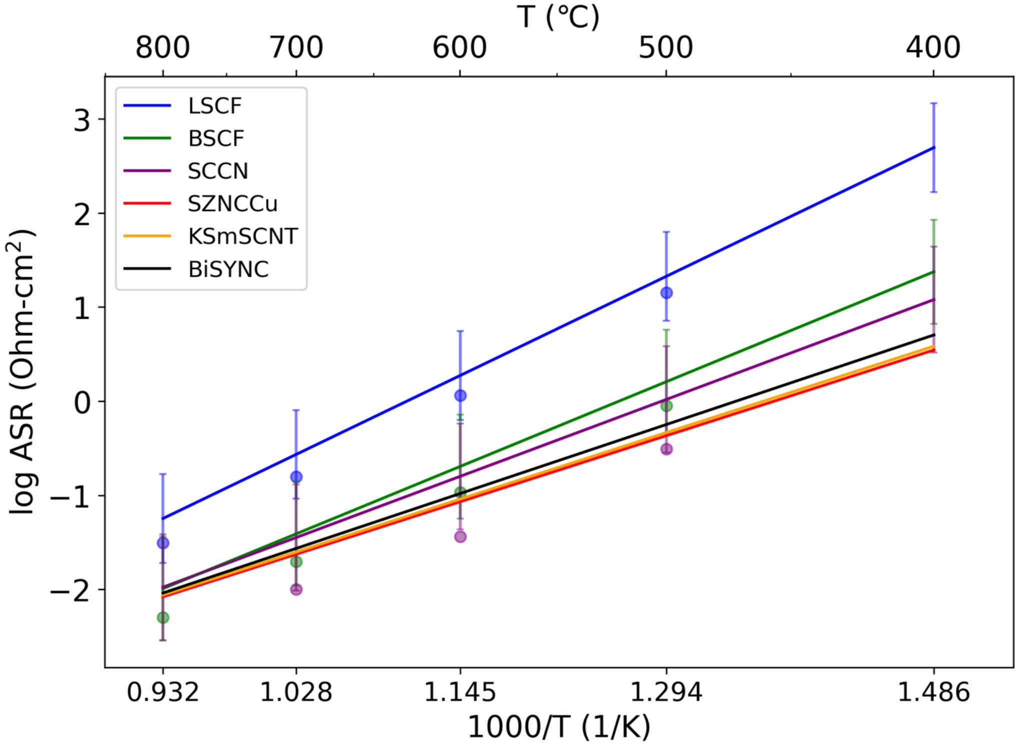
Property	Number of studies examined	Number of measurements extracted	Number of unique materials
k_{chem}	70	98	62
D_{chem}	56	83	58
k*	39	80	48
D*	37	66	42
ASR	235	422	257

Jacobs, R., et al. **Adv. Eng. Mat.** 14 (12), 2303684 (2024).

Machine learning predicted electrode materials

- Trained machine learning model could predict properties faster and at least as accurately than DFT-based study and could cover a larger space containing traditionally less-explored elements (e.g., K, Bi, Y, Ni, Cu).

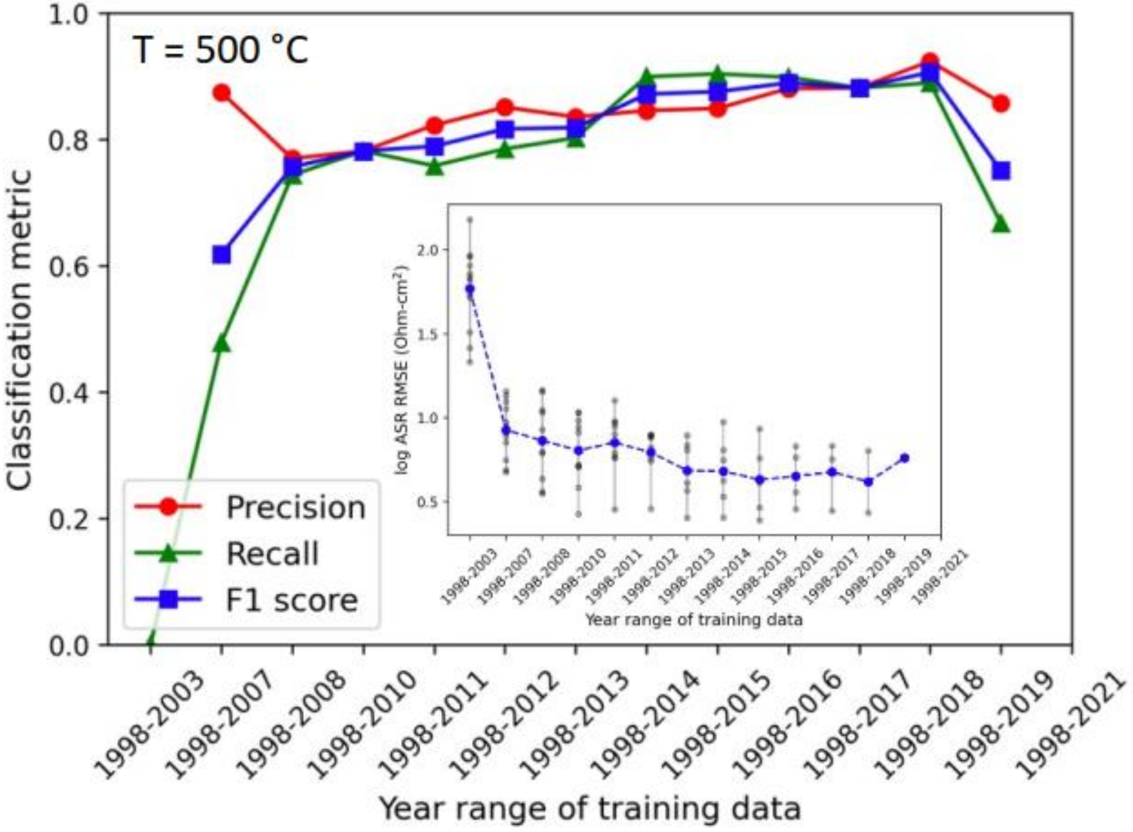




Jacobs, R., et al. **Adv. Eng. Mat.** 14 (12), 2303684 (2024).

Time-dependent cross validation

- Training on materials known prior to 2003 suggests high performing materials in the Ba(Fe, Co, Zr)O_3 space, suggesting materials such as BSCF and BFCZ could have been discovered using our model



Wrap Up

Conclusions

- Modeling is useful tool for deeper interpretation of performance data, designing more durable electrodes, and providing context to literature results
- Machine learning is useful tool for accelerating electrode/cell development and providing guidance for improving specific cells

How can NETL help you?

- NETL can collaborate with partners using partner data and conditions to run performance degradation-related simulations, especially if it aligns with H2NEW and R-SOFC Program objectives.
- R-SOFC Program FOA **DE-FOA-0003366**. Responses due **12/2/2024**. Topics: (1) Enhanced durability at high current density; (2) Thermodynamic database for SOC materials.
- Industry-specific simulations can also be done through DOE's High Performance Computing for Energy Innovation (HPC4EI) to gain access to NETL staff and its JOULE supercomputer.

Acknowledgements

- This work was performed in support of the U.S. Department of Energy's (DOE) (1) Fossil Energy and Carbon Management's R-SOFC Research Program and executed through the National Energy Technology Laboratory (NETL) Research & Innovation Center's FWP 1022411 and FWP 1025039 and (2) Hydrogen and Fuel Cell Technologies Office's H2NEW Program and executed through NETL RIC's CORE Project 1024574.

NETL Resources

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NETL and DOE SOC Research

NATIONAL ENERGY TECHNOLOGY LABORATORY

DOE HQ

Energy Efficiency and Renewable Energy (EERE)

Hydrogen and Fuel Cell Technology Office (HFTO)

H2NEW

FY24 HTE Budget: $10M

DOE Hydrogen Shot:
$2/kg H_2 by FY26
$1/kg H_2 by FY30

Fossil Energy and Carbon Management (FECM)

Advanced Energy Systems Program (AES)

R-SOFC Program

FY24 Budget: $5M