ENERGY earthshots U.S. DEPARTMENT OF ENERGY | Hydrogen

A New Generation of Innovation

Huyen Dinh, Director of HydroGEN, NREL

Hydrogen Shot Summit

HydroGEN
Advanced Water Splitting Materials

NREL Transforming ENERGY
BERKELEY LAB Bringing Science Solutions to the World
Sandia National Laboratories
INL Idaho National Laboratory
Lawrence Livermore National Laboratory

DOE Strategy for Green Hydrogen Challenges

Consortium Approach

Make	Move	Store	Use
H2NEW Hydrogen from Next-generation Electrolyzers of Water U.S. DEPARTMENT OF ENERGY	H-Mat Hydrogen Materials Compatibility Consortium SM	HyMARC Hydrogen Materials Advanced Research Consortium	MILLION MILE FUEL CELL TRUCK U.S. DEPARTMENT OF ENERGY
HydroGEN Advanced Water Splitting Materials	HyMARC Hydrogen Materials Advanced Research Consortium		ElectroCat Electrocatalysis Consortium
	HyBlend U.S. DEPARTMENT OF ENERGY		

Crosscutting:

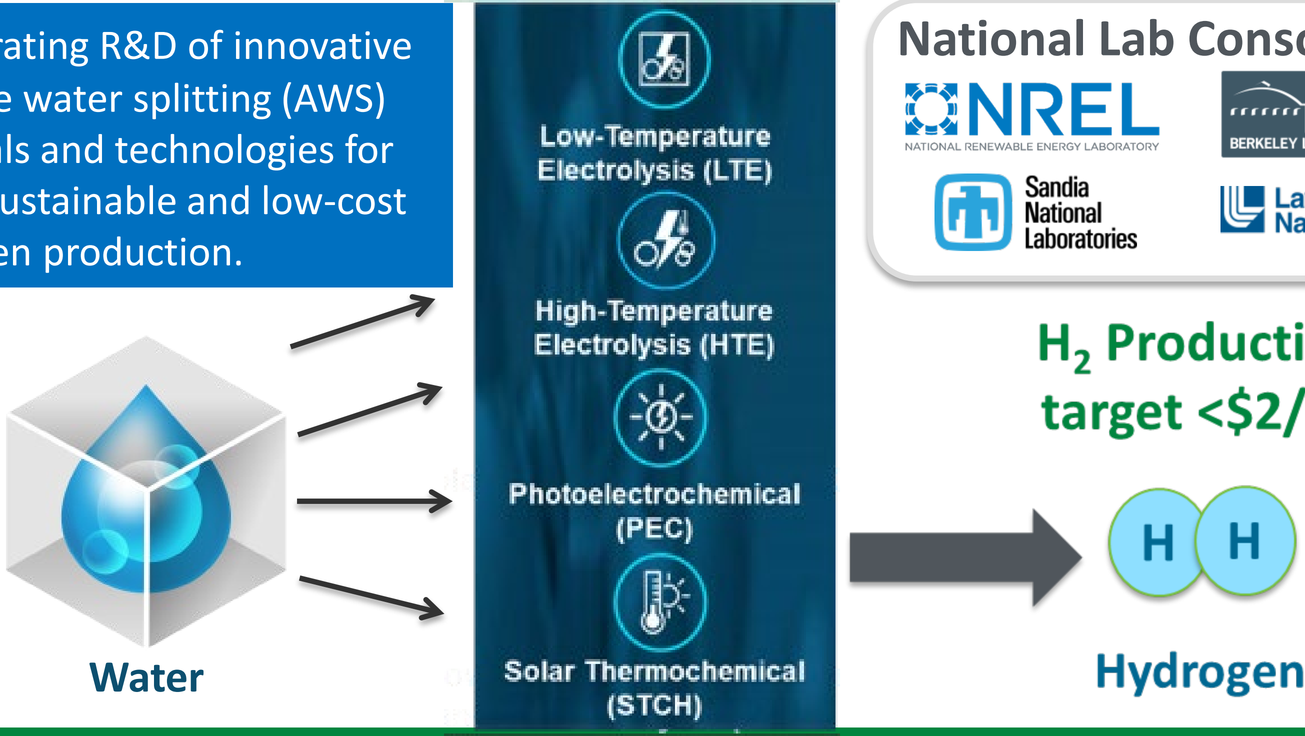
- Analysis
- Manufacturing
- Codes & Standards
- Prog. Mgmt

HydroGEN is advancing Hydrogen Shot

Website: https://www.h2awsm.org/

Goal: Accelerating R&D of innovative advance water splitting (AWS) materials and technologies for clean, sustainable and low-cost hydrogen production.

Challenges
- Cost
- Efficiency
- Durability



Water

Low-Temperature Electrolysis (LTE)

High-Temperature Electrolysis (HTE)

Photoelectrochemical (PEC)

Solar Thermochemical (STCH)

Hydrogen

National Lab Consortium Team

NREL NATIONAL RENEWABLE ENERGY LABORATORY
BERKELEY LAB
INL Idaho National Laboratory
Sandia National Laboratories
Lawrence Livermore National Laboratory

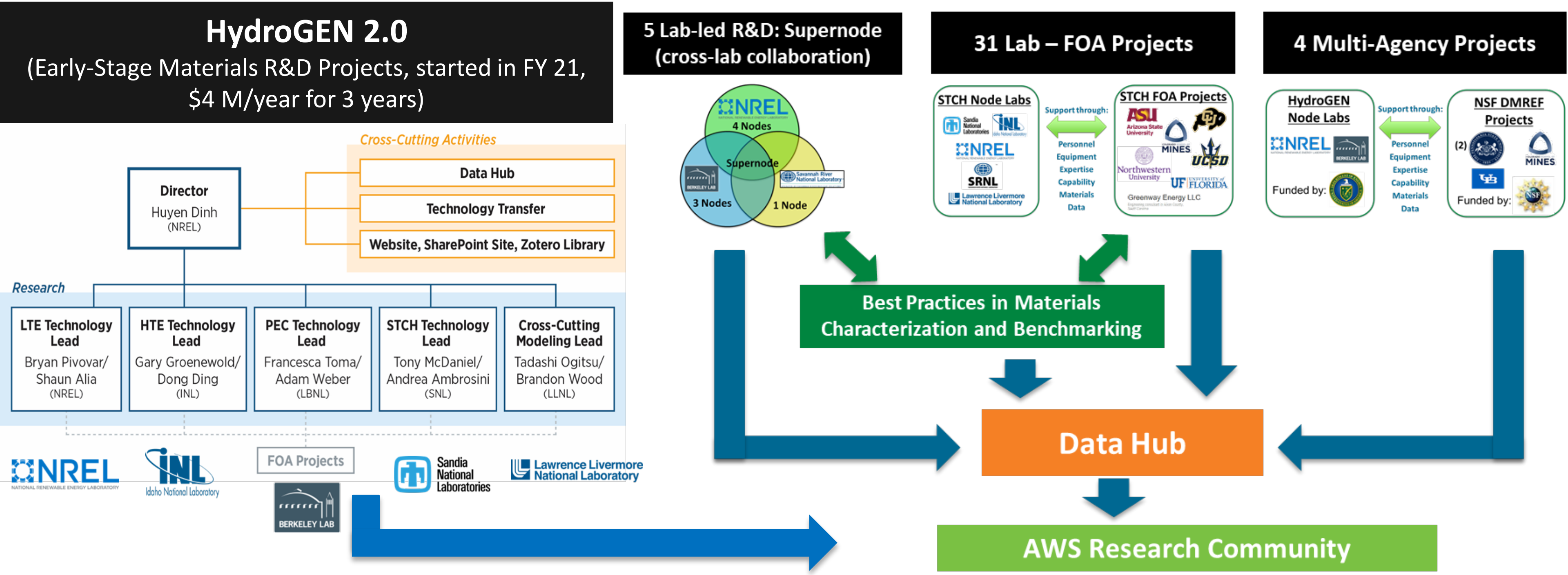
H_2 Production target <$2/kg

HydroGEN is advancing Hydrogen Shot goals by fostering cross-cutting innovation using theory-guided applied materials R&D to advance all emerging water-splitting pathways for hydrogen production

HydroGEN Energy Materials Network (EMN)

https://www.h2awsm.org/capabilities

HydroGEN Materials Capability Network *(Materials Theory, Synthesis, Characterization & Analytics)*



HydroGEN 2.0

(Early-Stage Materials R&D Projects, started in FY 21, $4 M/year for 3 years)

Director
Huyen Dinh
(NREL)

Cross-Cutting Activities

- Data Hub
- Technology Transfer
- Website, SharePoint Site, Zotero Library

Research

LTE Technology Lead	HTE Technology Lead	PEC Technology Lead	STCH Technology Lead	Cross-Cutting Modeling Lead
Bryan Pivovar/ Shaun Alia (NREL)	Gary Groenewold/ Dong Ding (INL)	Francesca Toma/ Adam Weber (LBNL)	Tony McDaniel/ Andrea Ambrosini (SNL)	Tadashi Ogitsu/ Brandon Wood (LLNL)

FOA Projects

5 Lab-led R&D: Supernode (cross-lab collaboration)

31 Lab – FOA Projects

STCH Node Labs

Support through:
Personnel
Equipment
Expertise
Capability
Materials
Data

STCH FOA Projects

4 Multi-Agency Projects

HydroGEN Node Labs

Funded by:

Support through:
Personnel
Equipment
Expertise
Capability
Materials
Data

NSF DMREF Projects

Funded by:

Best Practices in Materials Characterization and Benchmarking

Data Hub

AWS Research Community

Diverse HydroGEN Leadership and Community

Director
Huyen Dinh
(NREL)

Research

LTE Technology Lead
Bryan Pivovar/ Shaun Alia
(NREL)

HTE Technology Lead
Gary Groenewold/ Dong Ding
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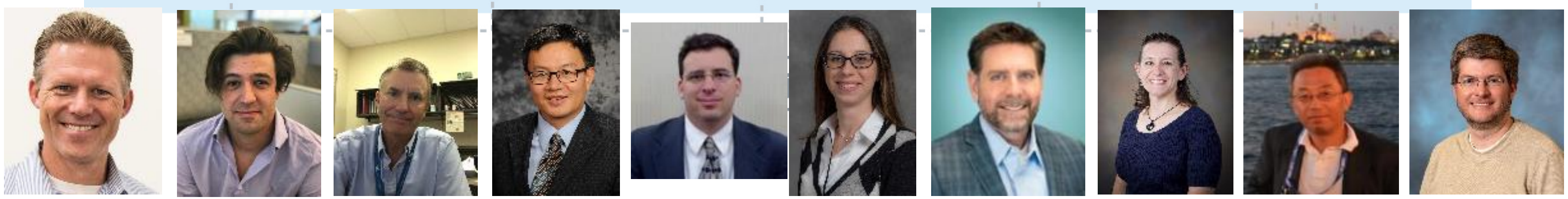
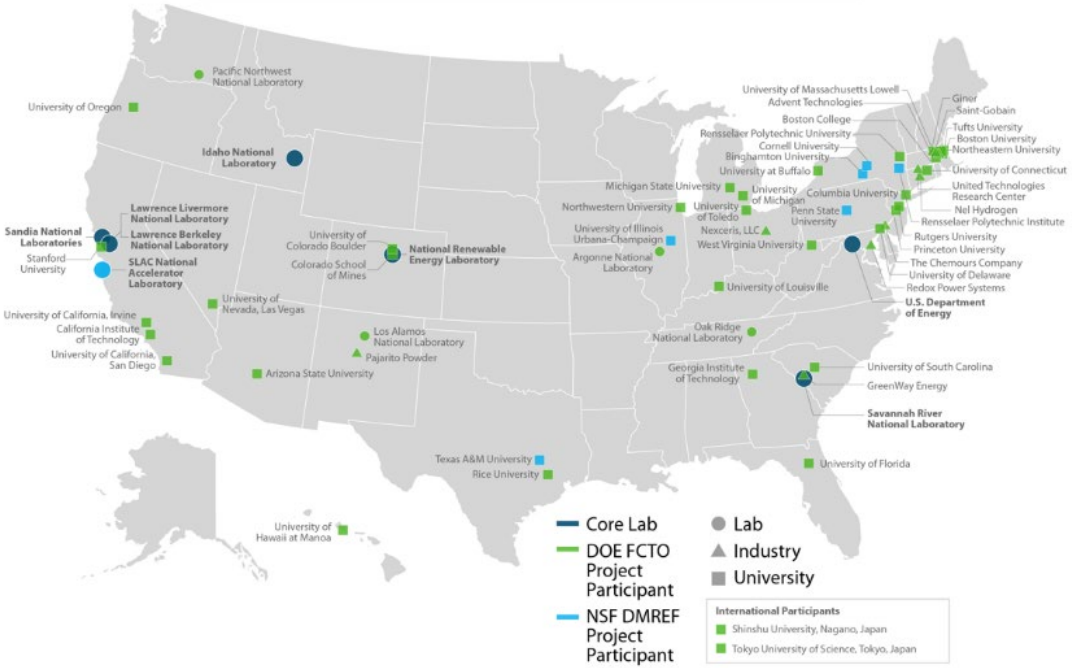


Ecosystem Enables Collaboration, Acceleration, and Diversity, Equity, and Inclusivity (DEI)

11 Labs **10** Companies **39** Universities **2** Funding Agencies



STEM Work Force Development Example

NSF DMREF – DOE EERE HydroGEN Inter-agency Collaboration: PSU – NREL PEC Project

Experimental Validation of Designed Photocatalysts For Solar Water Splitting

Catherine Badding,[1] Ismaila Dabo,[2] Raymond E. Schaak,[3] Héctor D. Abruña[1]
[1]Chemistry and Chemical Biology, Cornell, [2]Materials Science, Penn State, [3]Chemistry, Penn State

Cathy Badding
DOE *SULI Awardee* (2018)
Goldwater Scholar (2019)

NREL
NATIONAL RENEWABLE ENERGY LABORATORY

Collaboration enabled development of a screening procedure (with co-validation between experiment and theory) to expedite the synthesis, characterization, and testing of the computationally predicted, most attractive materials.

HydroGEN is a nationwide, inter-agency, collaborative consortium working to advance early-stage materials R&D and build a DEI community

Community Approach to Benchmarking and Protocol Development for AWS Technologies

Kathy Ayers, Proton OnSite (LTE)

Ellen B. Stechel, ASU (STCH);

Olga Marina, PNNL (HTE);

CX Xiang, Caltech (PEC)

Accomplishments:

- 3 Annual AWS community-wide benchmarking workshops
- 36 test protocols drafted and reviewed
- 40 additional protocols in drafting process
- Engaged with new HydroGEN projects and lab experts
- Disseminated info to AWS community

Development of best practices in materials characterization and benchmarking: critical to accelerate materials discovery and development

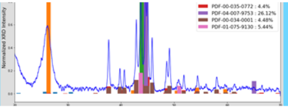
“Energy Material Network Data Hubs: Software Platforms for Advancing Collaborative Energy Materials Research”

NREL Authors: Robert White, Kris Munch, Nicholas Wunder, Nalinrat Guba, Kurt Van Allsburg, Huyen Dinh, and collaborators.

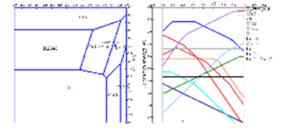
Published in: *International Journal of Advanced Computer Science and Applications, 12(6), 2021*. http://dx.doi.org/10.14569/IJACSA.2021.0120677

Materials properties

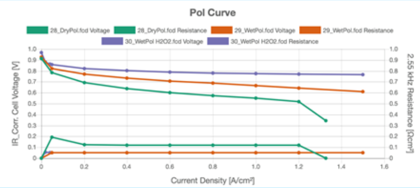
Structural information: XRD interface in collaboration with ElectroCat

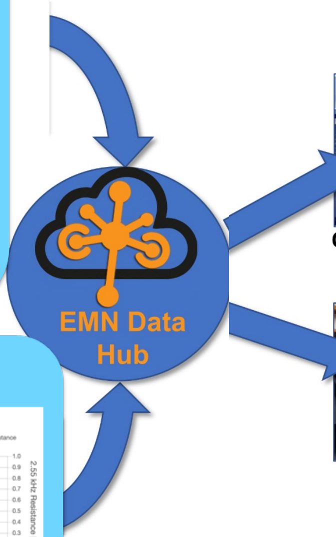


Phase stability & Defect properties



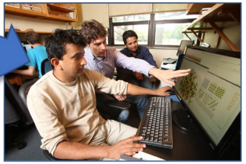
Device performance





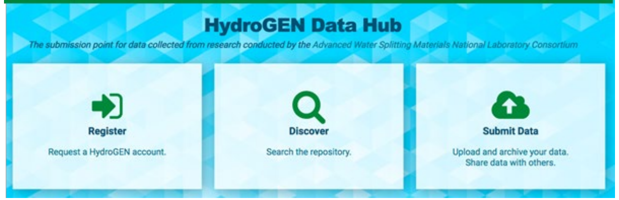
EMN Data Hub

Consortium researchers



Outside researchers and the public

Simple data interface developed



HydroGEN Data Hub

The submission point for data collected from research conducted by the Advanced Water Splitting Materials National Laboratory Consortium

Register
Request a HydroGEN account.

Discover
Search the repository.

Submit Data
Upload and archive your data.
Share data with others.

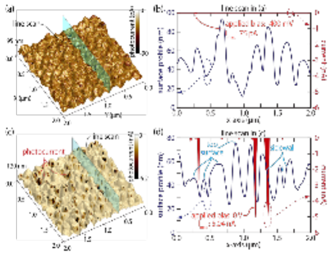
- Have proven capable of effectively leveraging geographically dispersed equipment resources and scientific expertise
- Enabled consortium in making significant advancements in their research and disseminate them the community.

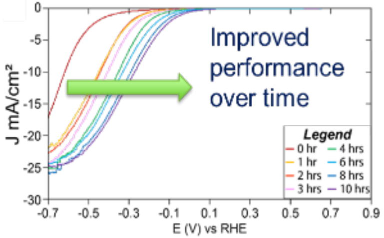
HydroGEN: Advanced Water Splitting Materials

Collaboration Results in High Impact Publication and Accelerates All AWS Technologies

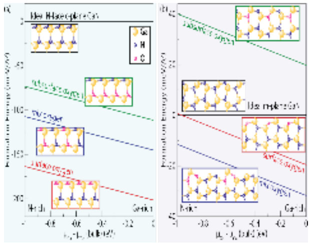
G Zheng, TA Pham, S Vanka, G Liu, C Song, J Cooper, Z Mi, T Ogitsu, FM Toma Development of a photoelectrochemically self-improving Si/GaN photocathode for efficient and durable H_2 production. *Nat. Mater.* **20,** 1130–1135 (2021). https://doi.org/10.1038/s41563-021-00965-w

Experiments





Theory



Highlight

Understanding the observed exceptional stability (> 3000 hr) is crucial for a commercial use of PEC hydrogen production.

Key Technical Accomplishments:

- **Achieved 70% PEM electrolyzer cell efficiency while improving durability & reducing cost**
- **Scaled up baseline cell by 8X with 9% STH efficiency & 100 h stability integrated PV-PEC system**
- **Discovered new STCH compounds with H_2 production capacities > state of the art at lower temperatures**
- **Demonstrated a metal-supported o-SOEC cell with dramatically improved stability**

NREL NATIONAL RENEWABLE ENERGY LABORATORY

BERKELEY LAB

INL Idaho National Laboratory

Sandia National Laboratories

Lawrence Livermore National Laboratory

MICHIGAN STATE UNIVERSITY

BERKELEY LAB

Lawrence Livermore National Laboratory

Acknowledgements

This work was fully supported by the U.S. Department of Energy (DOE), Office of Energy Efficiency and Renewable Energy (EERE), Hydrogen and Fuel Cell Technologies Office (HFTO).

Ned Stetson

Katie Randolph

David Peterson

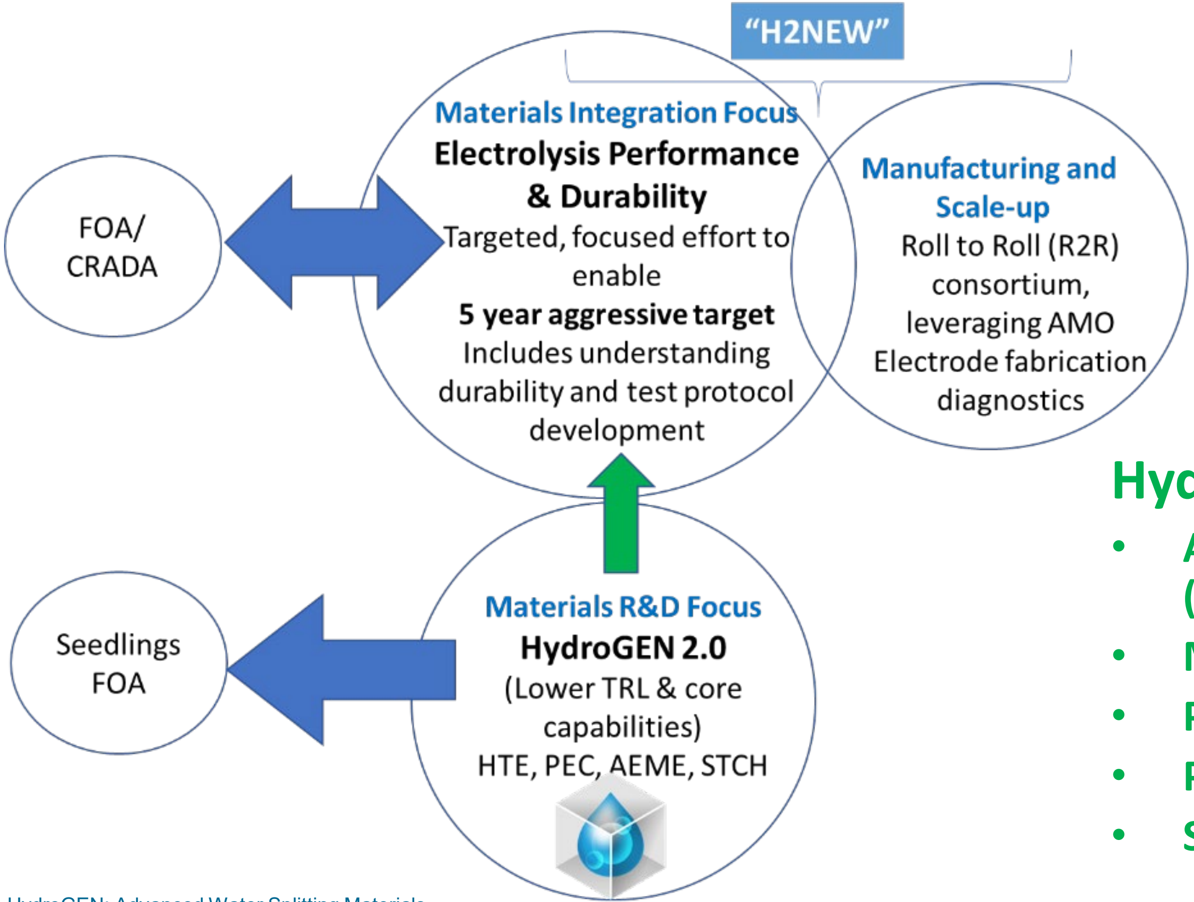
James Vickers

William Gibbons

Eric Miller

Interagency collaboration between NSF–DMREF projects and HFTO HydroGEN EMN
John Schlueter, Program Director, NSF–DMREF, Divisions of Materials Research

HydroGEN Materials R&D Feeds to H2NEW Materials Integration



"H2NEW"

FOA/
CRADA

Materials Integration Focus
Electrolysis Performance & Durability
Targeted, focused effort to enable
5 year aggressive target
Includes understanding durability and test protocol development

Manufacturing and Scale-up
Roll to Roll (R2R) consortium, leveraging AMO
Electrode fabrication diagnostics

Seedlings
FOA

Materials R&D Focus
HydroGEN 2.0
(Lower TRL & core capabilities)
HTE, PEC, AEME, STCH

H2NEW:

- **Polymer electrolyte membrane (PEM) Electrolysis**
- **Oxygen-conducting solid oxide electrolysis (SOEC)**

HydroGEN:

- **Alkaline exchange membrane (AEM) Electrolysis**
- **Metal-supported SOEC (MS-SOEC)**
- **Proton-conducting SOEC (p-SOEC)**
- **Photoelectrochemical (PEC)**
- **Solar thermochemical (STCH)**

Effectiveness of HydroGEN EMN Framework

Collaboration, Streamline Access

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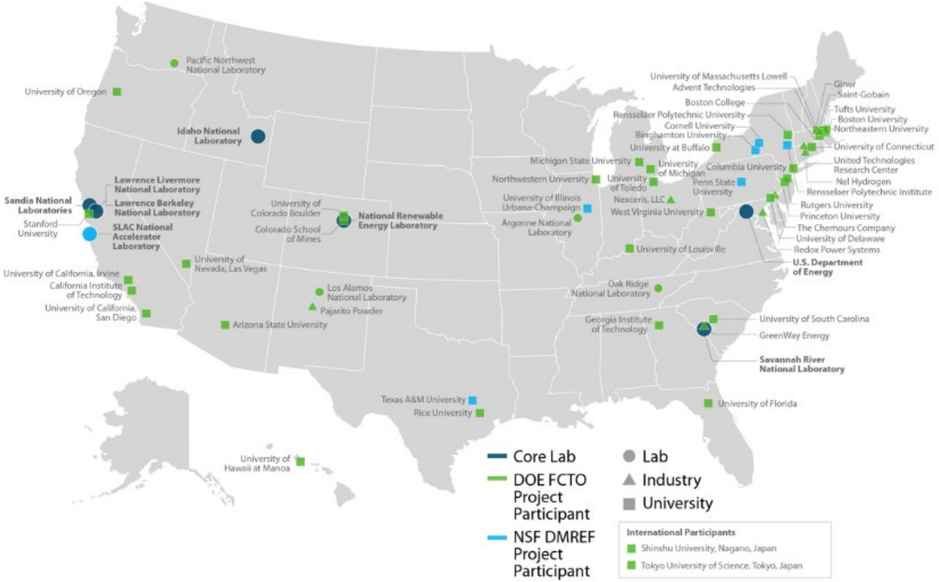
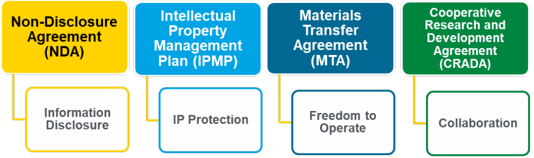
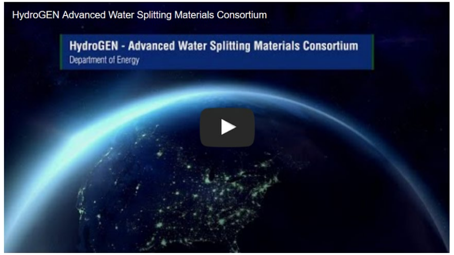




Non-Disclosure Agreement (NDA)	Intellectual Property Management Plan (IPMP)	Materials Transfer Agreement (MTA)	Cooperative Research and Development Agreement (CRADA)
Information Disclosure	IP Protection	Freedom to Operate	Collaboration

https://www.h2awsm.org/working-with-hydrogen



HydroGEN Advanced Water Splitting Materials Consortium

HydroGEN - Advanced Water Splitting Materials Consortium
Department of Energy

HydroGEN is vastly collaborative, has produced many high value products, and is disseminating them to the R&D community.

76 Publications, Impact factor* = 2.87
1,490 citations

HPC uses at NREL: 9,859,850 aus total:

- Across 3 AWS: STCH (95%), HTE, LTE
- 15 total HPC requests

33 project NDAs, 2 MTAs

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*Field-weighted citation impact (FWCI) indicates how the number of citations received by the Publication Set's publications compares with the average number of citations received by all other similar publications in Scopus.

A Balanced AWS Materials R&D Portfolio

Low Temperature Electrolysis (LTE)
(8 Projects)

- PEME component integration
- PGM-free OER catalyst
- Reinforced membranes

PEM Electrolysis

- PGM-free OER and HER catalyst
- Novel AEM and ionomers
- Bipolar membranes
- Electrodes

AEM Electrolysis

High Temperature Electrolysis (HTE)
(8 Projects)

- Degradation mechanism at high current density operation
- Nickelate-based electrode and scalable, all-ceramic stack design
- Neodymium and lanthanum nickelate

O^{2-} conducting SOEC

- High performing and durable electrocatalysts
- Electrolyte and electrodes
- Low-cost electrolyte deposition
- Metal supported cells

H^+ conducting SOEC

Photoelectrochemical (PEC)
(7 Projects)

- III-V and Si-based semiconductors
- Chalcopyrites
- Thin-film/Si
- Protective catalyst system
- Tandem cell

Semiconductors

- PGM-free catalyst
- Earth abundant catalysts
- Layered 2D perovskites
- Tandem junction

Perovskites

Solar Thermochemical (STCH)
(7 Projects)

- Computation-driven discovery and experimental demonstration of STCH materials
- Perovskites, metal oxides

STCH

- Solar driven sulfur-based process (HyS)
- Reactor catalyst material

Hybrid Thermochemical

PEME = proton exchange membrane electrolysis;
AEME = alkaline exchange membrane electrolysis
PGM = platinum group metal
SOEC = solid oxide electrolysis cells

BERKELEY LAB
Bringing Science Solutions to the World

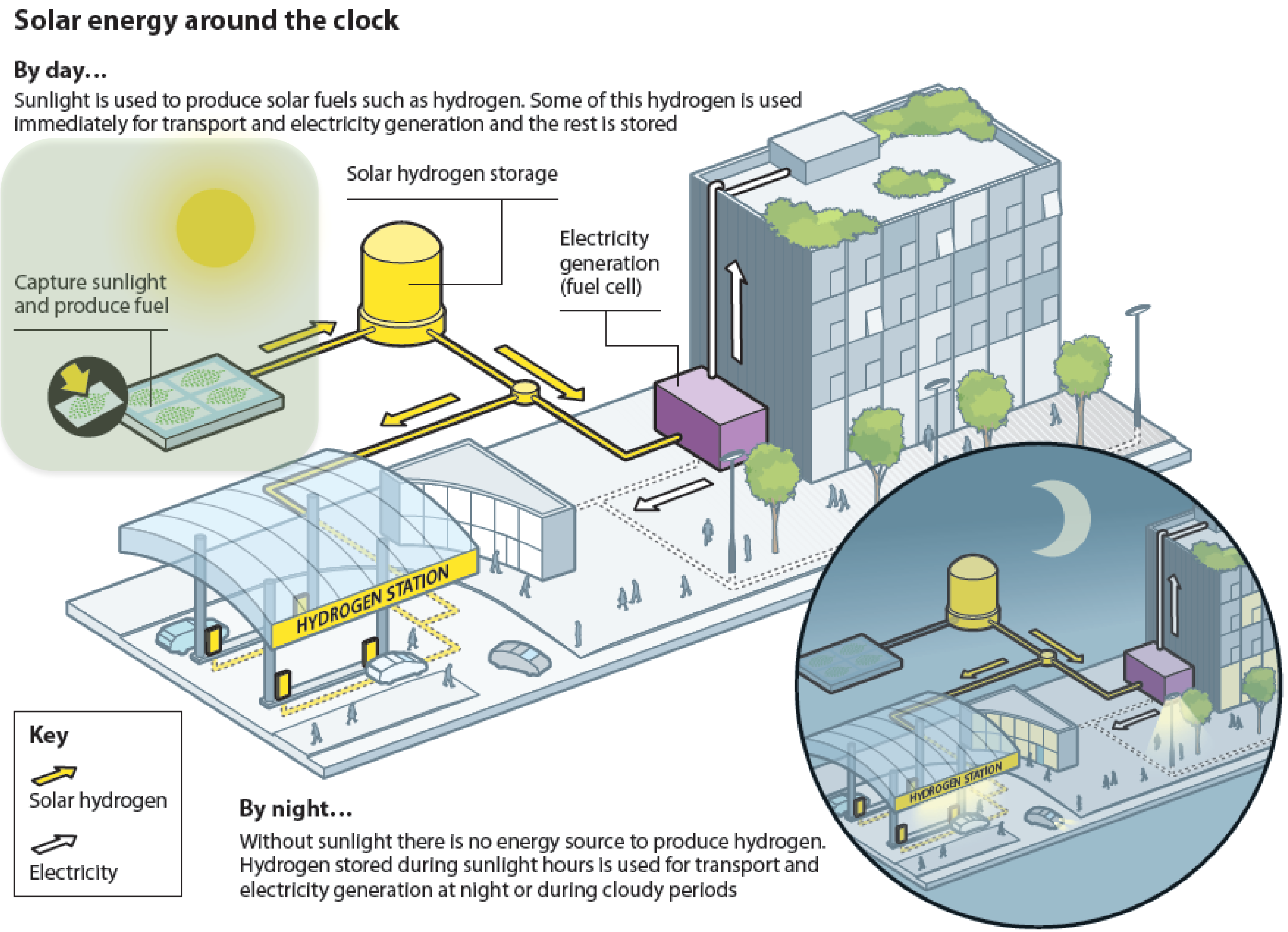
U.S. DEPARTMENT OF ENERGY
Office of Science

Challenges for the Hydrogen Economy

Kristin A. Persson

Director of the Molecular Foundry, The Materials Project and Professor at UC Berkeley, Materials Science and Engineering

The Hydrogen Economy



Solar energy around the clock

By day…

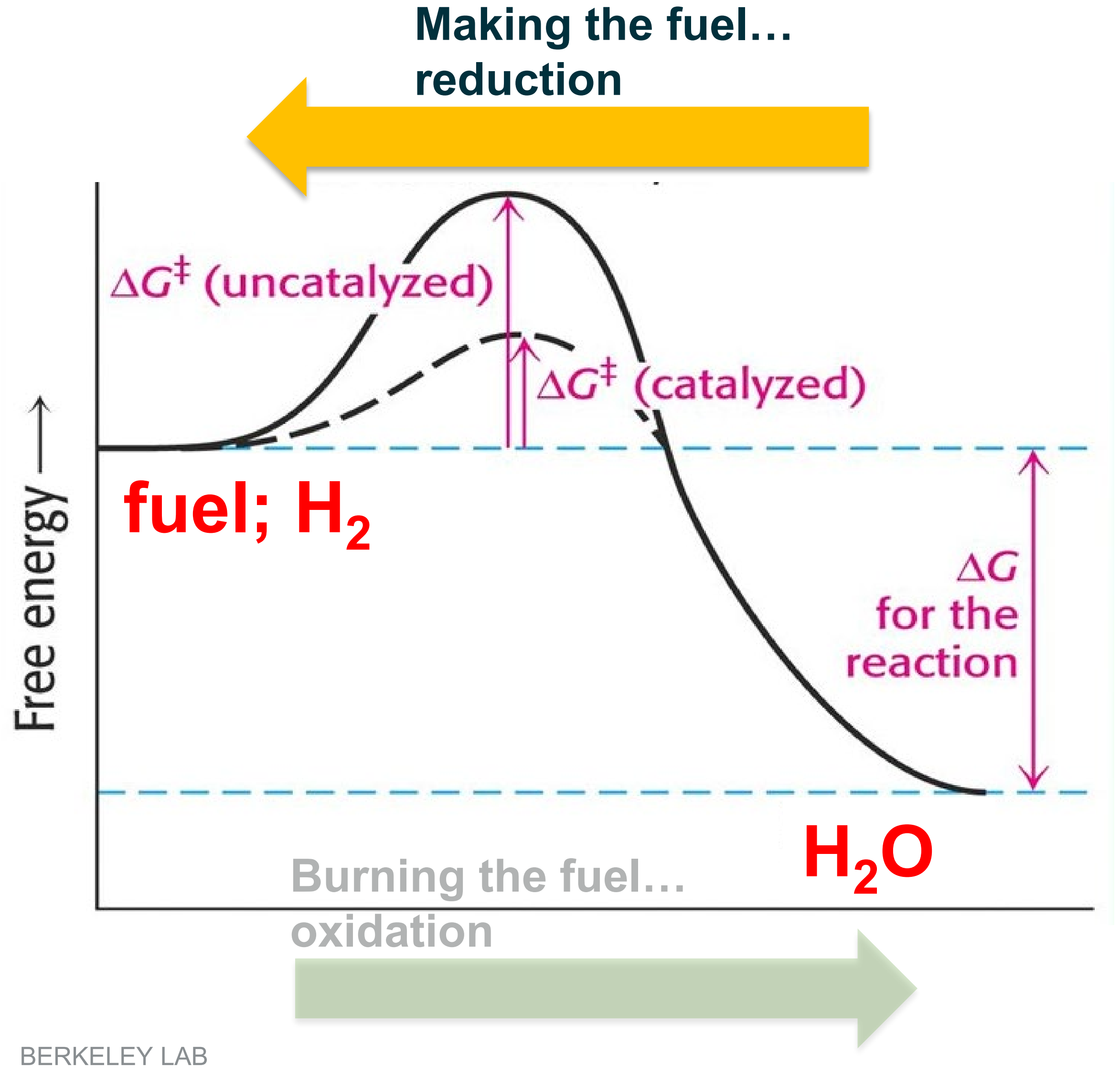
Sunlight is used to produce solar fuels such as hydrogen. Some of this hydrogen is used immediately for transport and electricity generation and the rest is stored

By night…

Without sunlight there is no energy source to produce hydrogen. Hydrogen stored during sunlight hours is used for transport and electricity generation at night or during cloudy periods

- Production
- Storage
- Refill
- Transportation
- Utilization

Production: Need to break a very stable molecule: H_2O

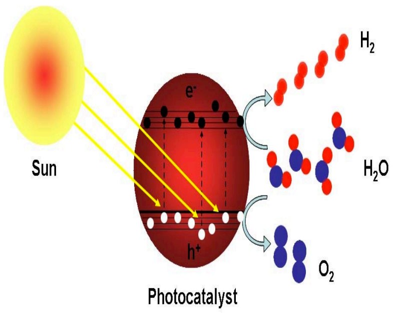


Making the fuel… reduction

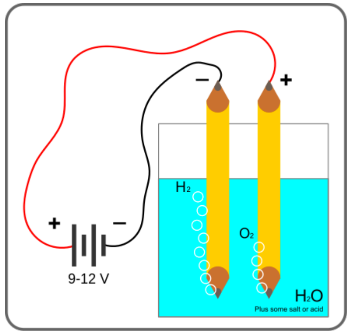
fuel; H_2

H_2O

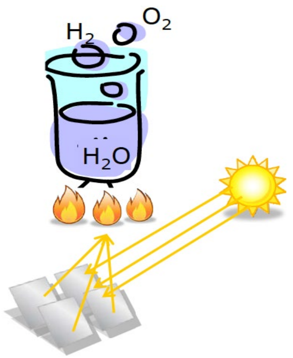
Burning the fuel… oxidation



Photo(cata)lysis

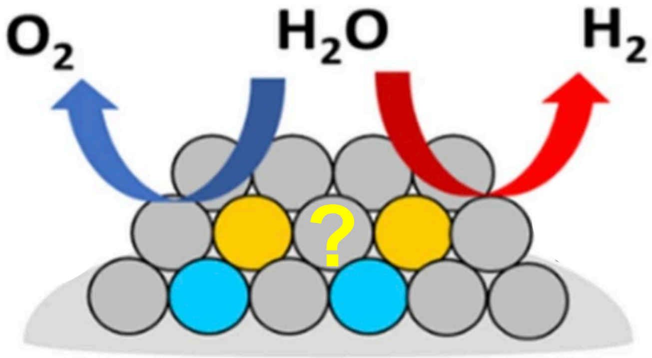


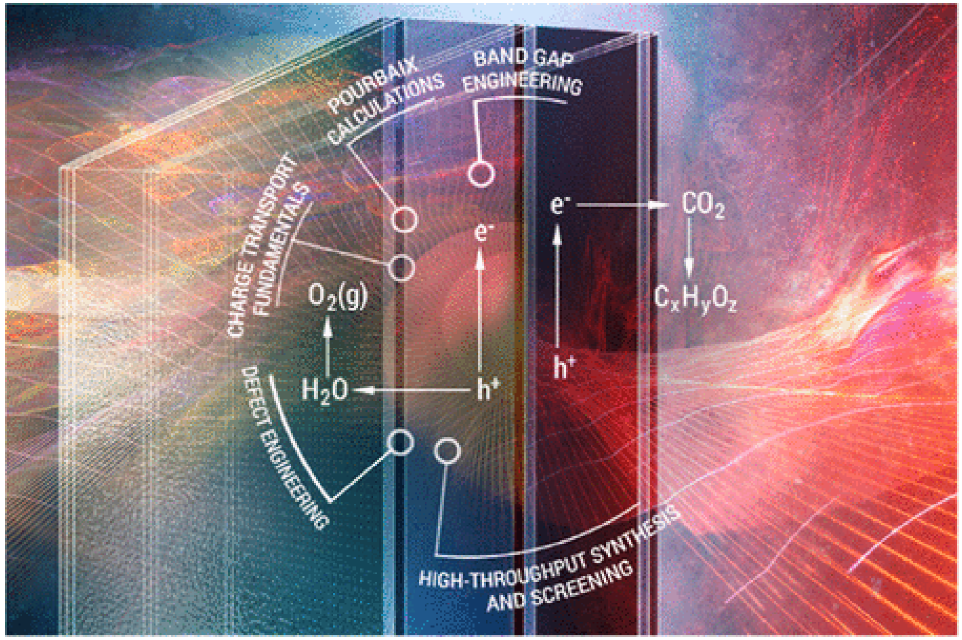
Electro(cata)lysis



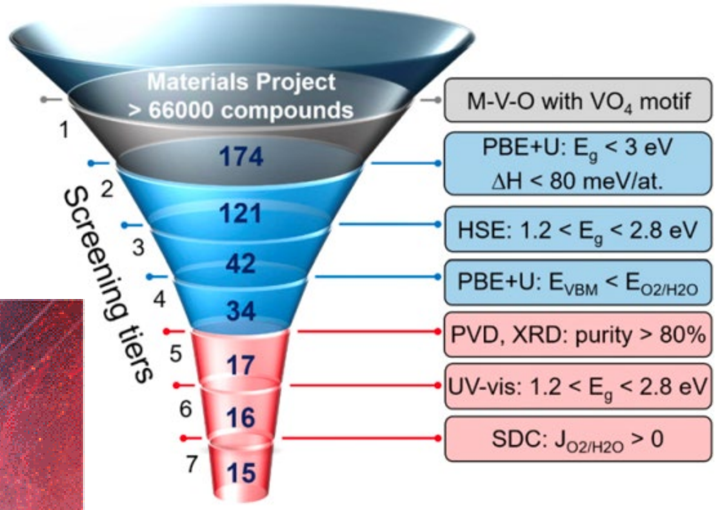
Thermo(cata)lysis

Research: Combining High-throughput Theory with High-throughput synthesis and characterization for Photocatalyst Design and Discovery





ACS Energy Lett. 2020, 5, 5, 1413−1421



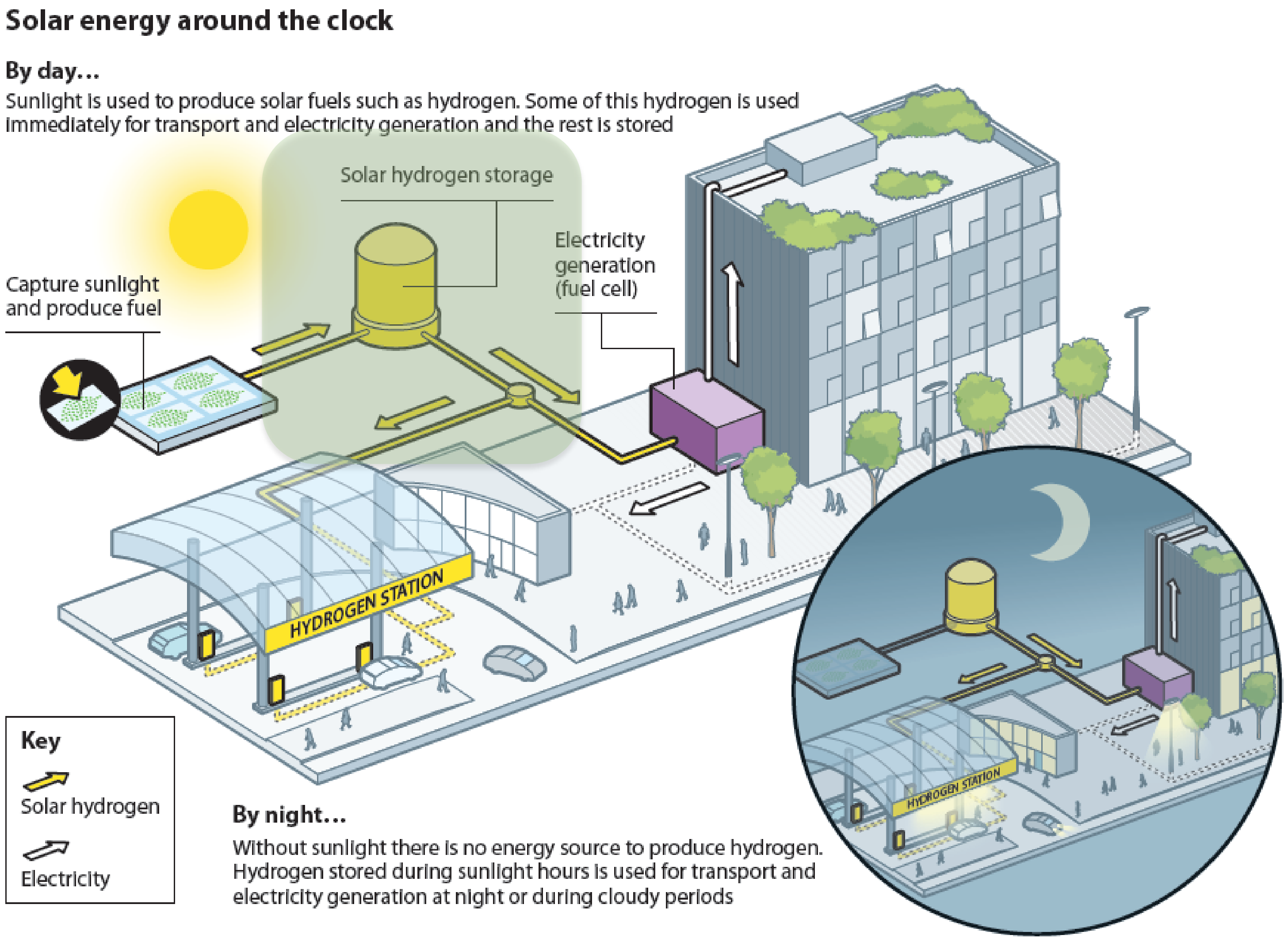
JCAP
JOINT CENTER FOR ARTIFICIAL PHOTOSYNTHESIS

John Gregoire, Caltech

Combinatorial synthesis combined with high throughput electrochemistry enabled discovery of 29 ternary oxide photoanodes, 15 with visible light response for oxygen evolution. $Y_3Fe_5O_{12}$ and trigonal V_2CoO_6 emerge as particularly promising candidates due to their photorepsonse at sub-2.4 eV illumination.

MATERIALS
PROJECT

The Hydrogen Economy: Storage and Refill



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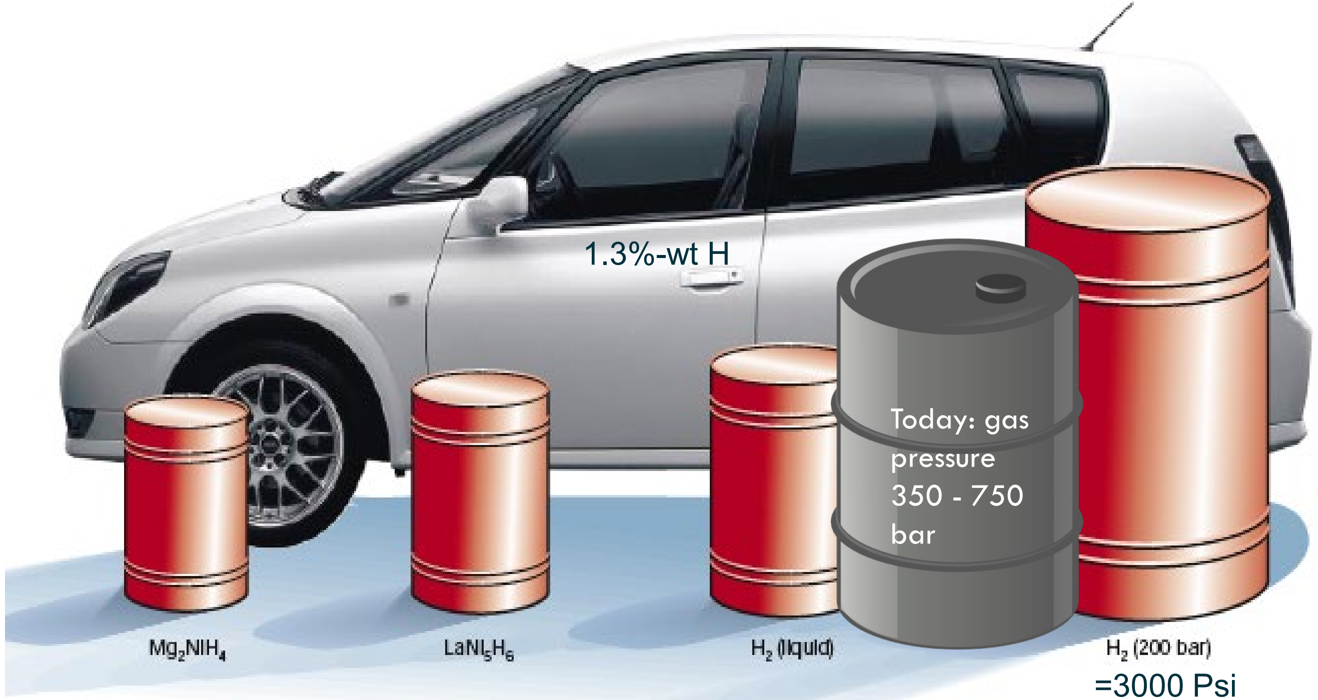
Storage: gas or solid?

Fuel	Storage system	P (bar)	ρ (kg m^{-3})	M (kg mol^{-1})	g (kJ mol^{-1})	g.. (MJ kg^{-1})	g.. (GJ m^{-3})	g_{eff} (GJ m^{-3})	T_B (K)	T_{Des} (K)
Octane[a] C_8H_{18}	Liquid tank	1	703	0.114	5430	47.5	33.4	37.6	399.0	
Methane CH_4	Gas-storage system[b]	250	188	0.016	891.8	55.6	10.5	27.0	109.0	
Methanol CH_3OH	Liquid tank	1	790	0.032	637.6	19.9	15.7	16.0	338.0	
Hydrogen H_2	Cryogenic-liquid tank	>1	67.8	0.00202	285.8	141.5	9.6	30.0	20.3	
Hydrogen H_2	Gas standard condenser	1	0.085	0.00202	285.8	141.5	0.01	112.0	20.3	
Hydrogen H_2	Gas pressurized	300	21.5	0.00202	285.8	141.5	3.04	35.0	–[c]	

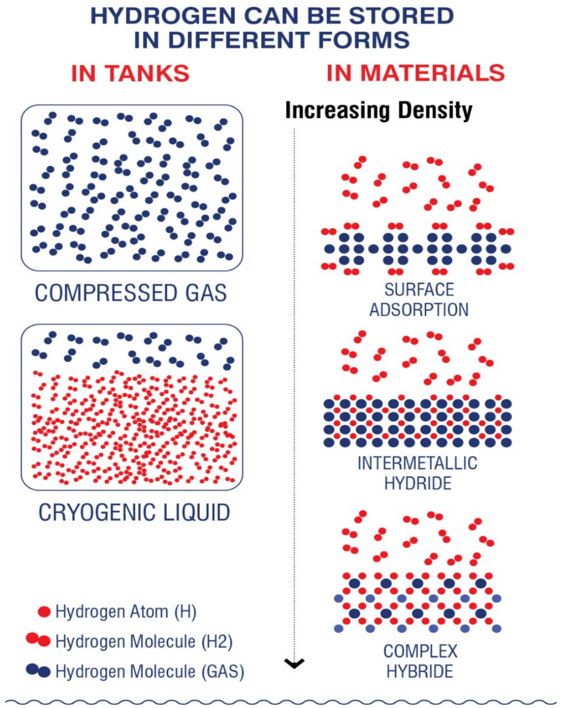


1.3%-wt H

Today: gas pressure 350 - 750 bar

=3000 Psi

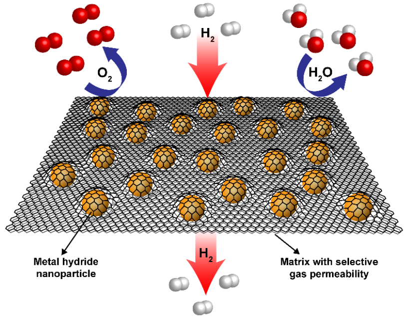
Image of car courtesy of Toyota Motor Co., Tokyo Motor Show 1999



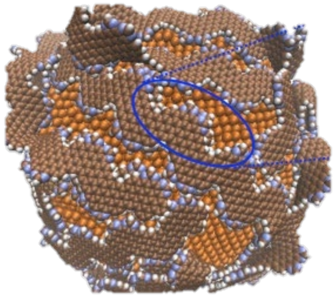
Driving range of 300 miles requires high volumetric and gravimetric H_2 storage densities

C. Jooss, H. Tributsch, Solar Fuels (Chap. 47) in Fundamentals of Materials for Energy and Environmental Sustainability,D. Ginley and D. Cahen Eds, Cambridge Univ. Press (2012)

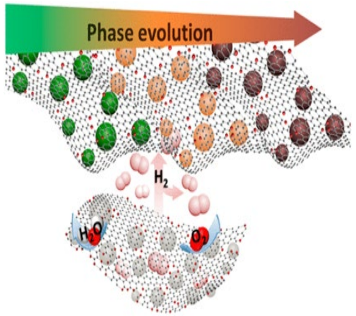
Storage Challenges: Materials Discovery and Heat Management



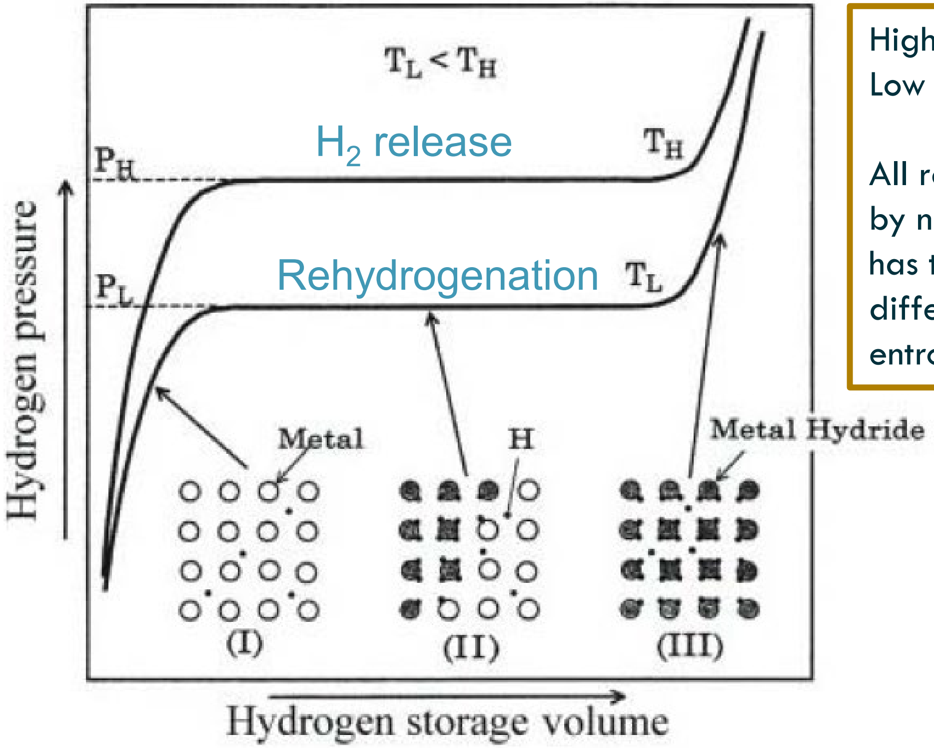
Atomically-thin interfacial suboxide key to hydrogen storage performance enhancements of magnesium nanoparticles encapsulated in reduced graphene oxide.
Wan et al. Nano Lett. 17, 5540 (2017)



Edge-Functionalized Graphene Nanoribbon Encapsulation To Enhance Stability and Control Kinetics of Hydrogen Storage Materials. Wan et al. Chem. Mater. 31, 2960-2970 (2019)



A Mechanistic Analysis of Phase Evolution and Hydrogen Storage Behavior in Nanocrystalline $Mg(BH_4)_2$ within Reduced Graphene Oxide, Jeong et al., ACS Nano (2020). Doi: 10.1021/acsnano.9b07454

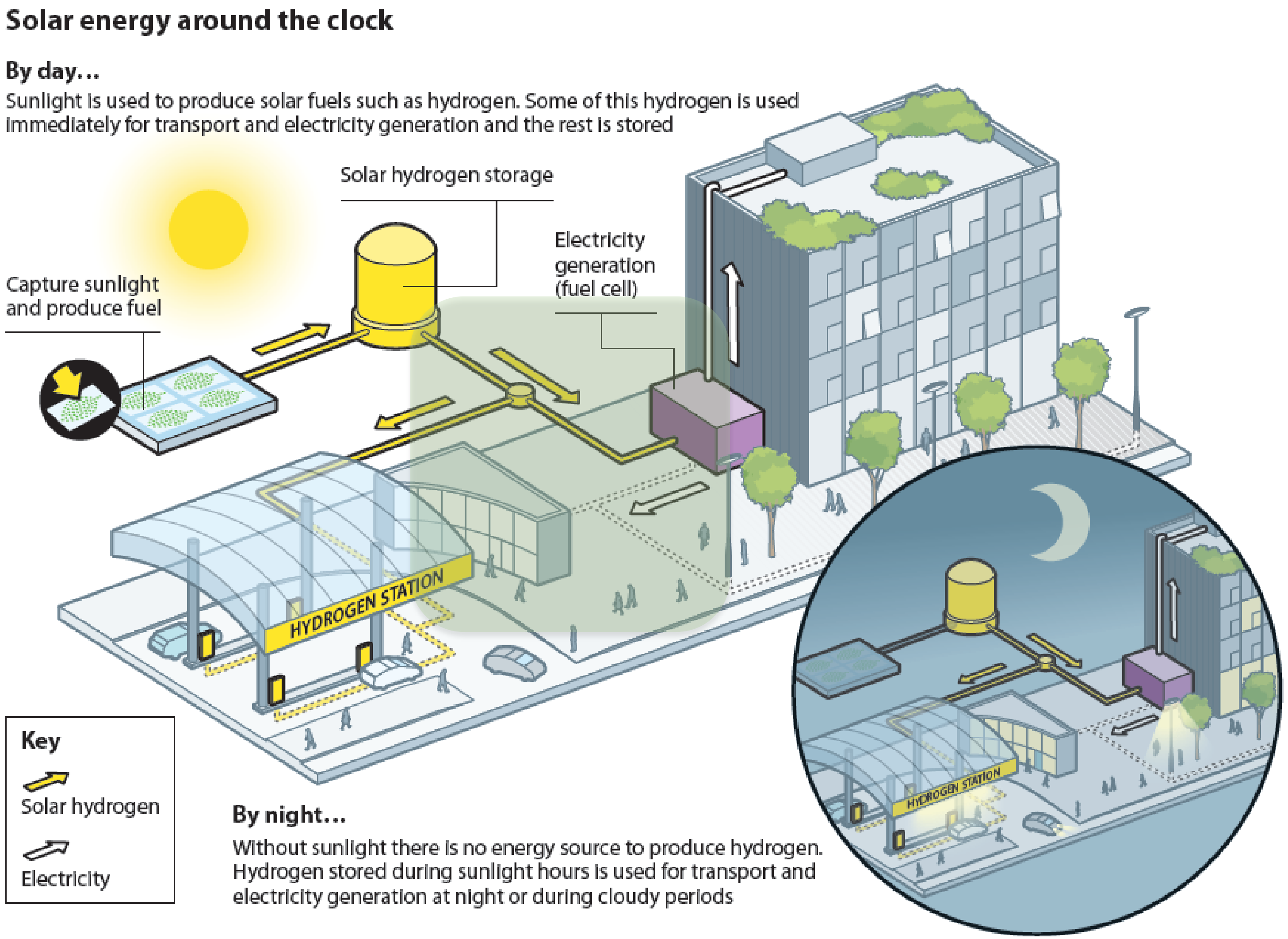


I. a solid solution of hydroge (α phase)
II. a coexistant region of hydrogen solid solution & metal hydride
III. metal hydride (β phase)

High T drives H_2 release
Low T drives H_2 absorption

All rehydrogenation reactions are by nature exothermic since ΔH has to balance a large ΔS difference to due loss of gas entropy -> heat release

The Hydrogen Economy: Transportation



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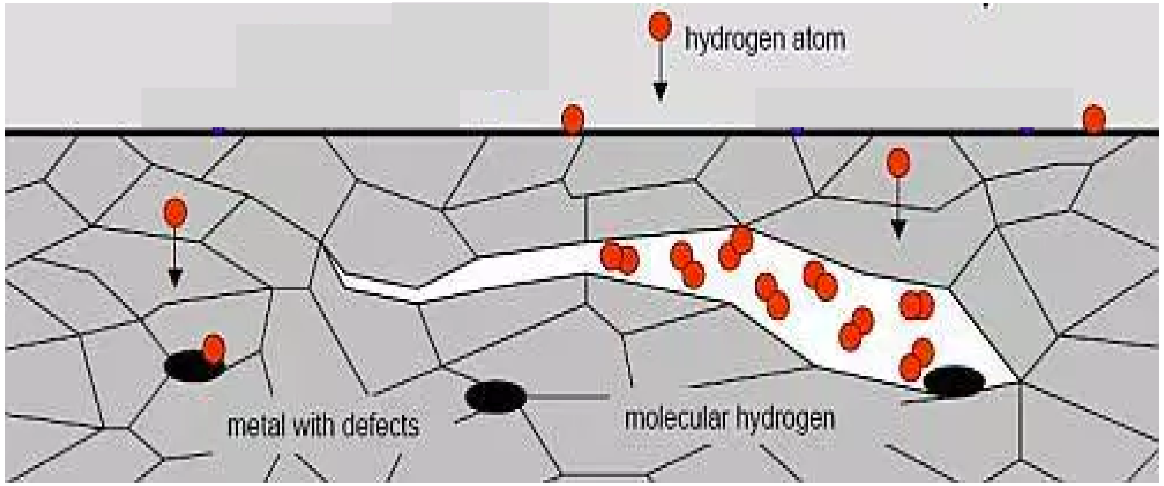
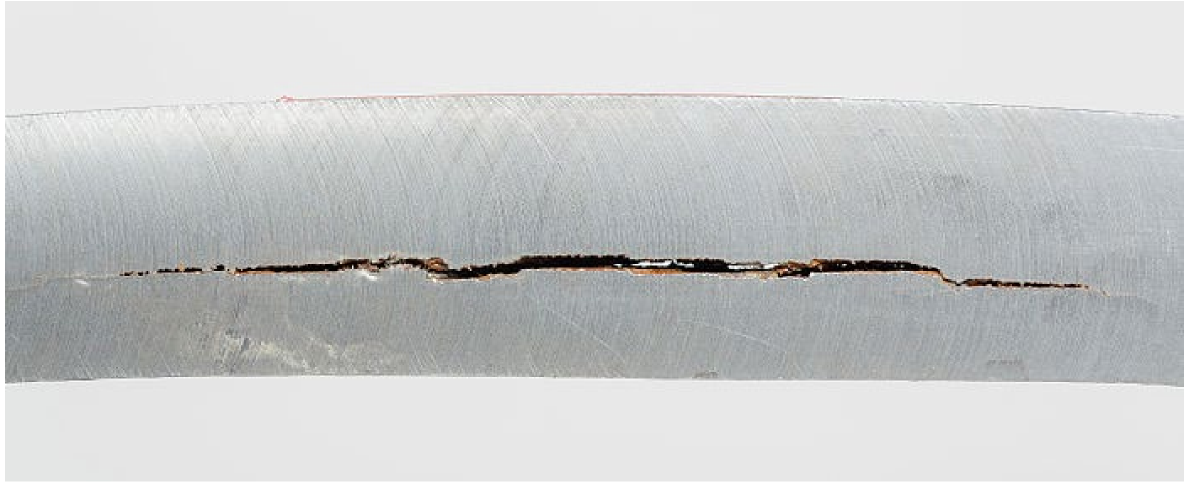
Handling Hydrogen: Embrittlement

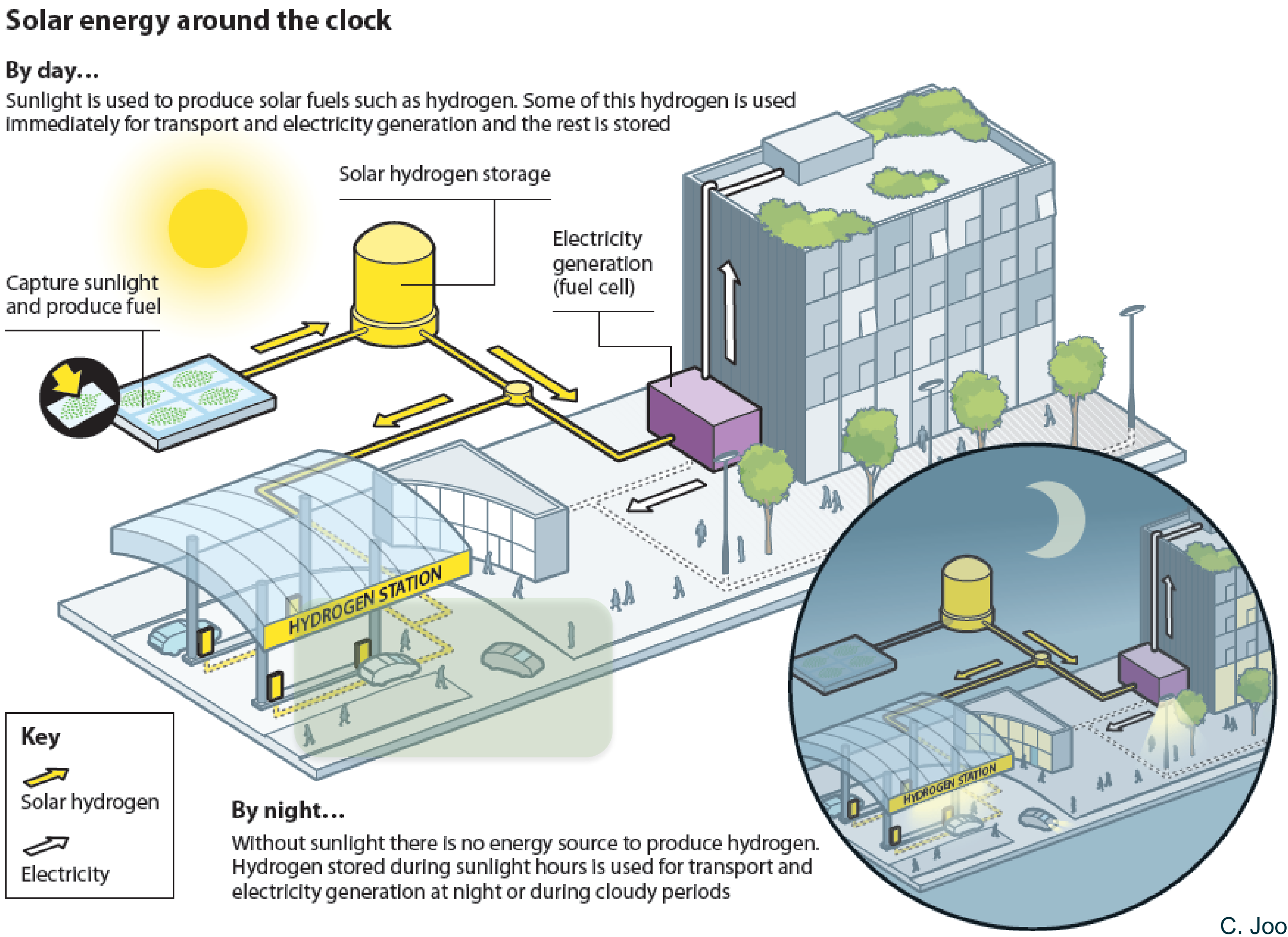
Most metals and alloys are susceptible to different levels of H_2 embrittlement. Because embrittlement **occurs slowly** and can cause catastrophic failures of hydrogen storage containers, it creates **a materials science challenge**





Research: coatings, trapping phases, gas blends (natural gas), careful selection of materials and processing conditions

The Hydrogen Economy: Utilization



Solar energy around the clock

By day…

Sunlight is used to produce solar fuels such as hydrogen. Some of this hydrogen is used immediately for transport and electricity generation and the rest is stored

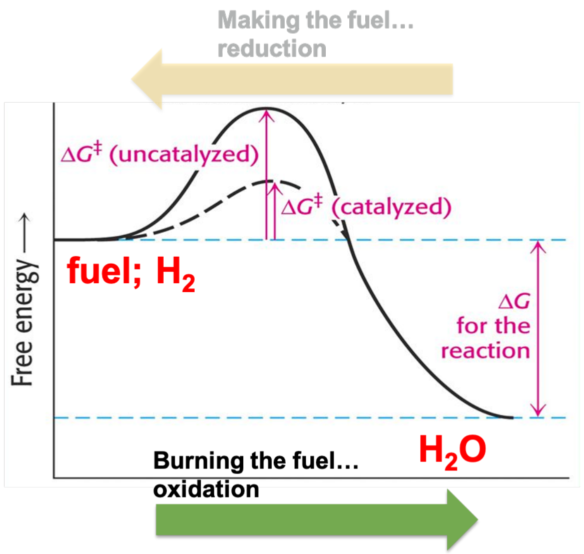
By night…

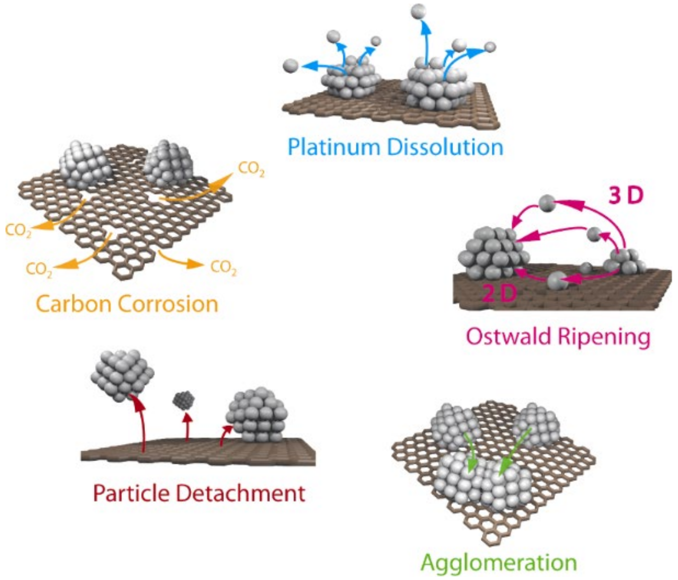
Without sunlight there is no energy source to produce hydrogen. Hydrogen stored during sunlight hours is used for transport and electricity generation at night or during cloudy periods

- Production
- Storage
- Refill
- Transportation
- Utilization

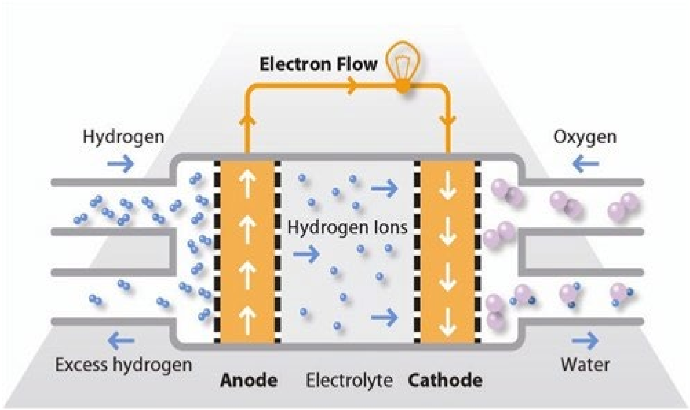
C. Jooss, H. Tributsch, Solar Fuels (Chap. 47) in Fundamentals of Materials for Energy and Environmental Sustainability, D. Ginley and D. Cahen Eds, Cambridge Univ. Press (2012)

Utilization: burning the fuel: catalyst stability and cost





Catalyst stability, durability, cost, and support



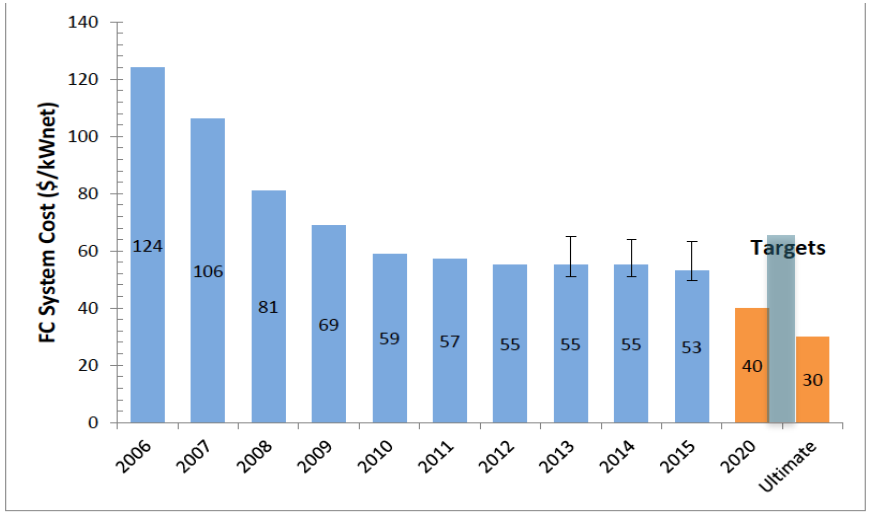


Figure 1. Modeled cost of an 80-kW$_{net}$ PEM fuel cell system based on projection to high-volume manufacturing (500,000 units/year). Reported values from 2012 and earlier were adjusted to

The 2020 estimated cost of an 80-kWnet automotive polymer electrolyte membrane (PEM) fuel cell system is projected to be $76/kWnet when manufactured at a volume of 100,000 units/year (hydrogenenergy.gov)

Beilstein J. Nanotechnol. **2014,** *5,* 44–67. https://doi.org/10.3762/bjnano.5.5; *Membranes* 2019, *9*(7), 83; https://doi.org/10.3390/membranes9070083

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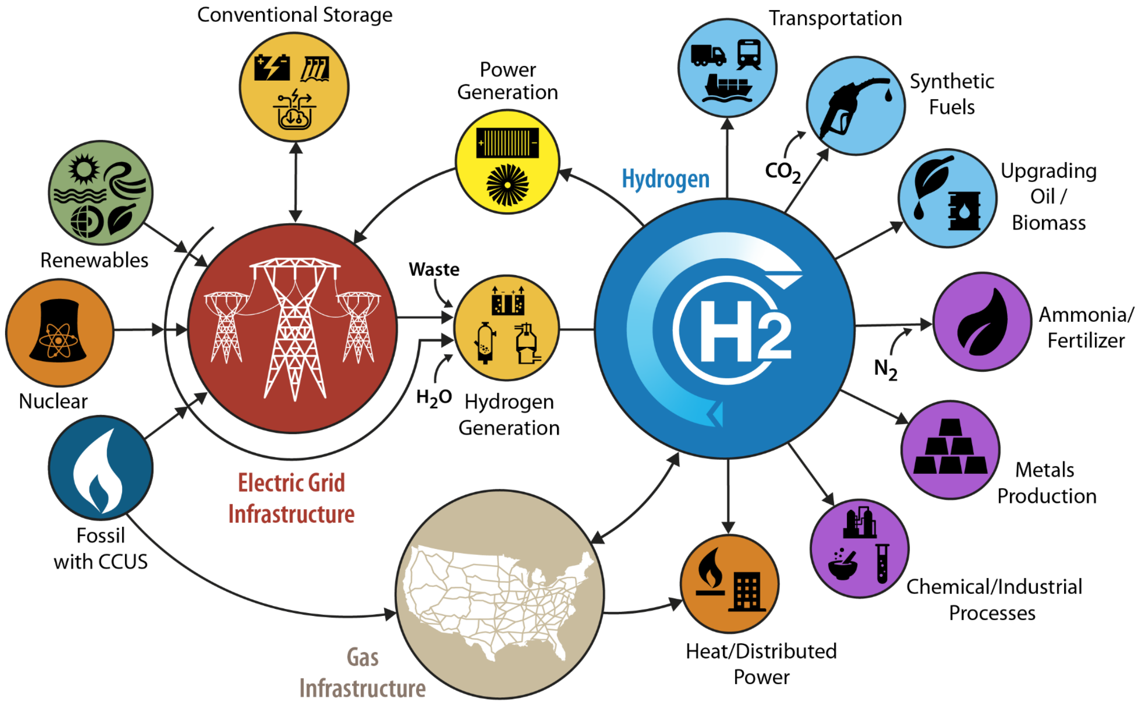
- Materials discovery
- Materials optimization
- Engineering solutions
- Infrastructure investments



Thank You

QUESTIONS?