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Fueling the Future through Chemical Energy of Fuel Cells, Solar Cells, and More

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MASSCREST
CLEAN ENERGY THROUGH CHEMISTRY

Center for Fueling the Future

Fueling the Future through Chemical Energy of Fuel Cells, Solar Cells, and More

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Center for Fueling the Future

http://www.chem.umass.edu/masscrest/fuelingthefuture/

- Supported by the National Science Foundation through Center for Chemical Innovations Program

- Research Investigators from Chemistry, Physics and Polymer Science & Engineering

"The Center for Fueling the Future carries out research that addresses fundamental aspects of proton transport, the molecular-level process that underlies the functioning of a central component of fuel cells."

Hydrogen as an Energy Source

$$H_2(g) + \frac{1}{2} O_2(g) \rightarrow H_2O(l) + \text{Energy}$$

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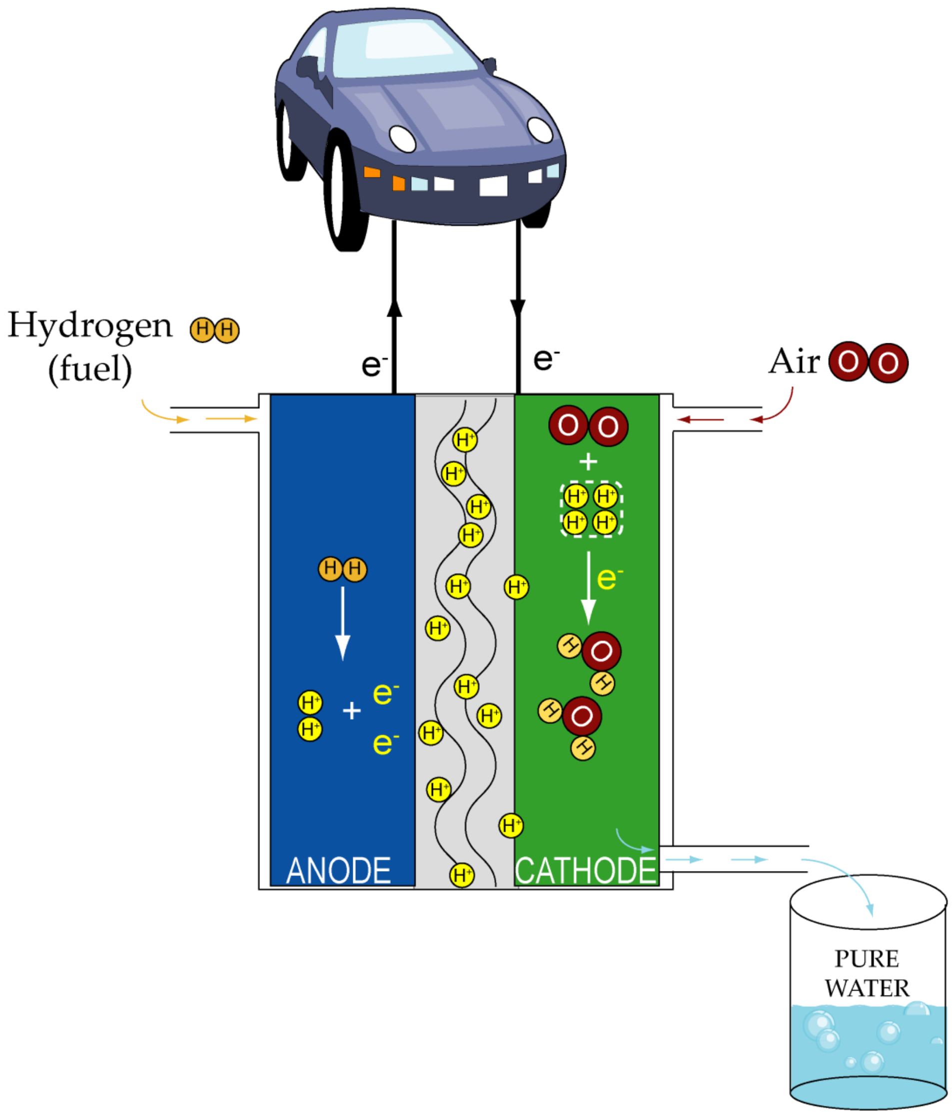
Fuel Cells and Automobiles



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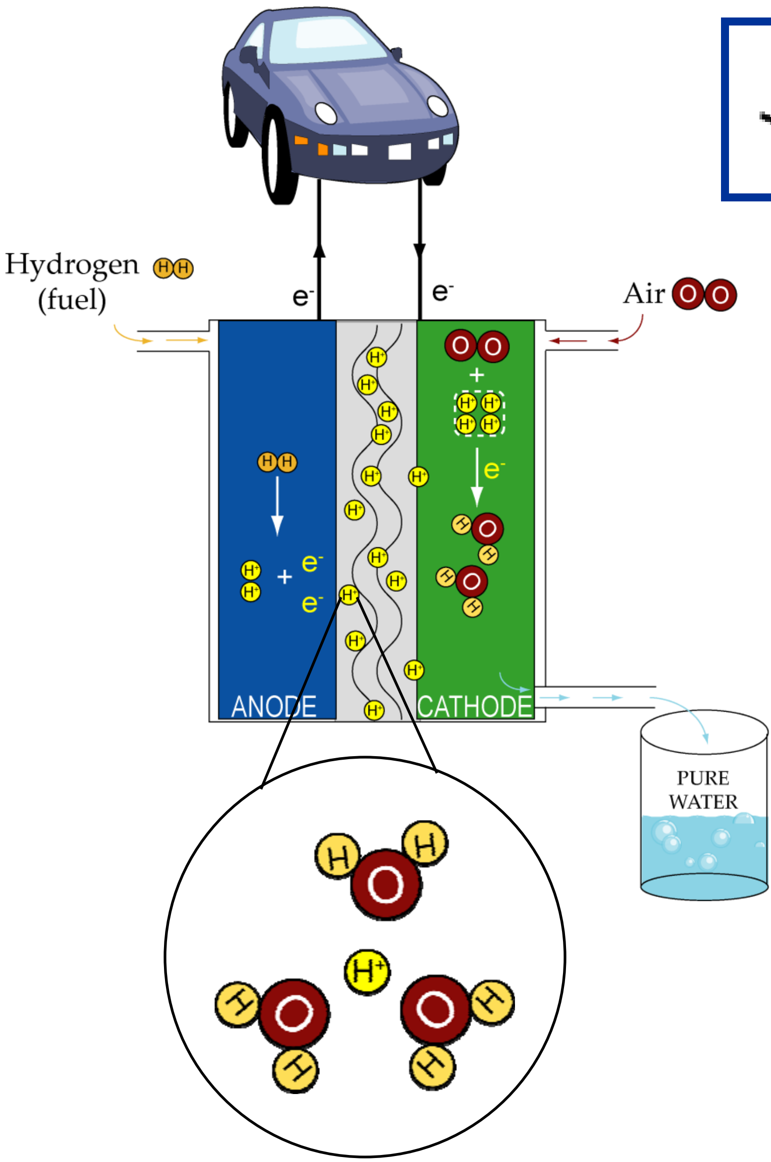
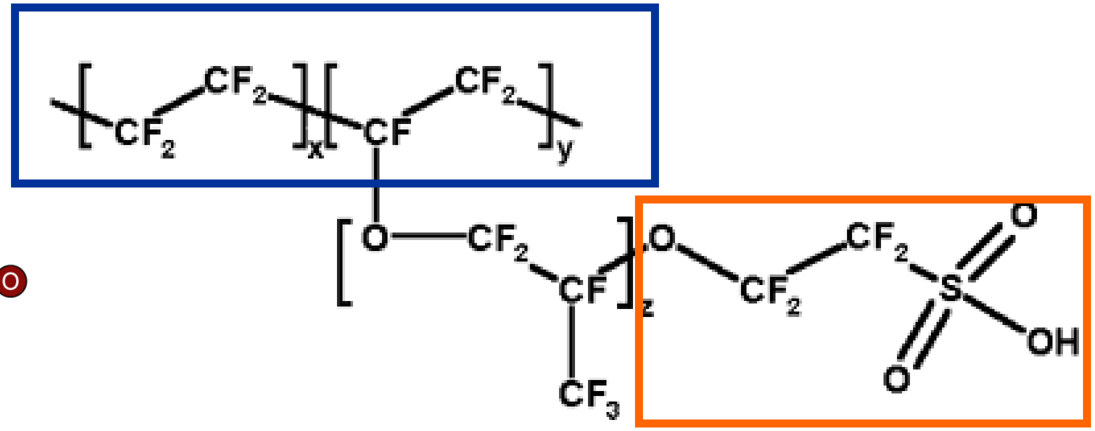
Need for Better Membranes





Nafion

❖Expensive

❖Breaks down at high temps

❖Bleeds Fuel

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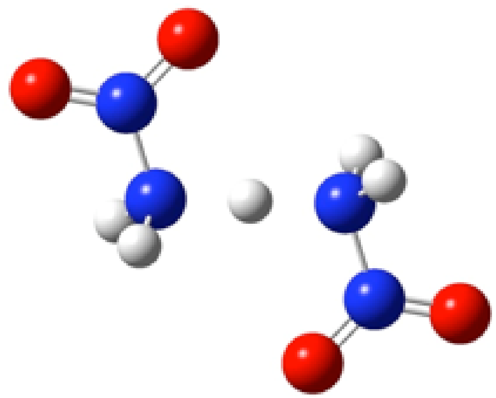
What Controls Proton Transfer?

$$NH_2NO_2 \cdot\cdot H^{+} \cdot\cdot NH_2NO_2$$



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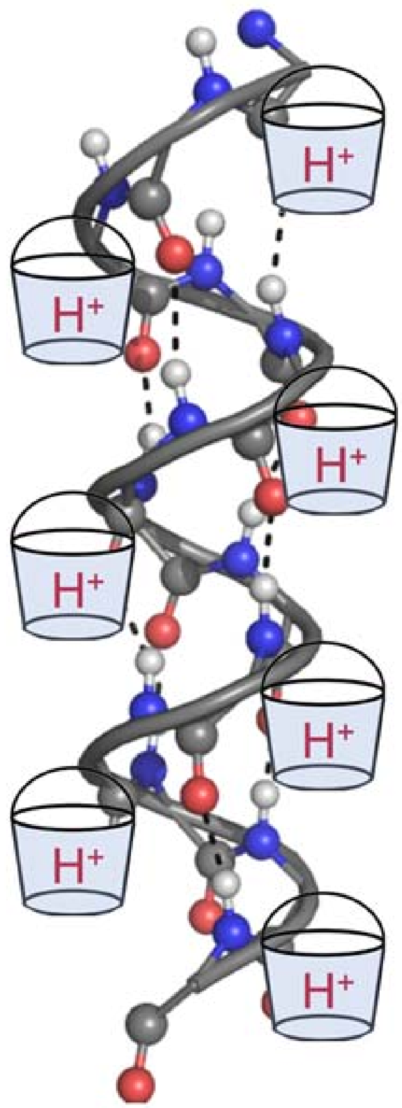
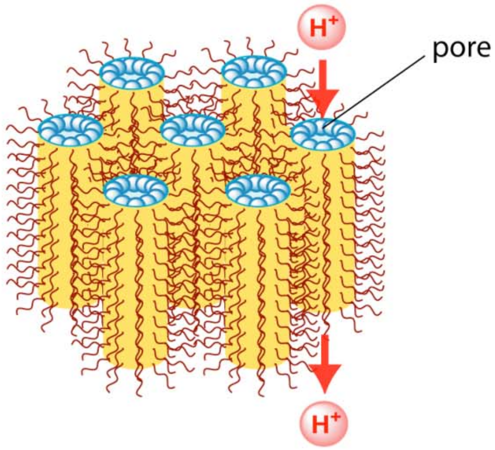
What Controls Proton Transport?

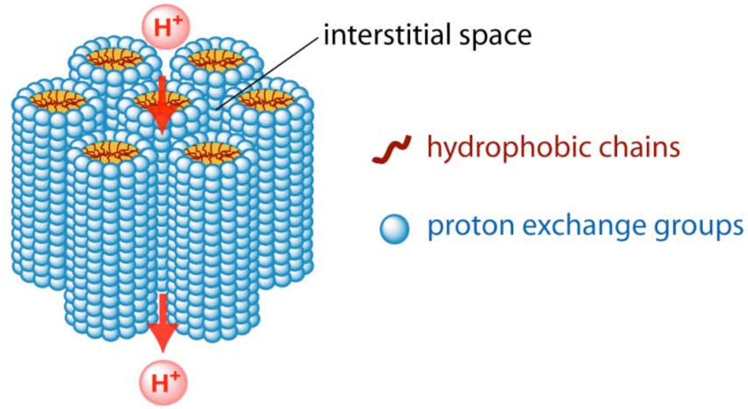


inverse cylindrical micelle



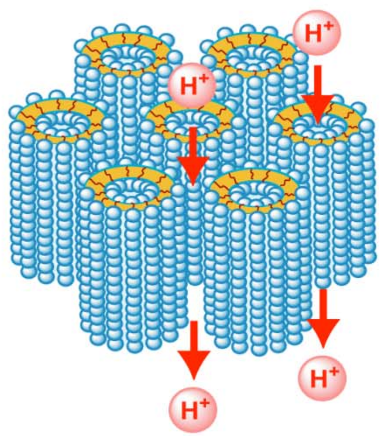
Proton conduction through pores of the assembly

cylindrical micelle



Proton conduction through interstitial space of the assembly

vesicle



Proton conduction through both

- **Do we need organized structure?**
- **Which ordered structure is better?**
- **Which is the best for H^+ conductivity?**

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Hydrogen Economy: Fundamental Questions

Efficient, Cost effective, Environmentally Friendly , Storage and Transport

- How to break H-O-H bonds at lower temperatures?
- How to break C-H bonds at lower temperatures?
- How to reversibly convert H- to H_2?
- Can H_2 be physisorbed on surfaces?

Efficient Fuel Cells for Energy Generation

- What is the structure of H^+ ions in water?
- How to design membranes that could transport H^+ ions?
- How to stop methanol or hydrogen from moving across the membrane?

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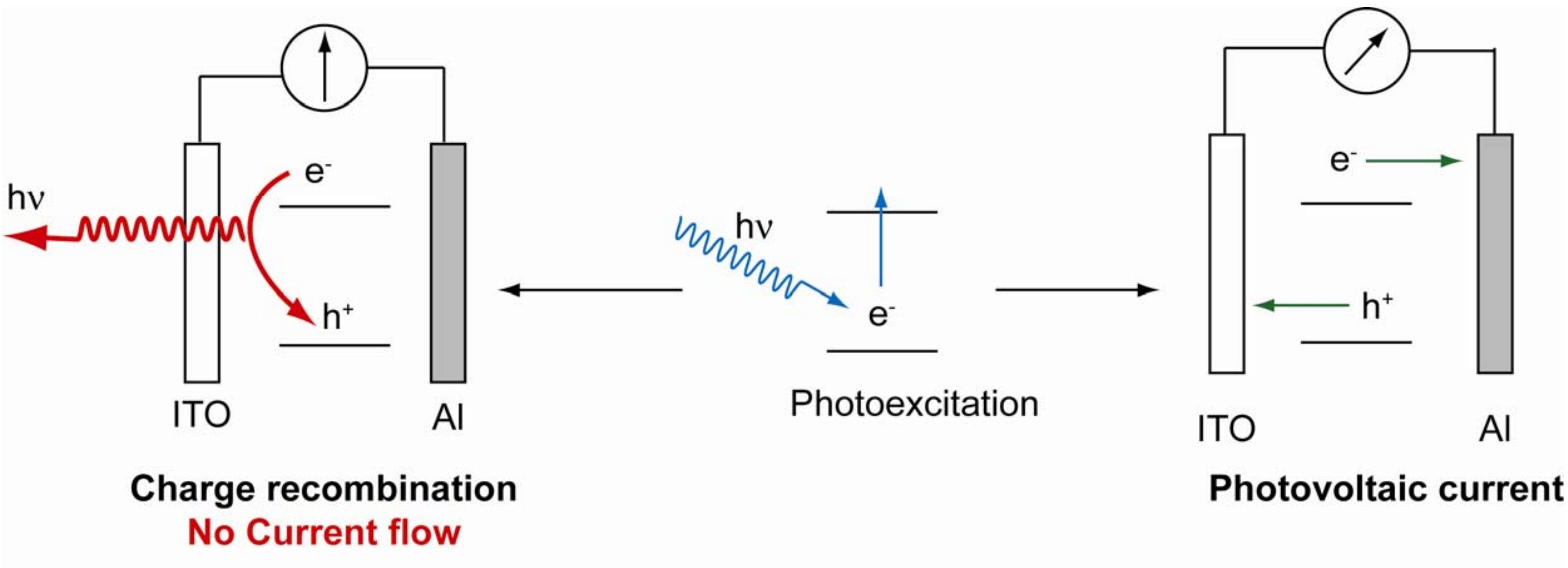
Photovoltaic Cells



Efficiency of Photovoltaic Cells Depend on
- Absorption in Solar Spectrum
- Charge Separation Efficiency
- Charge Mobility

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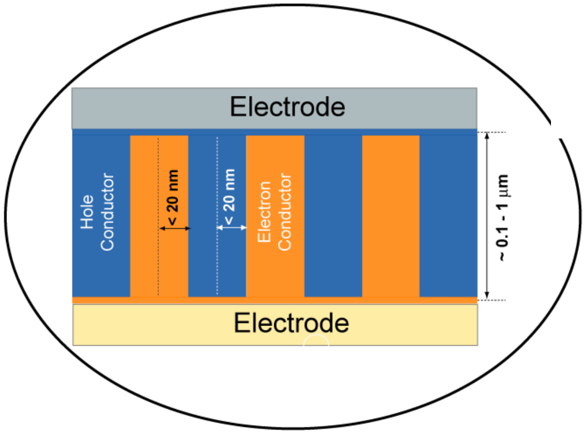
Elusive Heterojunctions

WELL-DEFINED HETEROJUNCTIONS



PV Cells: Fundamental Questions

PV Cells:
Efficient, cost effective, environmentally friendly energy production

❖How to assemble semiconductors for efficient charge separation and mobility? How to assemble heterojunctions without macrophase segregation (interplay of intermolecular forces)?

❖Design of molecules and macromolecules for efficient capture of solar energy. Strategies to capture Solar Energy

❖Design and synthesis of transparent semiconductors to replace expensive Indium tin oxide

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National Chemical Energy Research Network (NCERN)

http://www.chem.umass.edu/masscrest/NCERN/

National Chemical Energy Research Network (NCERN) is designed to facilitate communication between energy researchers and the public, and provides enhanced public understanding, visibility, and publicity to chemical energy research. It is a public portal for educators, students and public to get accurate information on topics related to chemical energy. NCERN is also a dynamic interface between research centers engaged in chemical energy and the surrounding community that is impacted by that research.

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National Chemical Energy Research Network (NCERN)

- ❖Education and Outreach
- ❖Energy Blogs
- ❖Energy Wiki
- ❖Research
- ❖Technology

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Contact Info:

http://www.chem.umass.edu/masscrest/NCERN/

http://www.chem.umass.edu/masscrest/

http://www.umass.edu/research/energy/

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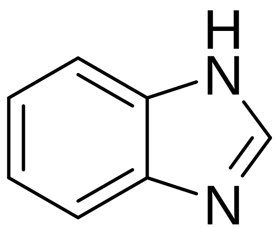
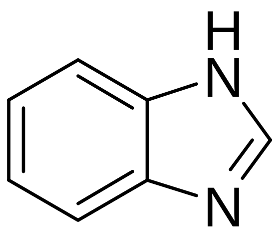
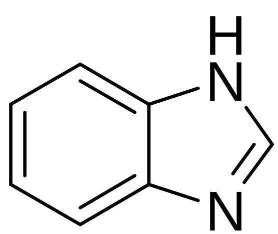
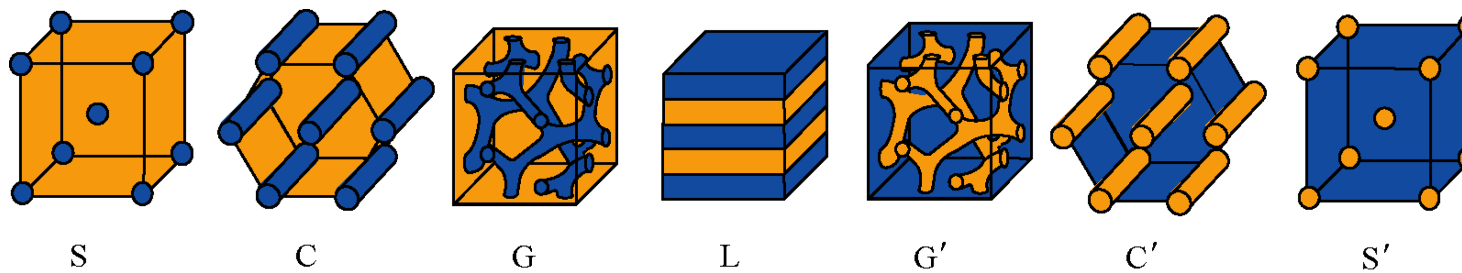
New Membrane Materials at Centre for Fueling the Future



1. Controlling distance between the sites
2. Controlling the assembly of molecules
3. Creating new molecules for proton transport







Benzimidazole

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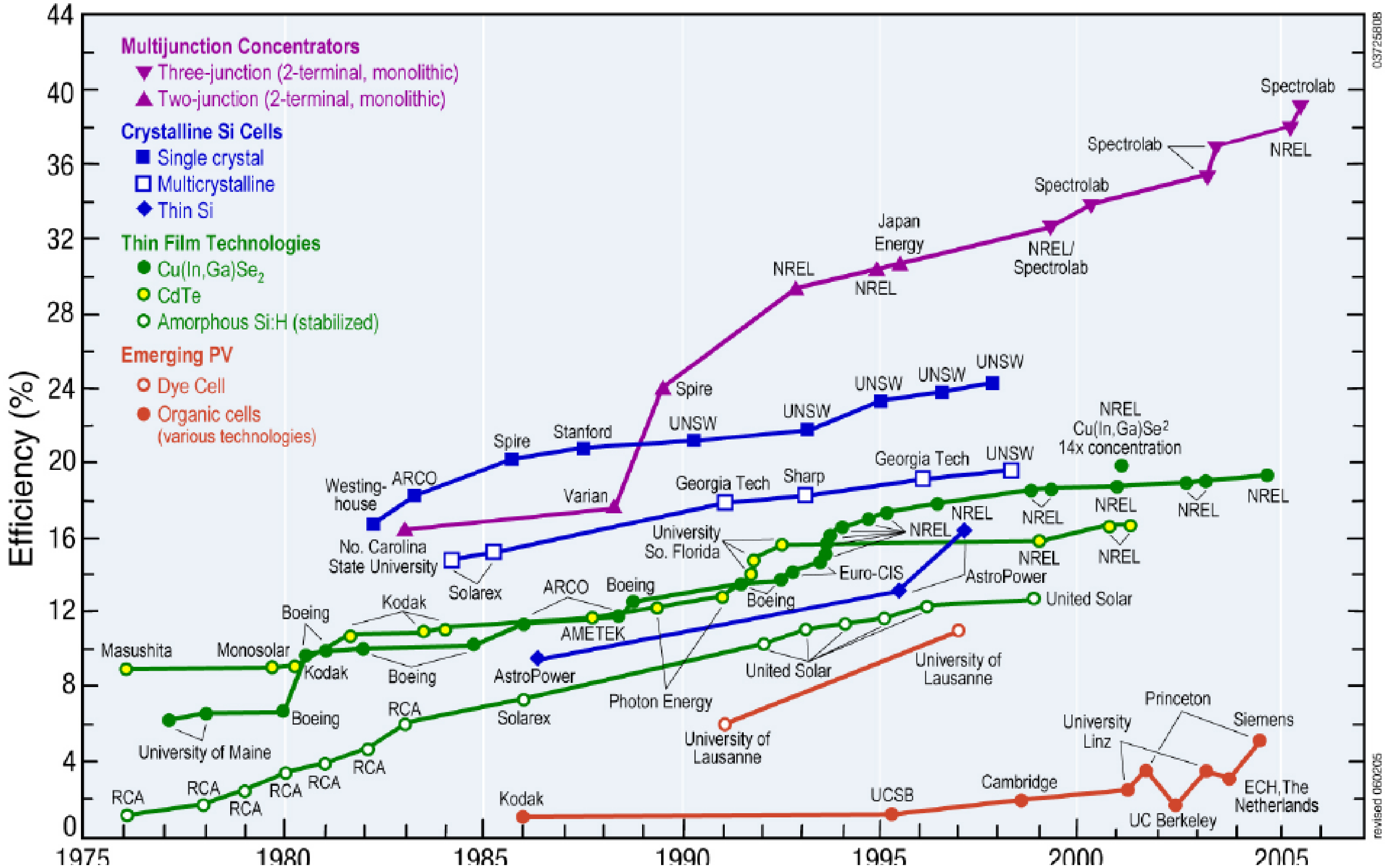
Efficiency of Current Photovoltaics Devices



Source: Basic Research Energy Needs for Solar Energy Utilization, US Department of Energy

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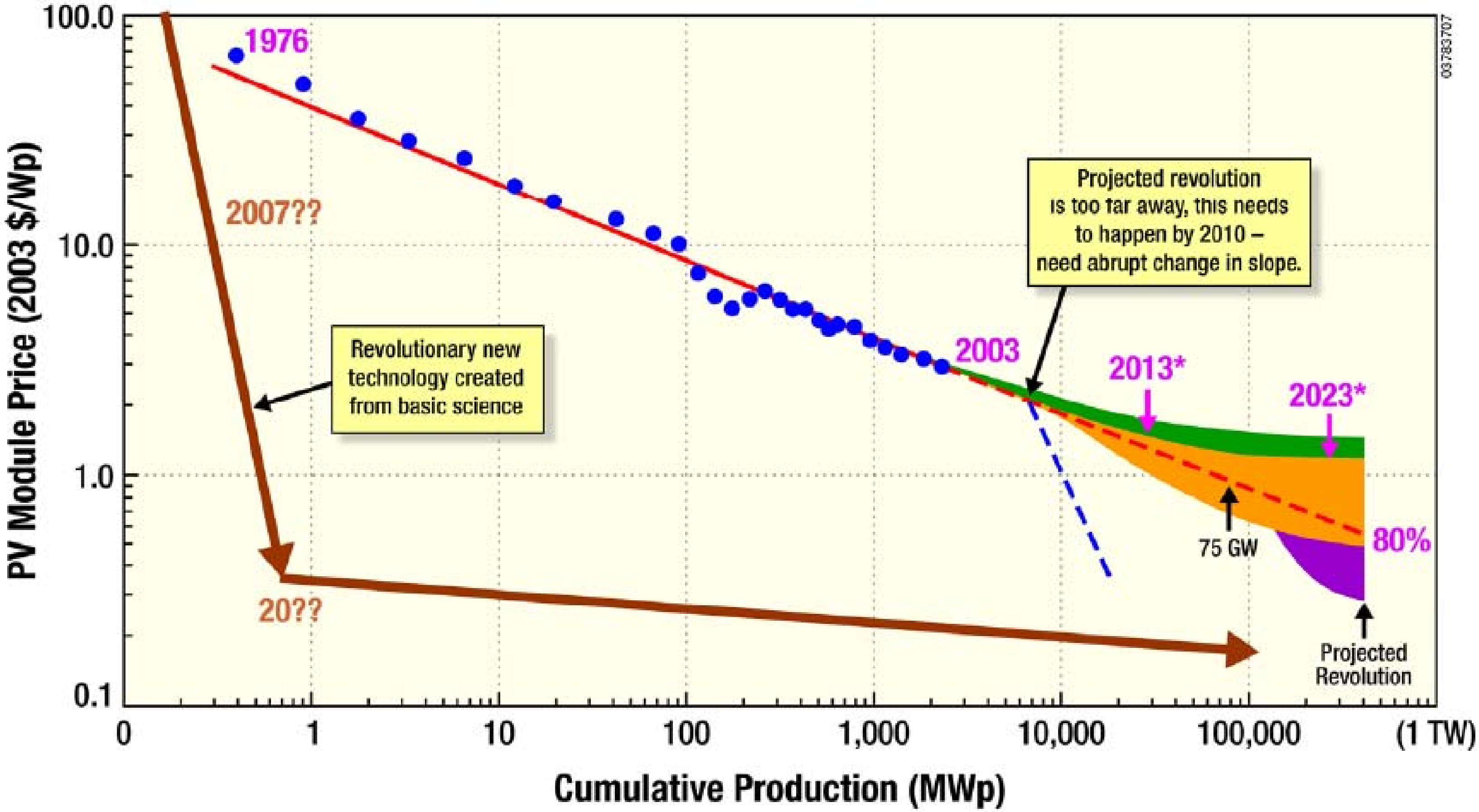
Fuel Cells in Develpment

Fuel Cell Type	Electrolyte	Cond. Ion	Temp. (ºC)	Features
Polymer **Fuel: H_2**	$CF(CF_2)_nOCF_2SO_3^-$ NAFION	H^+ hydrated	0–80	High power density, Pt catalyst, must be kept wet, poisoned by CO, S, Cl
Alkaline **Fuel: H_2**	KOH gel	OH^-	90	High power density, cannot tolerate CO_2, impurities (NASA)
Phosphoric acid **Fuel: H_2**	H_3PO_4	H^+	250	Medium power density, Pt catalyst, sensitive to CO, poisoned by S, Cl
Molten carbonate **Fuel: H_2**	Li_2CO_3 / K_2CO_3	CO_3^{2-}	650	Low power density, Ni catalyst, needs CO_2 recycle
Solid oxide **Fuel: CH_4, H_2**	$Zr_{0.92}Y_{0.08}O_{1.96}$	O^{2-}	700–1,000	Medium-to-high power density, much less sensitive to impurities
Direct methanol **Fuel: CH_3OH**	$CF(CF_2)_nOCF_2SO_3^-$ NAFION	H^+ hydrated	0–80	Medium power density, low efficiency, high Pt content. Sensitive to S and Cl impurities

Efficiency and Cost



Source: Basic Research Energy Needs for Solar Energy Utilization, US Department of Energy

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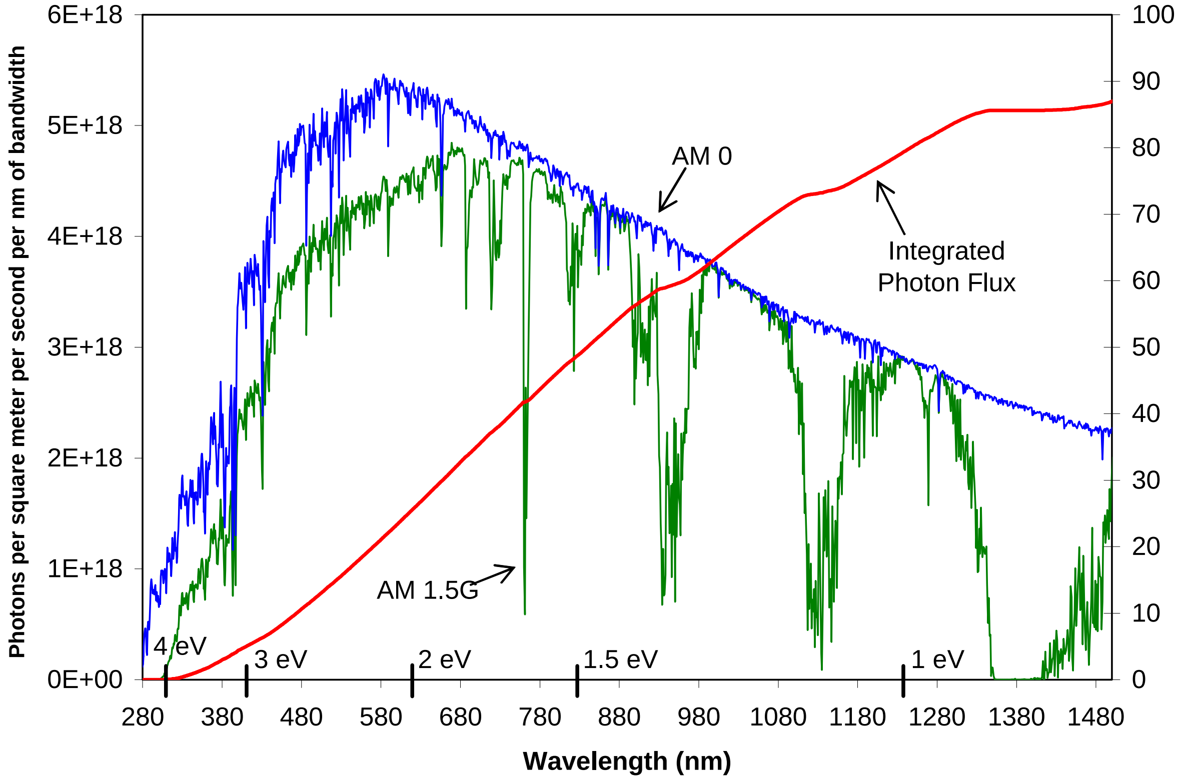
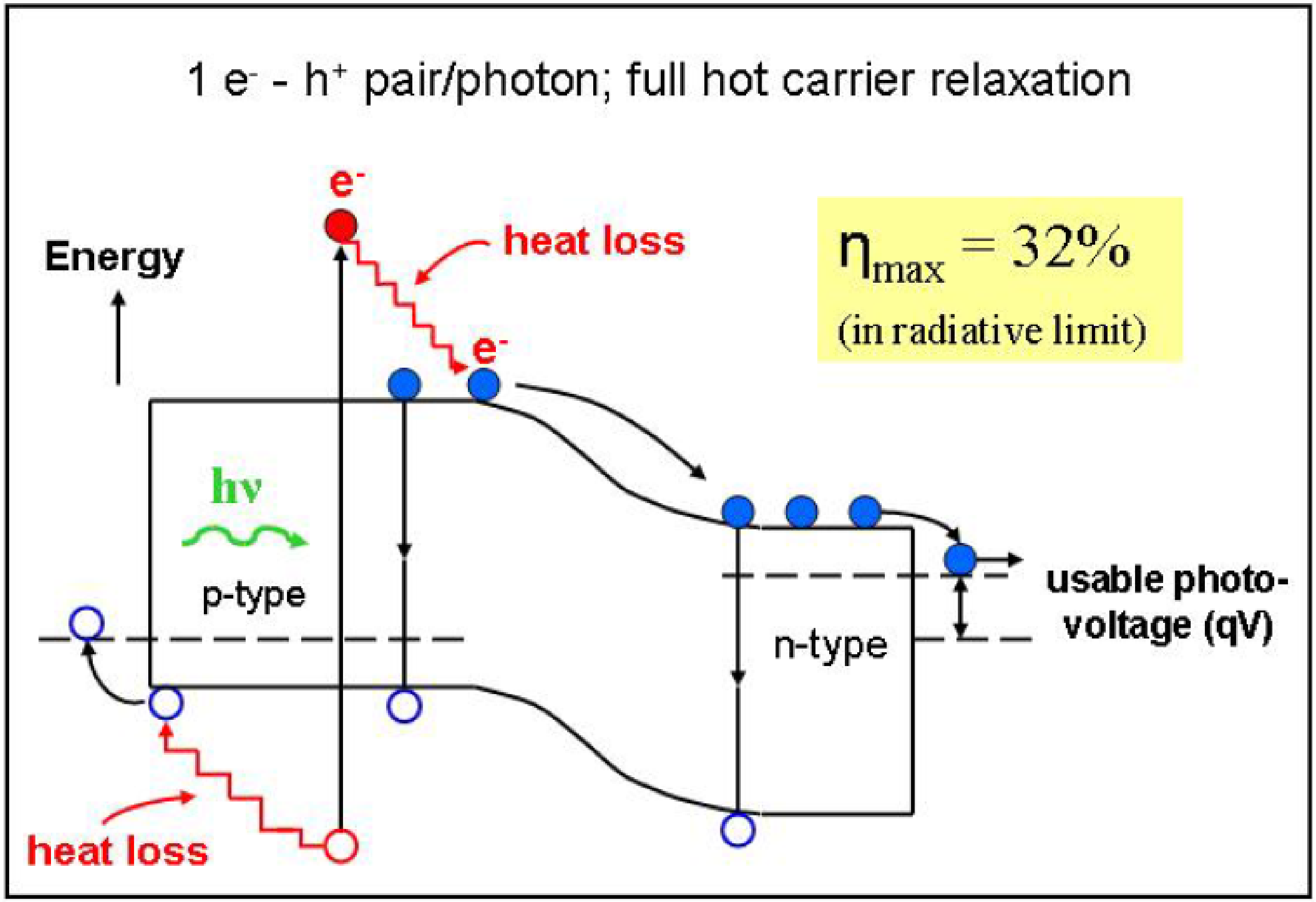
Solar Insolation



Shockley-Queisser Limit: Better Photon Management



Source: Basic Research Energy Needs for Solar Energy Utilization,
US Department of Energy

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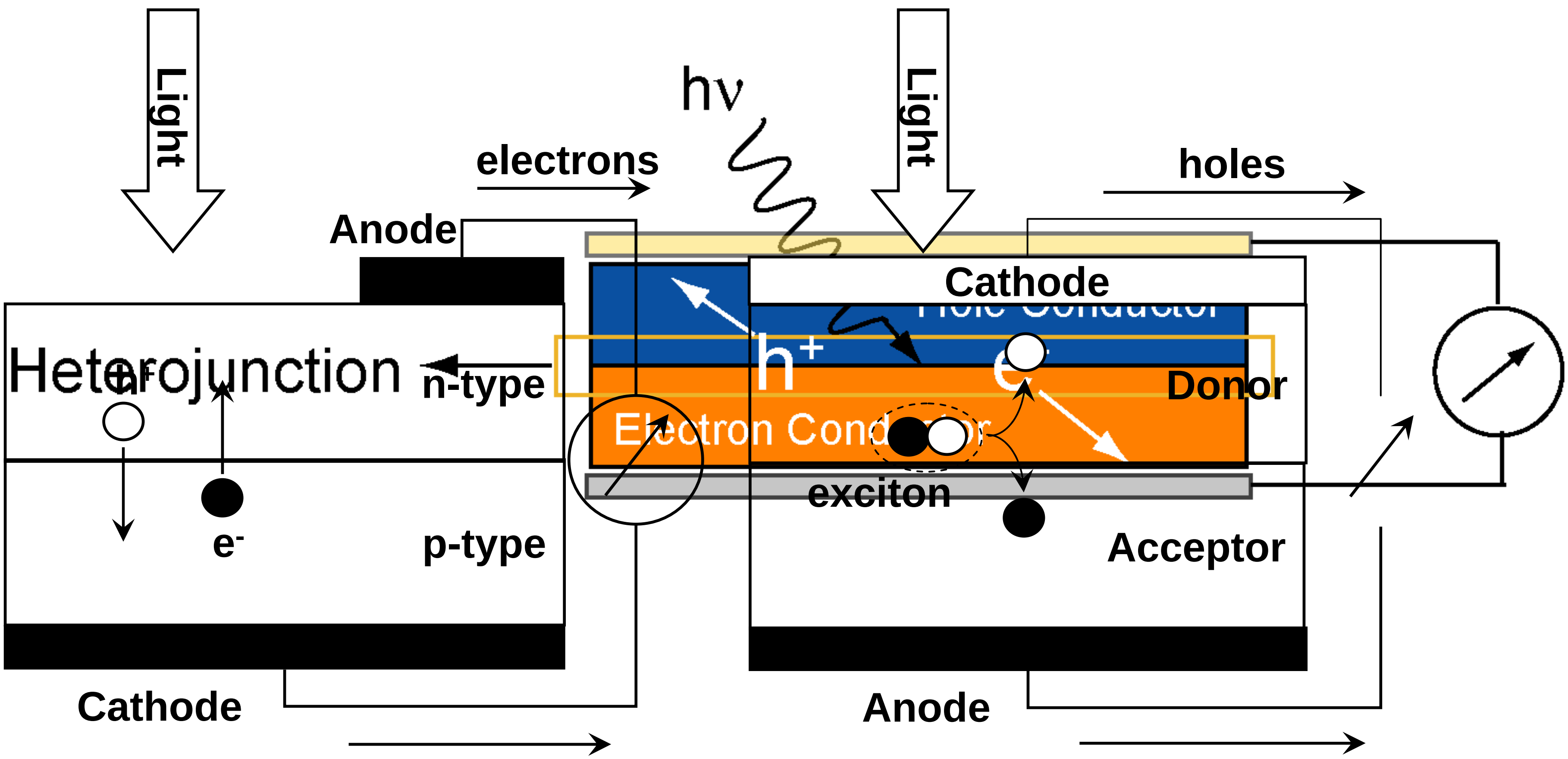
P-N junctions and Photovoltaic Cells

Conventional Solar Cell **Organic Heterojunction Solar Cell**



Spanggaard, H.; Krebs, F. C. "A brief history of the development of organic and polymeric photovoltaics," *Solar Energy Materials and Solar Cells* **2004**, *83*, 125-146.

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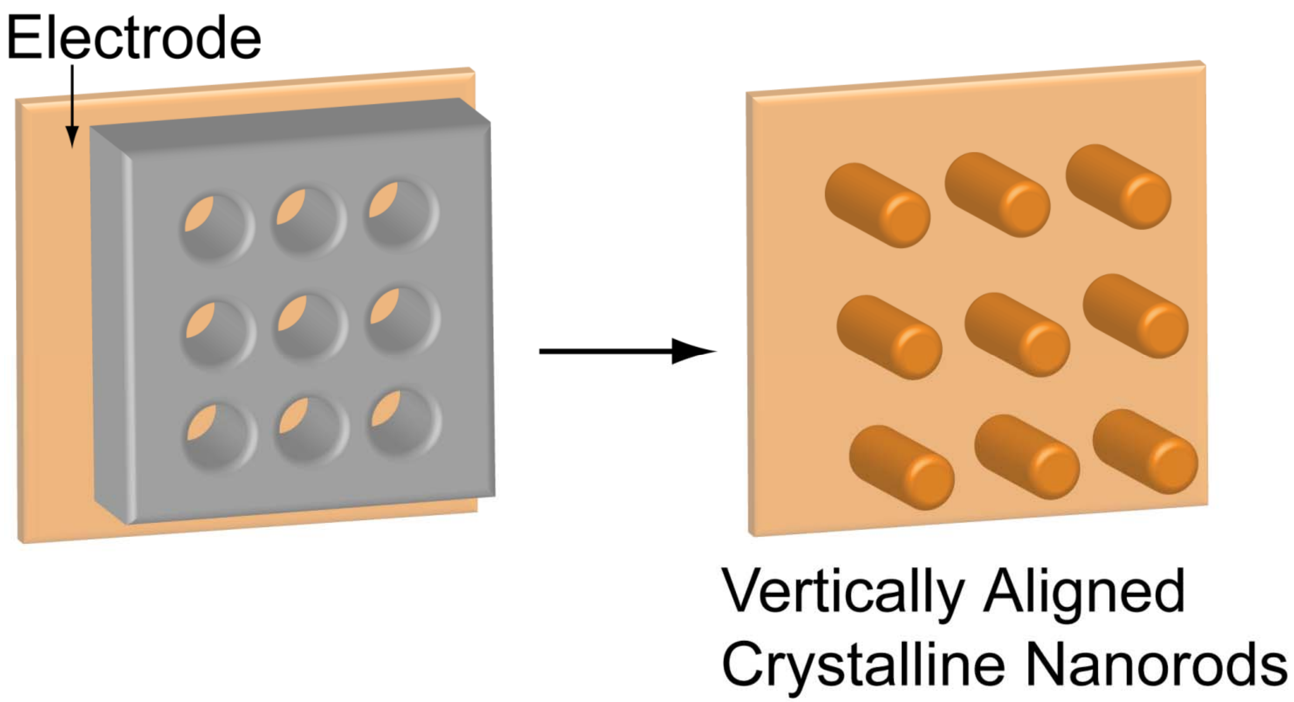
Templated-Directed Electrodeposition



'a simple, high-throughput, and cost-effective procedure...' to create 1D nanostructures

Xia, Y. N.; Yang, P. D.; Sun, Y. G.; Wu, Y. Y.; Mayers, B.; Gates, B.; Yin, Y. D.; Kim, F.; Yan, Y. Q. "One-Dimensional Nanostructures: Synthesis, Characterization, and Applications," *Advanced Materials* **2003,** *15*, 353-389.

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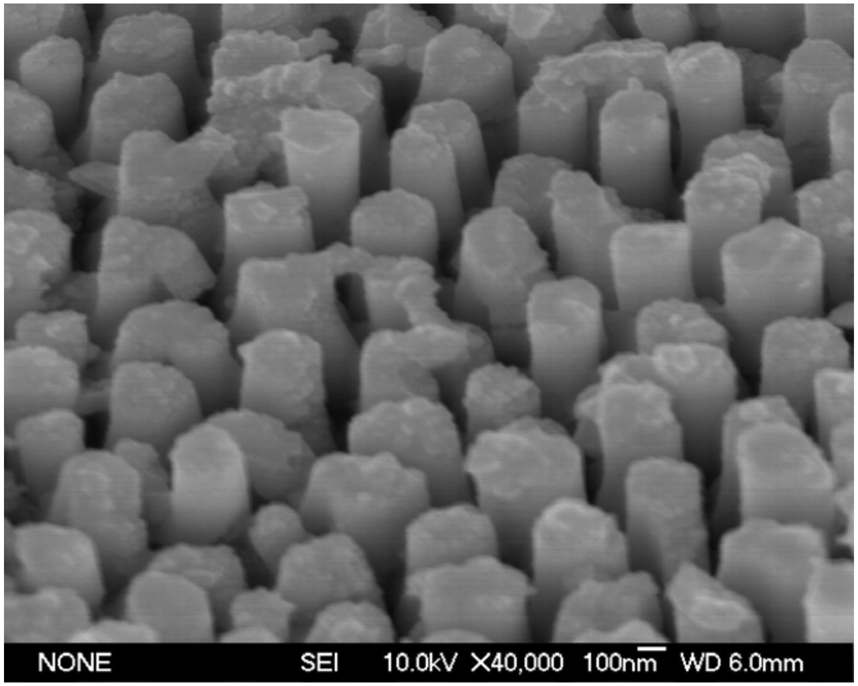
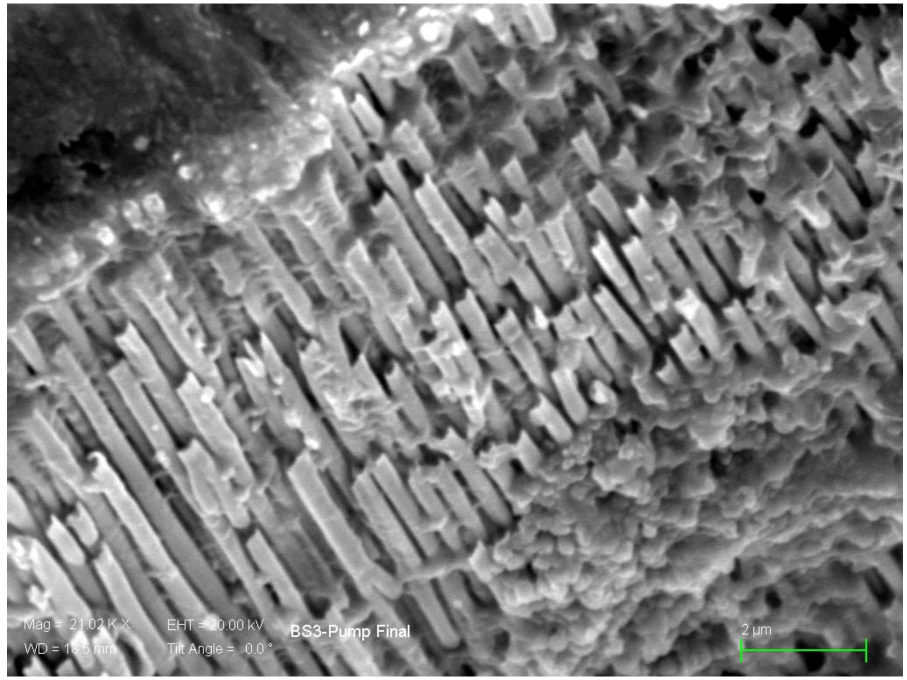
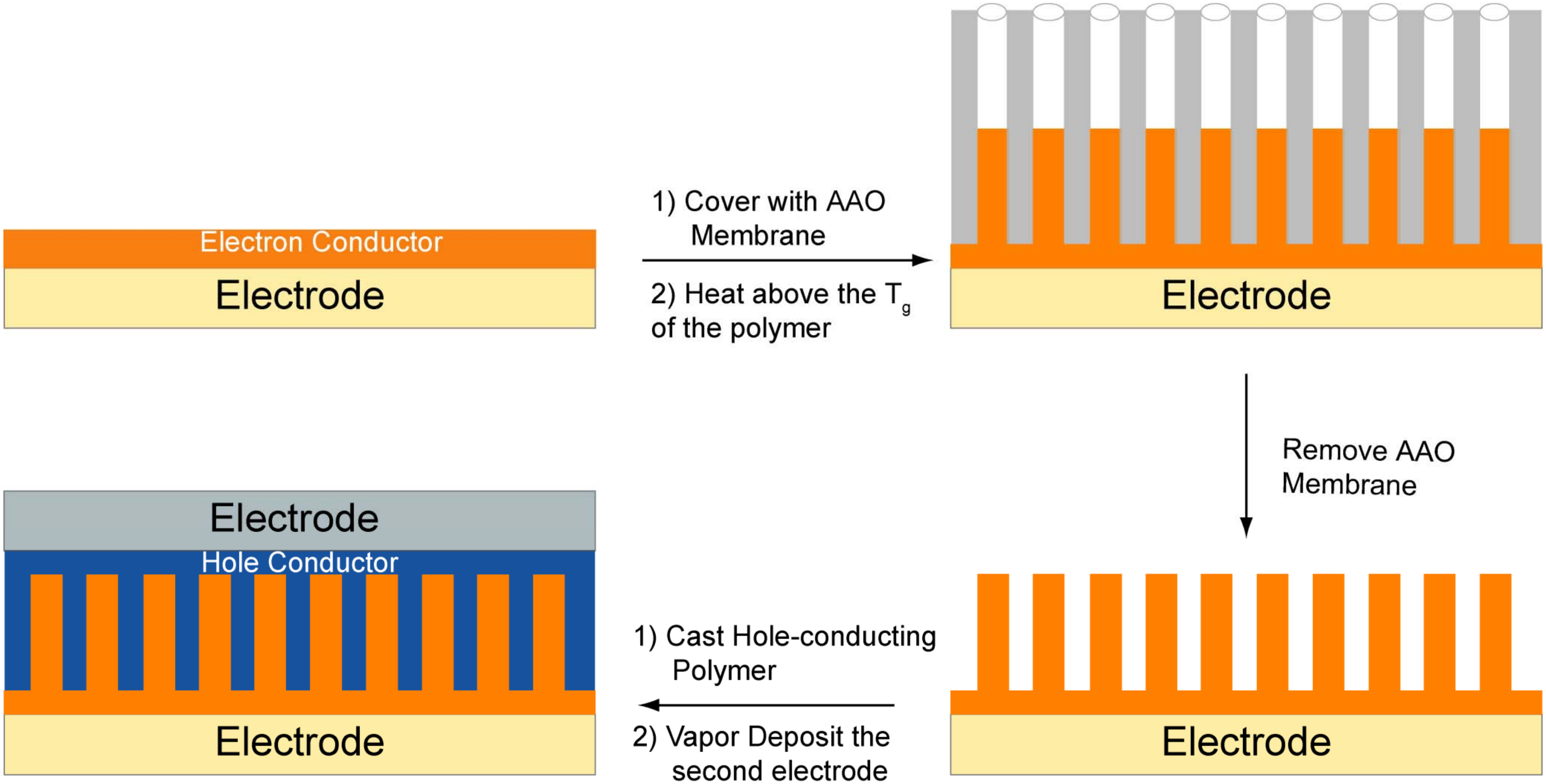
Templated-Directed Cadmium Selenide Electrodeposition





UMass Researchers Focus on Efficient PV Cells



Prof. Thayumanavan, Chemistry
Prof. Thomas Russell, PSE

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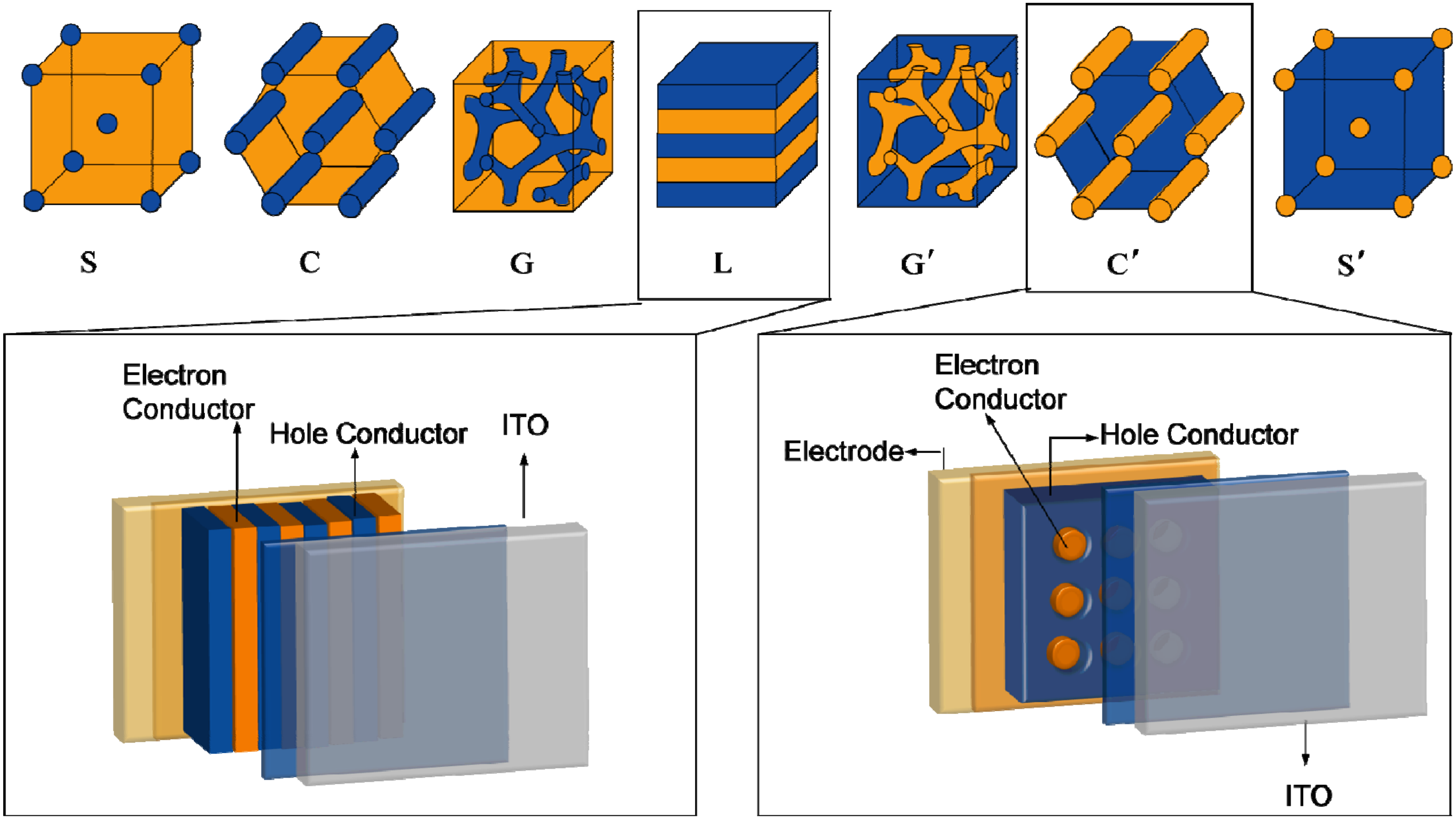
UMass Researchers Focus on Efficient Morphologies



THE DV RESEARCH GROUP AT UMASS AMHERST

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Hydrogen Production from Carbon Sources

Methane

$$CH_4\,(g) + H_2O\,(g) \rightarrow CO_2\,(g) + 4\,H_2$$

At 650 °C, the reaction is spontaneous.

Water- Gas Shift Reaction

$$CO + H_2O \rightarrow CO_2 + H_2$$

From Coal

$$C + H_2O \rightarrow CO + H_2$$

$$C + 2\,H_2O \rightarrow CO_2 + 2H_2$$

Expected H_2 Demand in 2040

- 150 Mtons

Current Production

- 10 Mtons

- **1 ton of H_2 = 5 tons of CO_2**

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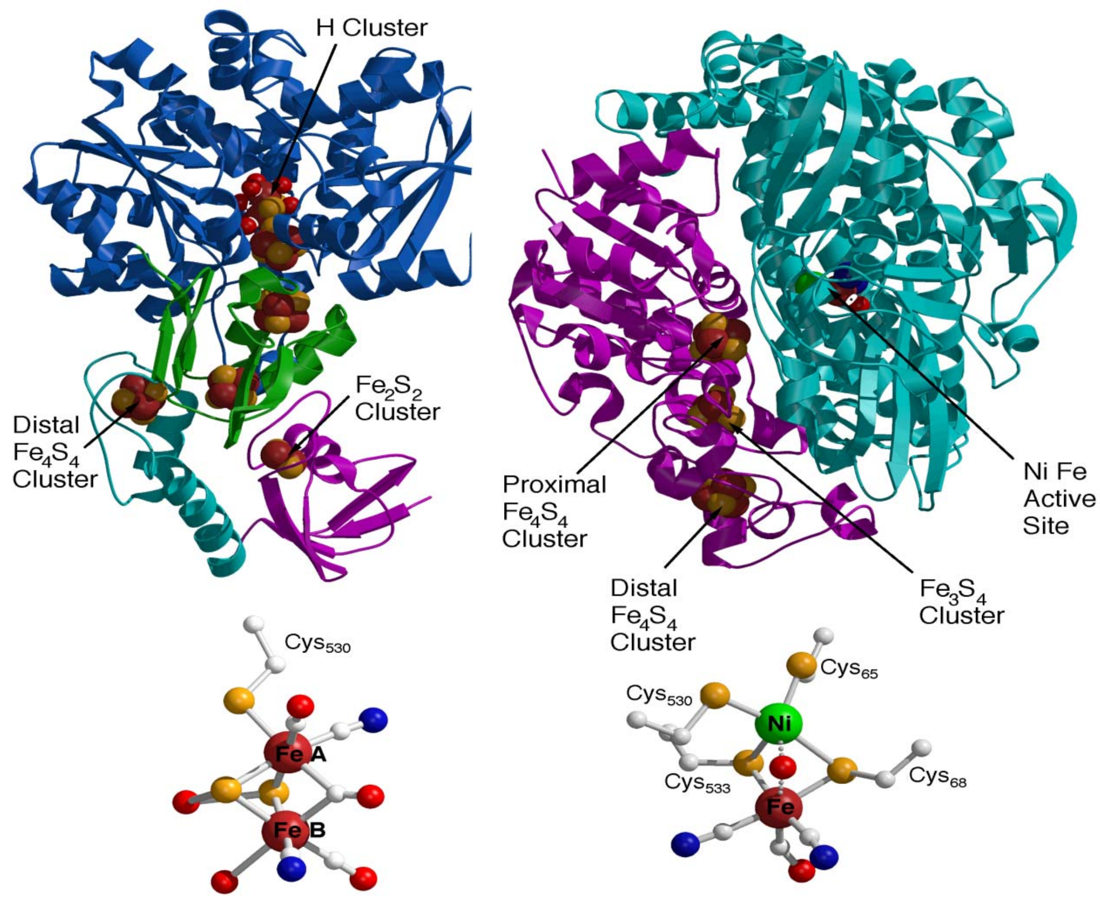
Breaking Water Using Enzymes –UMass at the Forefront

Hydrogenase



Clostridium pasteuianum Fe-Fe H2ase-I and *Desulfovibrio gigas* NiFe H2ase.

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Hydrogenase as a catalyst of H_2 Production

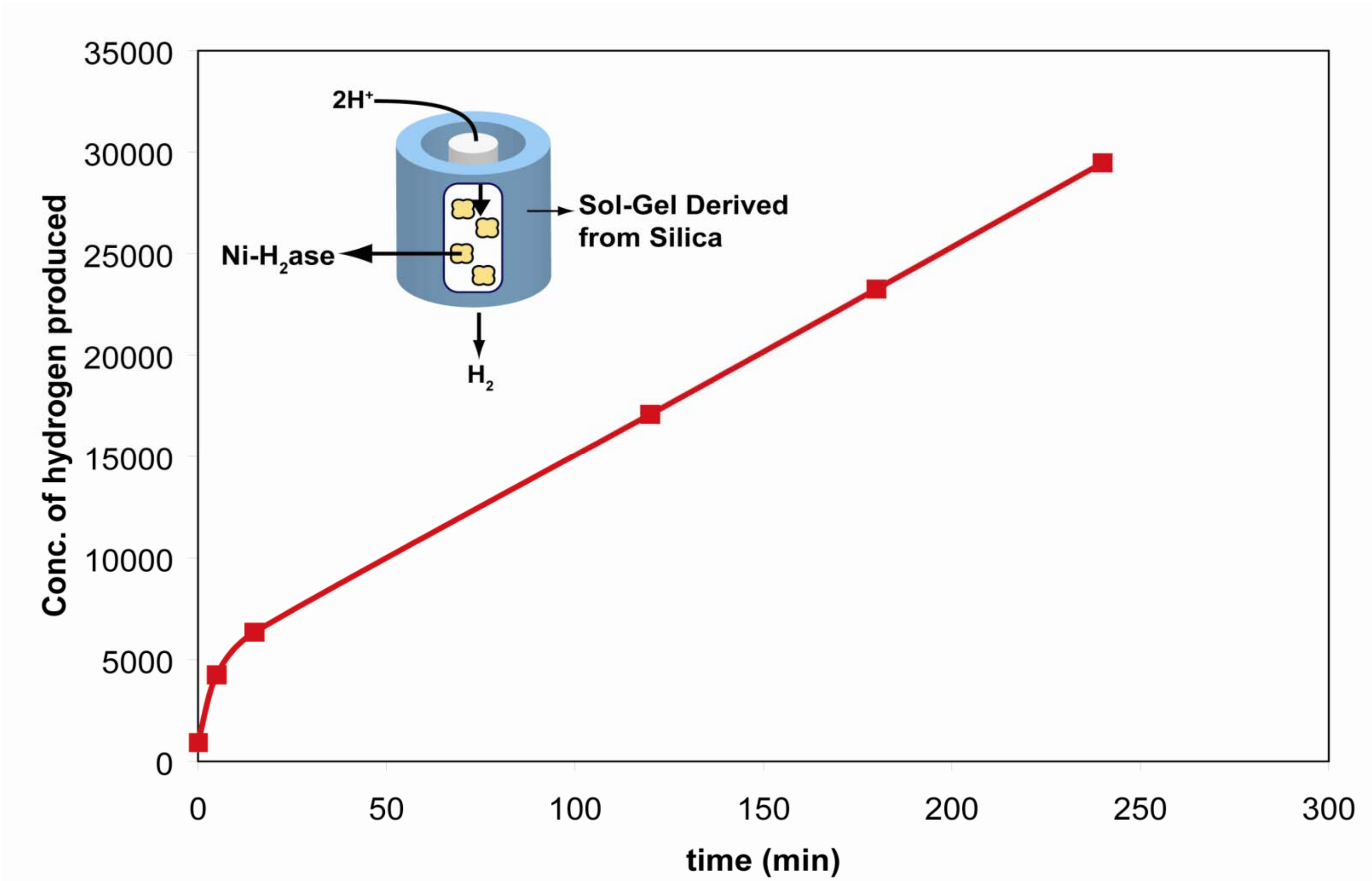


Figure 4: A plot of the amount of hydrogen produced with respect to time in a hydrogenase encapsulated in a sol-gel glass.

Maroney (UMass Amherst) and Elgren (Hamilton College)

Hydrogen Generation through Nanobiotechnology

$$2\,H^+ + 2\,e^- \rightleftharpoons H_2$$

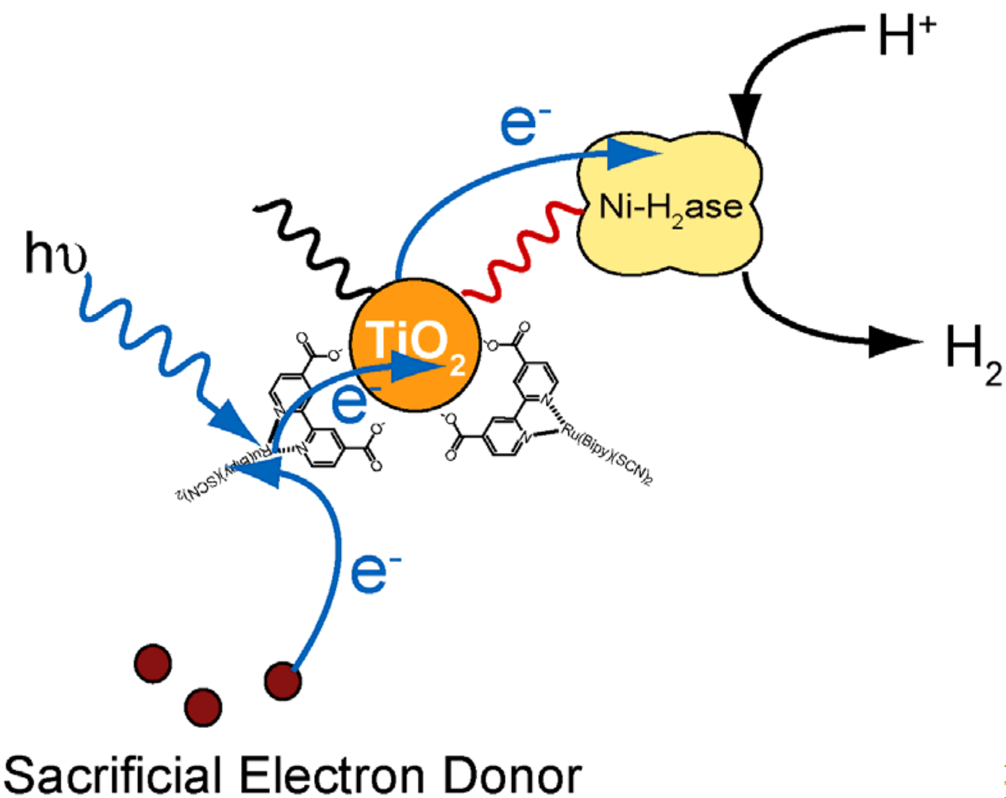


Chart 1

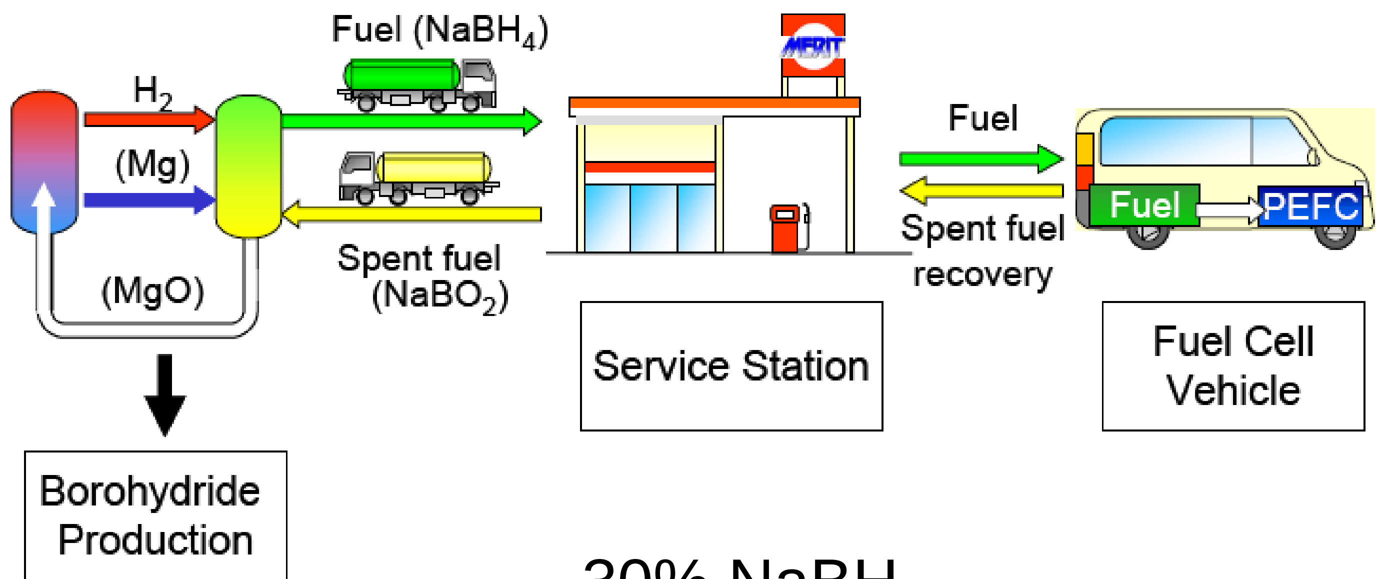
D. Venkataraman and Maroney

Hydrogen Storage and Transport : Sodium Borohydride

Millennium Cell

catalyst

$$NaBH_4 + 2\,H_2O \rightarrow 4\,H_2 + NaBO_2$$



"Hydrogen on demand"

30% $NaBH_4$
3% NaOH
67% Water

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Hydrogen Storage and Transport

Hydrogen storer	Mass, kg	Volume, l	Cost, US$
LiH	1.7	3.7	109
CaH_2	4.5	4.0	104
$NaBH_4$ (35 wt% aqueous)	6.21	6.21	102
H_3BNH_3	2.38	3.21	390-525

Source: National Renewable Energy Laboratory, USA

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