

Hydrogen Production from Photoelectrochemical Cells: Theoretical Considerations and Experimental results



M Curie RTN “Hydrogen”
Warsaw, Poland

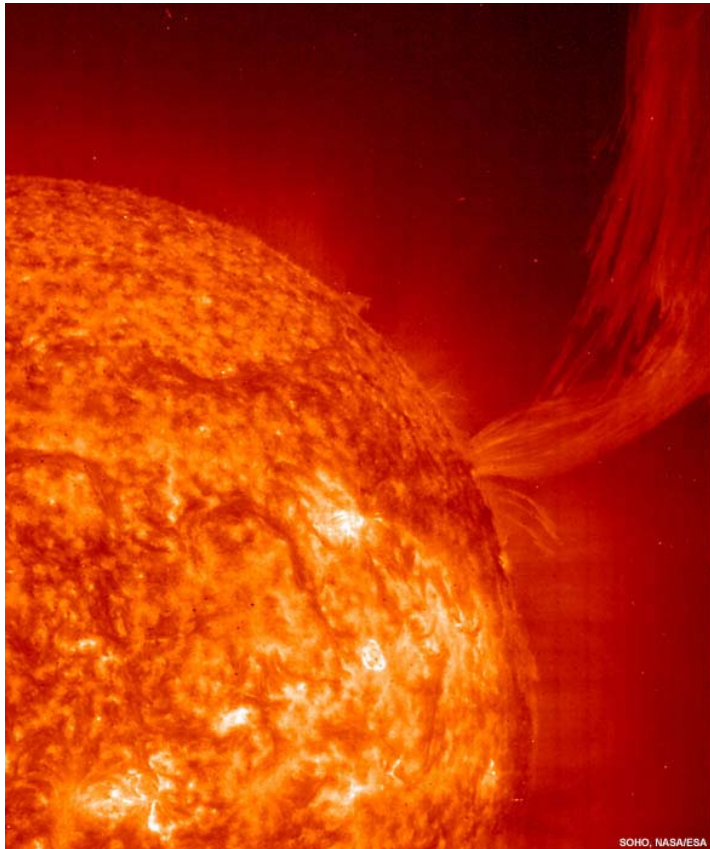
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October 25, 2009

Direct Conversion Systems

Visible light has sufficient energy to split water (H_2O) into **Hydrogen and Oxygen**

Requires the combination of a **Light Harvesting System** and a **Water Splitting System**



- ✓ Semiconductor photoelectrolysis
- ✓ Photobiological Systems
- ✓ Homogeneous water splitting
- ✓ Heterogeneous water splitting
- ✓ Thermal cycles

(Sunlight and Water to Hydrogen with No External Electron Flow)

Historical Perspective - Setting Goals

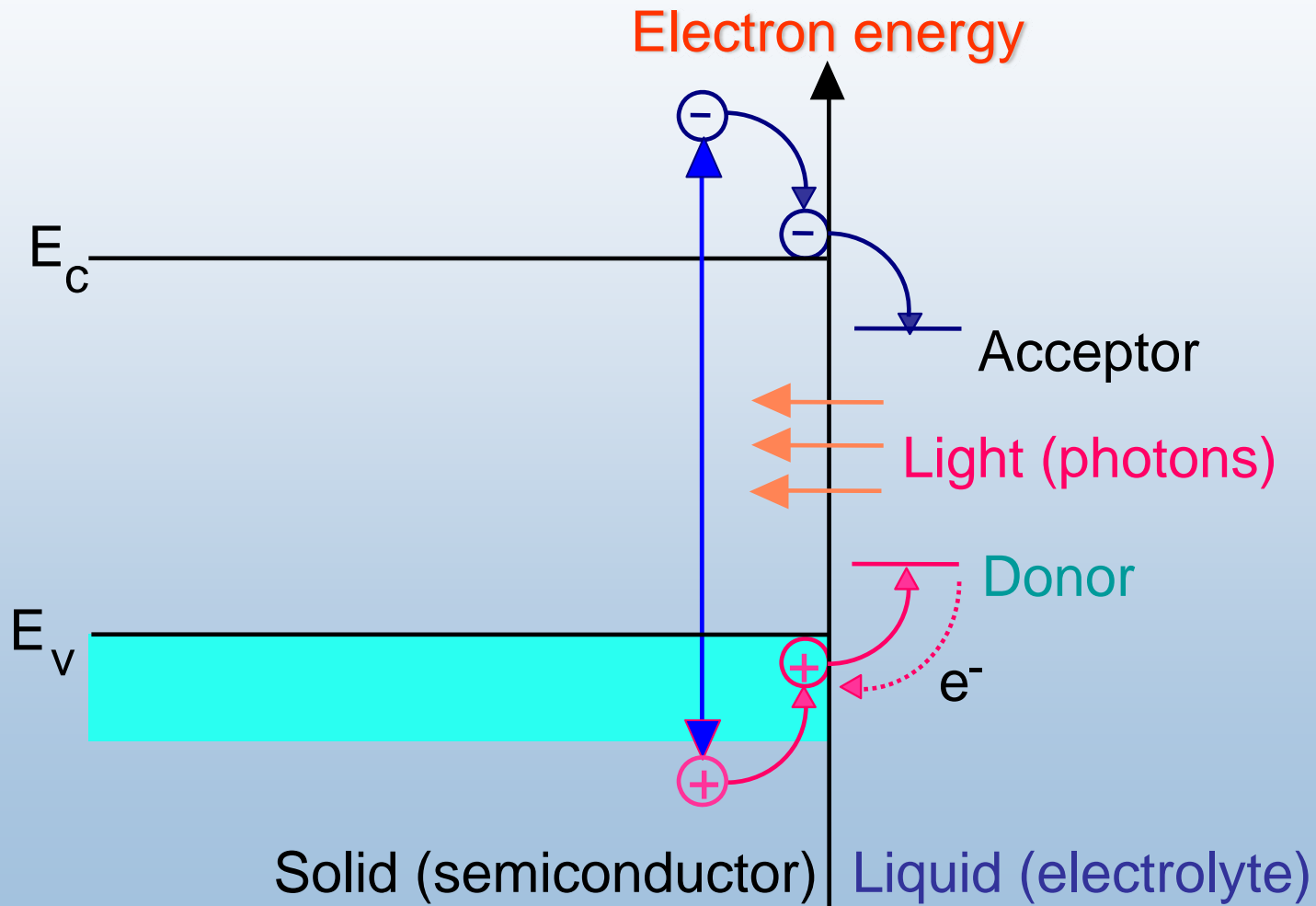
“Holy Grails of Chemistry”, *Accounts of Chemical Research*,
vol 28 (1995)

Allen J. Bard & Marye Anne Fox “Artificial Photosynthesis:
Solar Splitting of Water to Hydrogen and Oxygen”

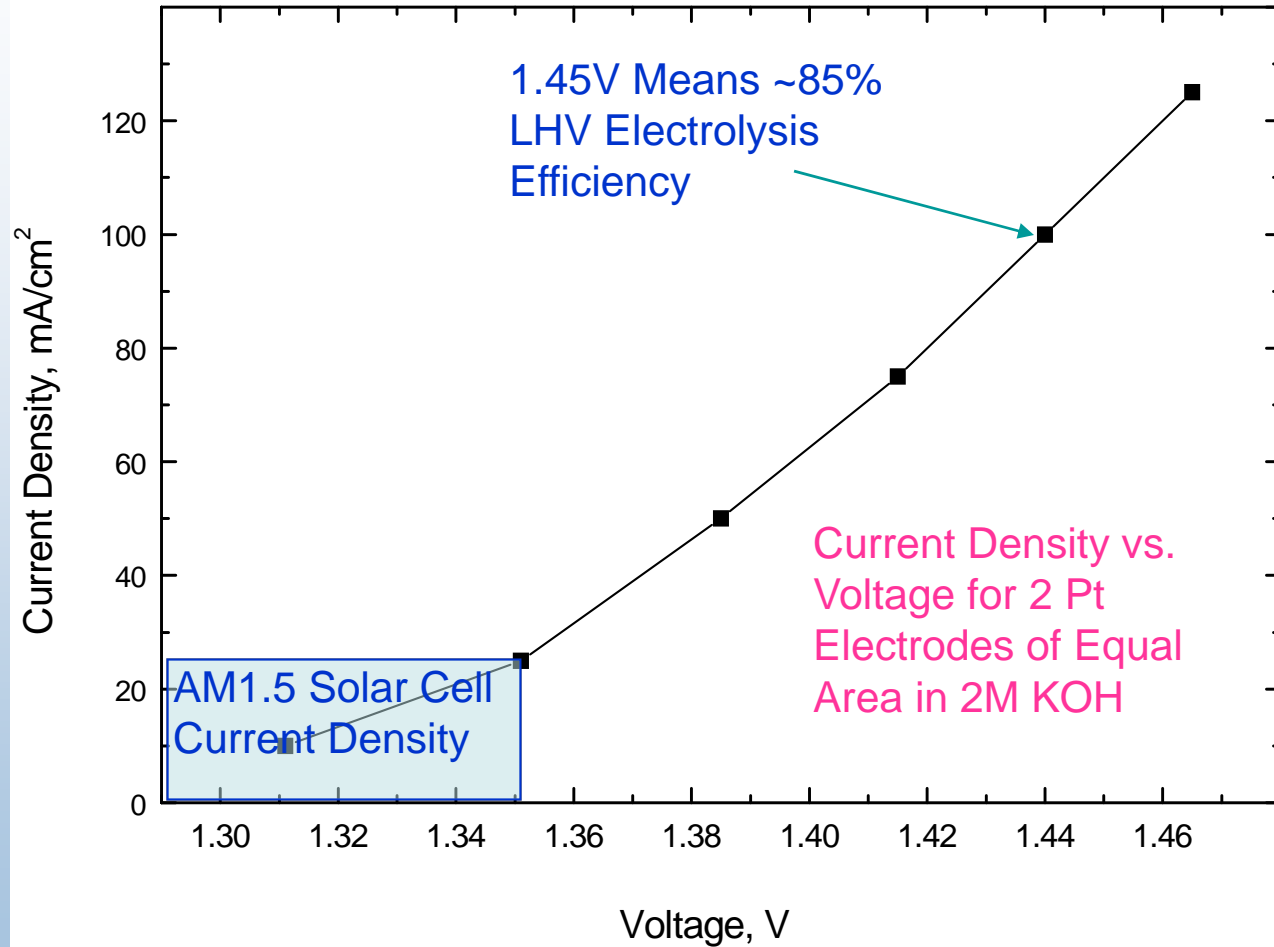
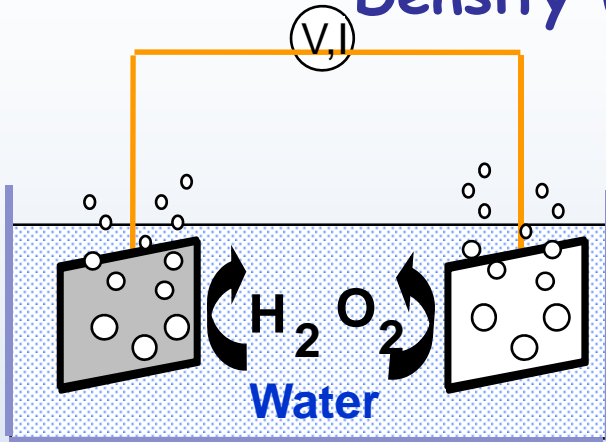


Water splitting “Holy Grail” definition: “We want an efficient and long-lived system for splitting water to H_2 and O_2 with light in the terrestrial (AM1.5) solar spectrum at an intensity of one sun. For a practical system, an energy efficiency of at least 10% appears to be necessary. This means that the H_2 and O_2 produced in the system have a fuel value of at least 10% of the solar energy incident on the system....and will not be consumed or degraded under irradiation for at least 10 years.”

Chemical Reactions at a Semiconductor Electrolyte Interphase



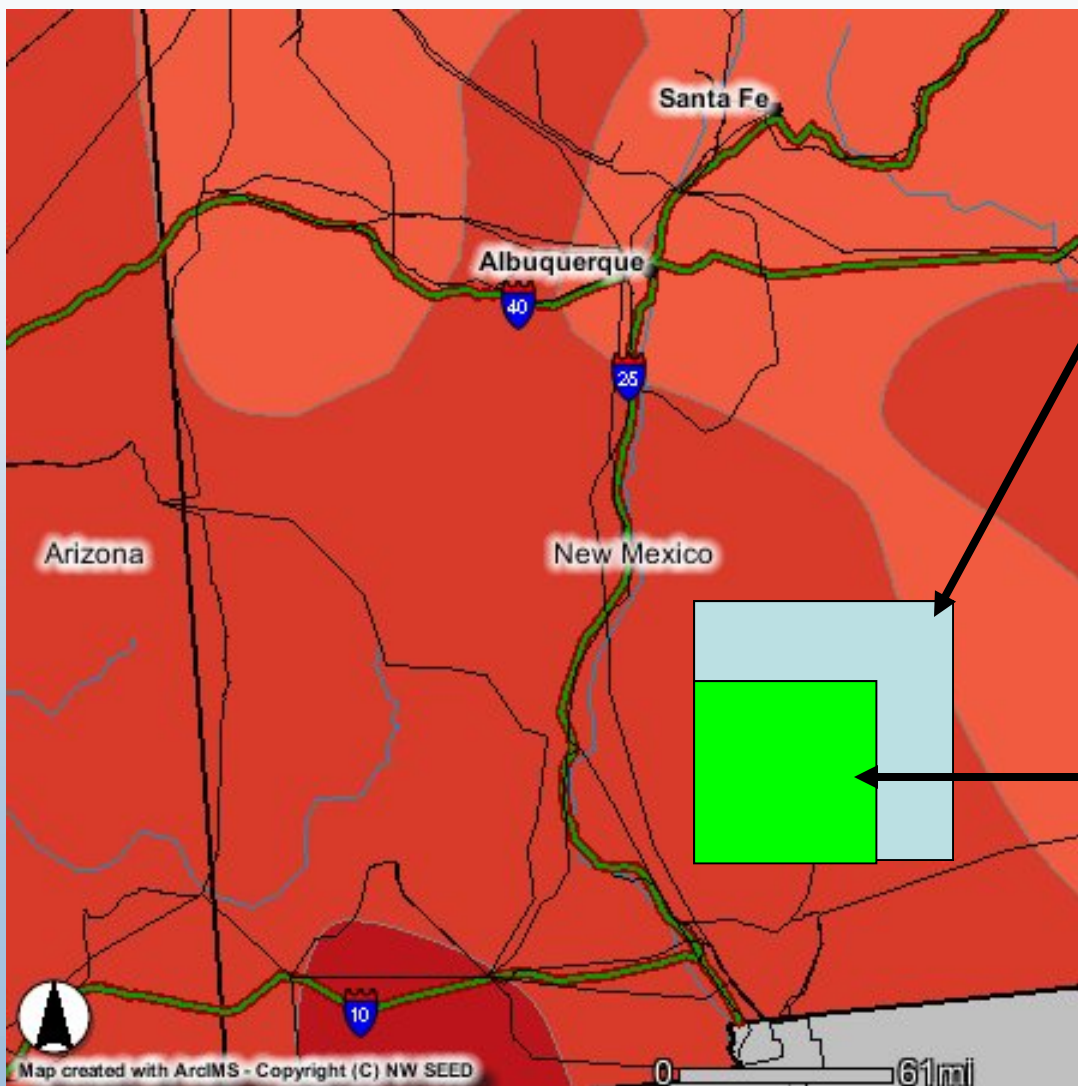
Higher Efficiency from PEC Devices (as Compared to PV/Electrolysis) Stems from the Lower Operational Current Density when using Direct Solar Light



O. Khaselev, A. Bansal, and J. A. Turner, *International Journal of Hydrogen Energy*, 26, p 127-132 (2001)

Hydrogen from Solar Energy and Water

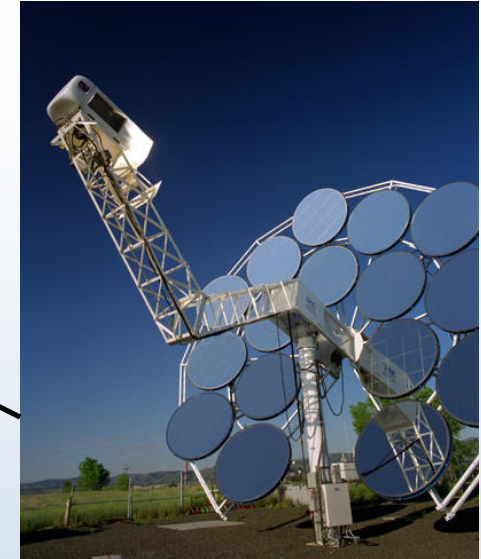
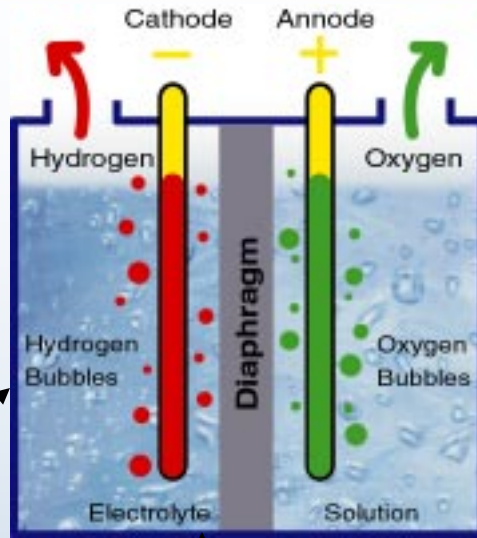
PV/Electrolysis vs. PEC Direct Conversion



PV panel area to produce hydrogen for current U.S. fleet (10% system, 70% electrolysis efficiency)

10% efficient PEC direct conversion system for same amount of hydrogen

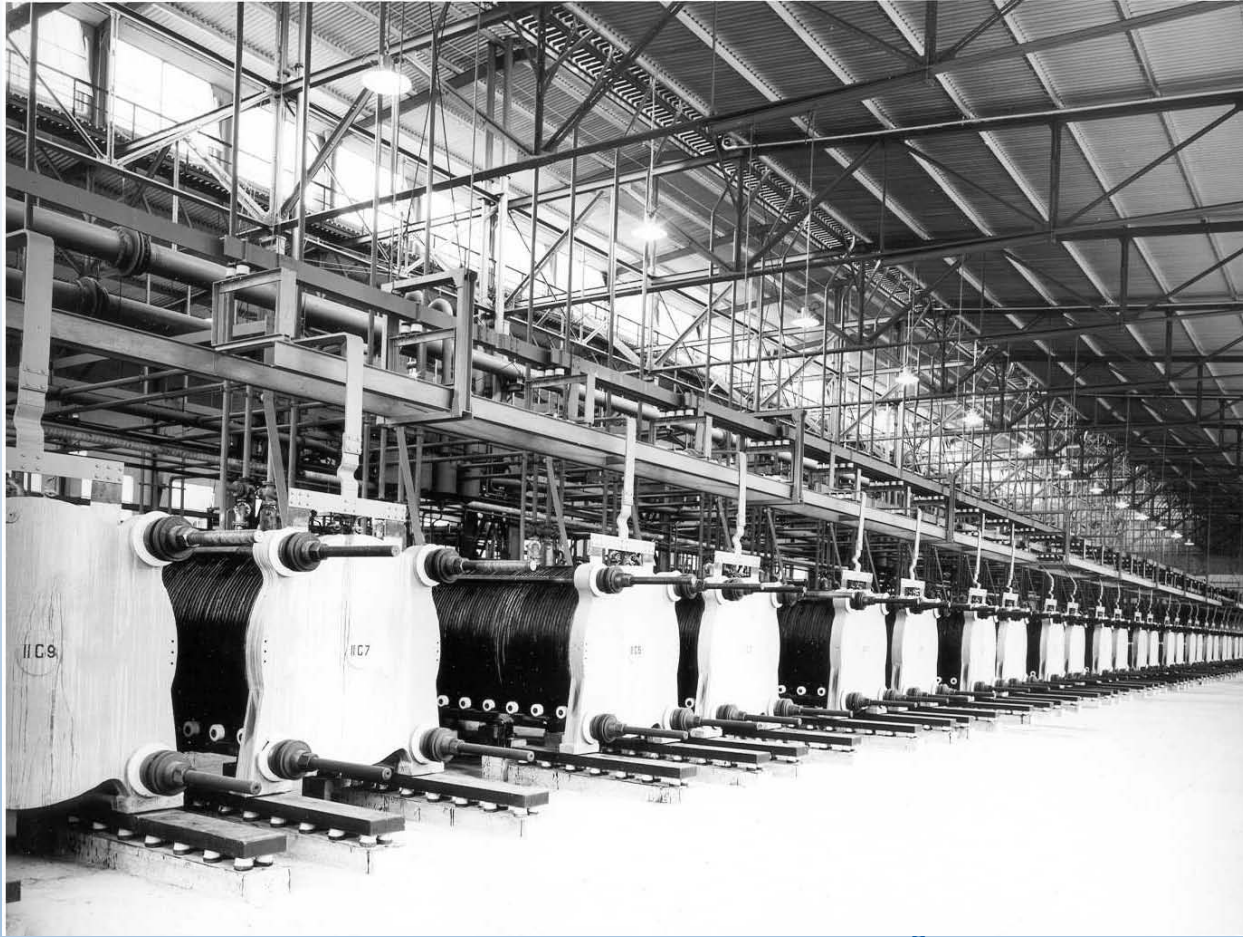
Renewable Hydrogen Production via Electrolysis



An electrolyzer is an energy conversion device, converting electrical energy into chemical energy in the form of chemical bonds.

150 MW: It has been done before!

Norsk Hydro's 30,000 Nm³/h (~150 MW) Electrolyzer Plant (1948 - 90)

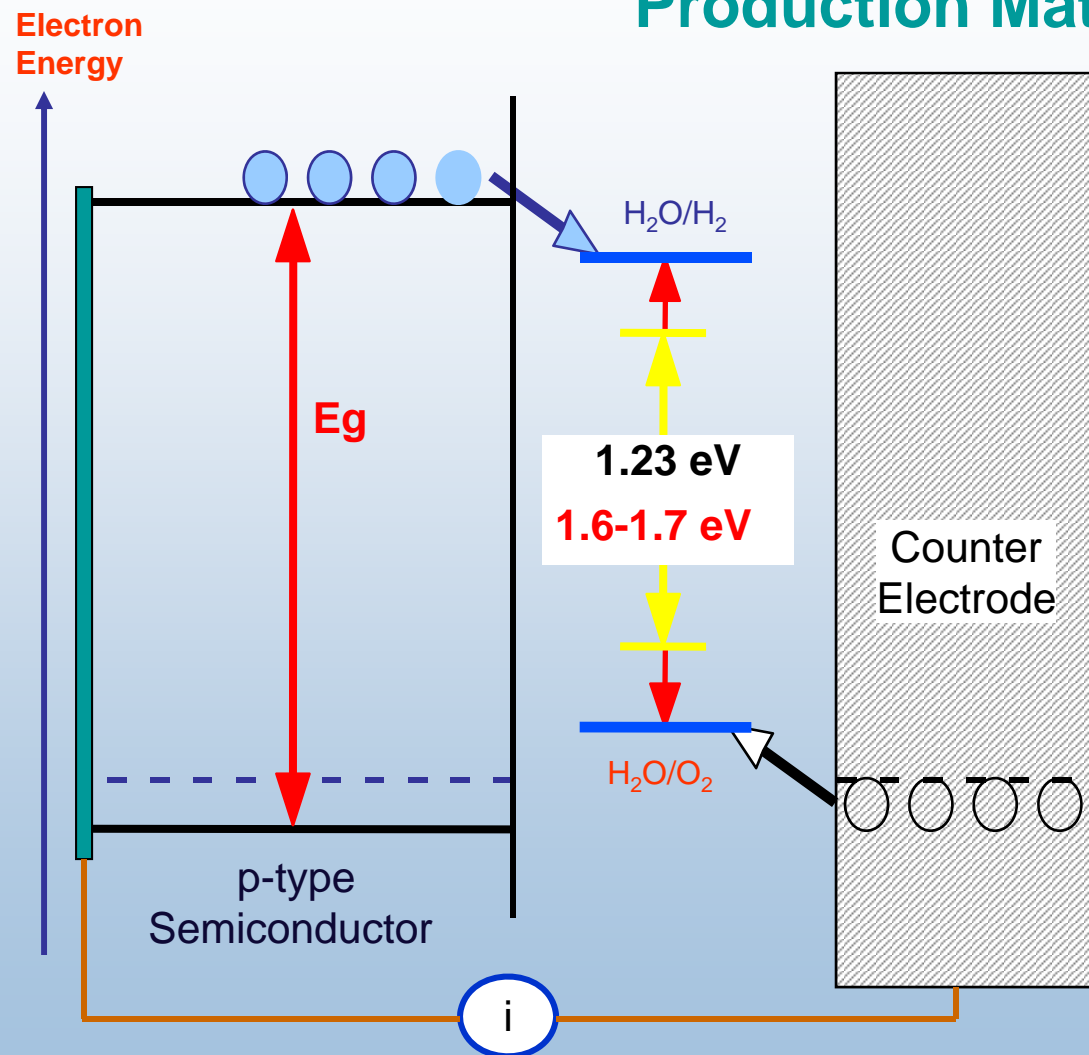


Connected to a hydroelectric plant, generating about 70,000 kg/day, enough for 7,500,000 km/day for FCVs. (100km/kg)

Knut Harg, Hydro Oil & Energy, Hydrogen Technologies
NAS – Hydrogen Resource Committee, April 19, 2007

Material Challenges (*the big three*)

Characteristics for Ideal Photoelectrochemical Hydrogen Production Material



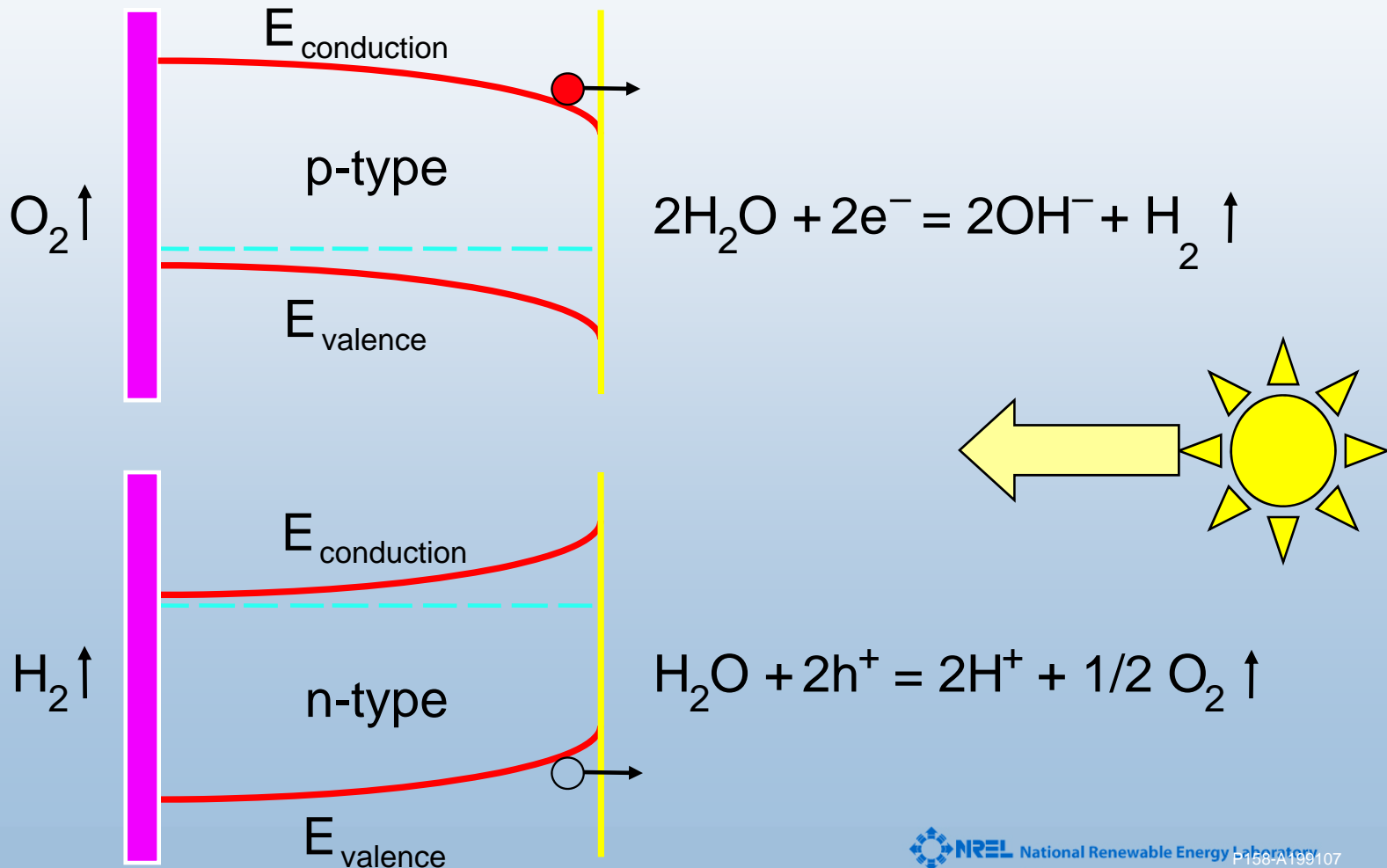
➤ **Efficiency** – the band gap (E_g) must be at least 1.6-1.7 eV, but not over 2.2 eV; must have high photon to electron conversion efficiency (**Grand Challenge**)

➤ **Material Durability** – semiconductor must be stable in aqueous solution

➤ **Energetics** – the band edges must straddle H_2O redox potentials

All must be satisfied simultaneously

Band Edges of p- and n-Type Semiconductors Immersed in Aqueous Electrolytes to Form Liquid Junctions



Efficiency Considerations

Any viable PEC device must have the same external quantum efficiency as commercial PV devices

- Solar Energy conversion efficiency for photoelectrolysis =

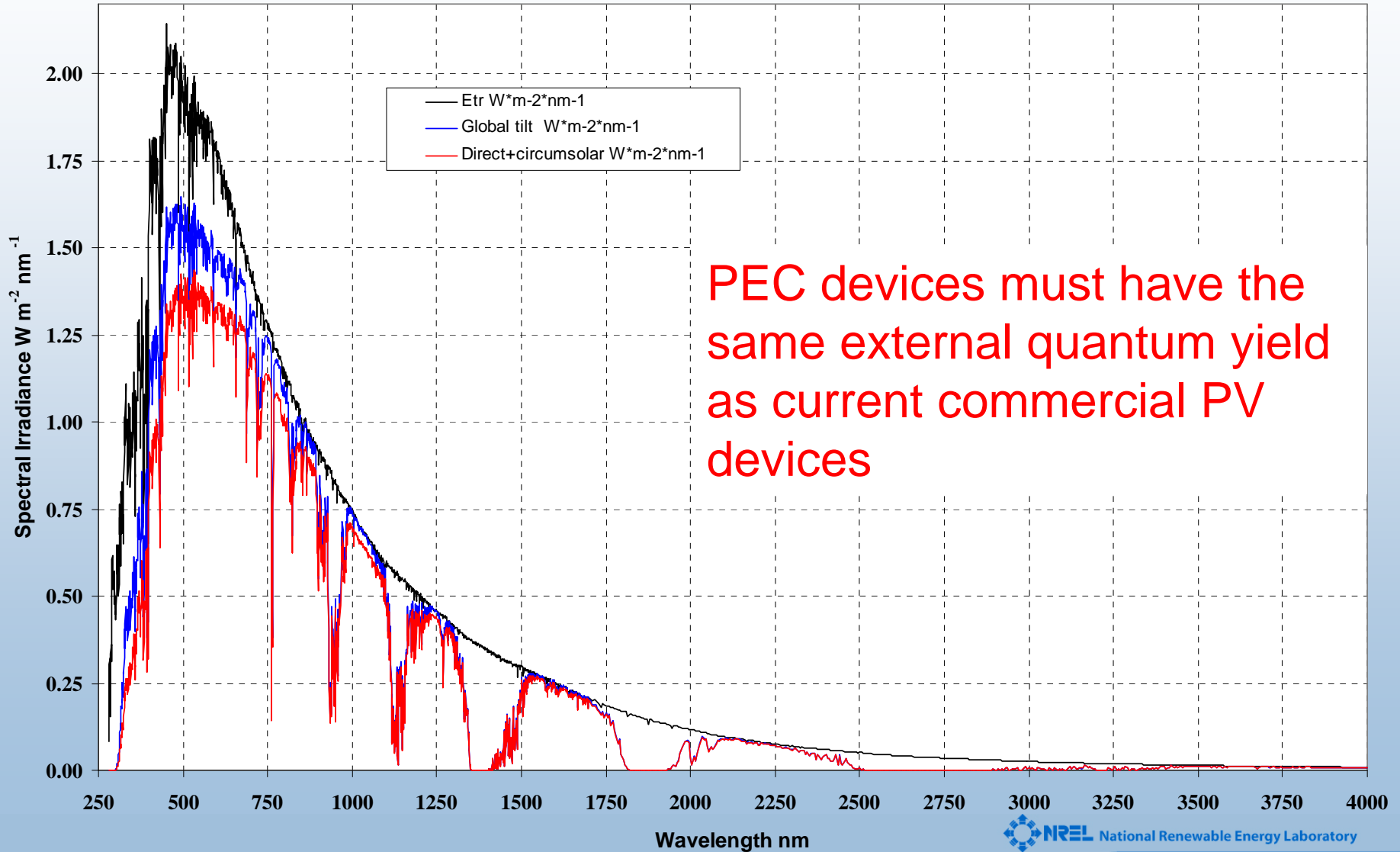
$$\frac{(\text{Chemical potential}) * (\text{rate})}{\text{Light intensity}} = \frac{1.23\text{V} * \text{current}(\text{mA}/\text{cm}^2)}{100\text{mW}/\text{cm}^2}$$

- Unlike solar cells, for PEC hydrogen, the potential is fixed. The only variable in the efficiency is the rate of the production of hydrogen – the current.



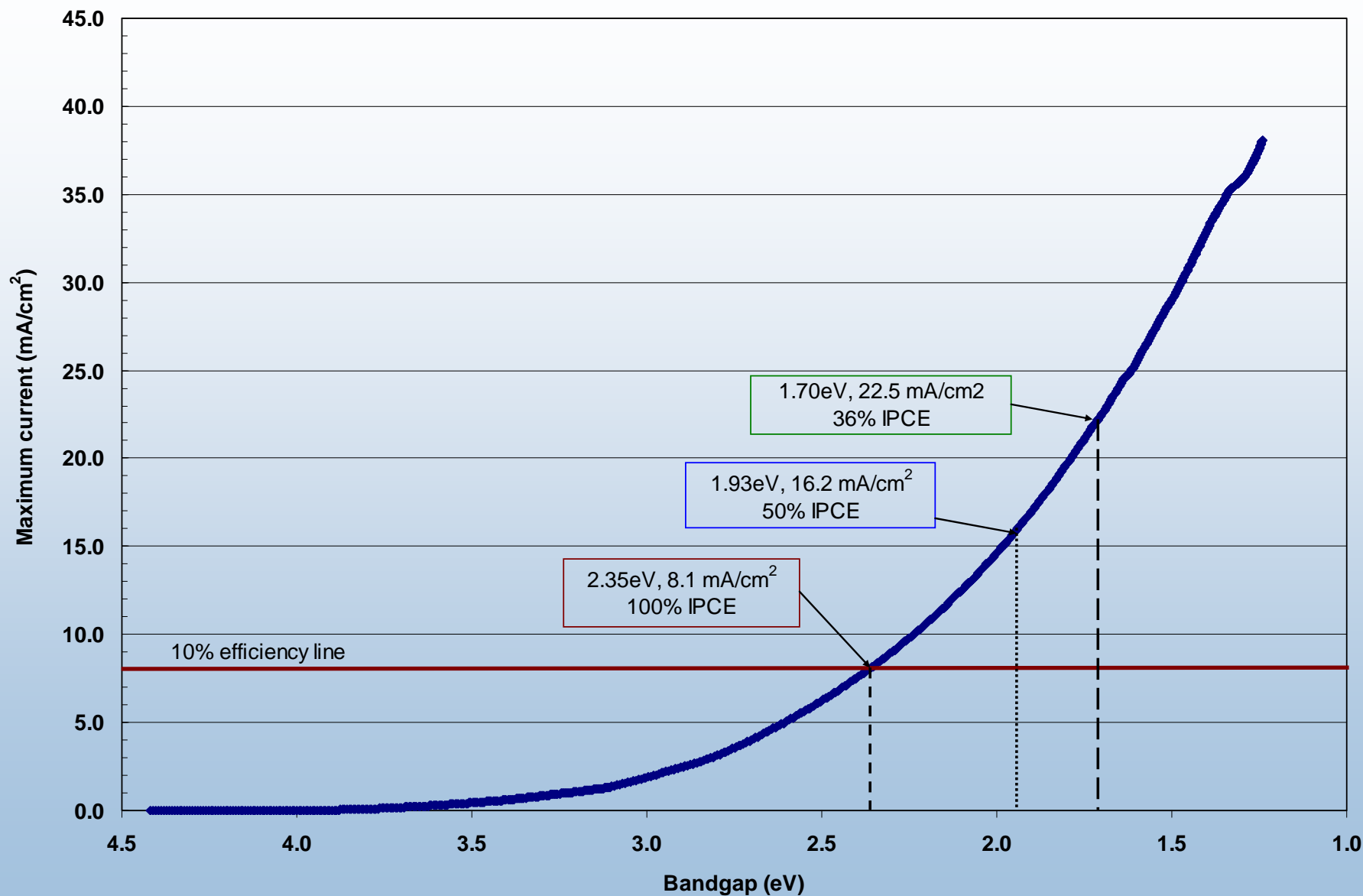
Solar Spectra

ASTM G173-03 Reference Spectra



PEC devices must have the same external quantum yield as current commercial PV devices

Maximum Current vs. Bandgap for AM 1.5



Materials

Break down the very large set of possible materials into two general categories

Non-Oxides

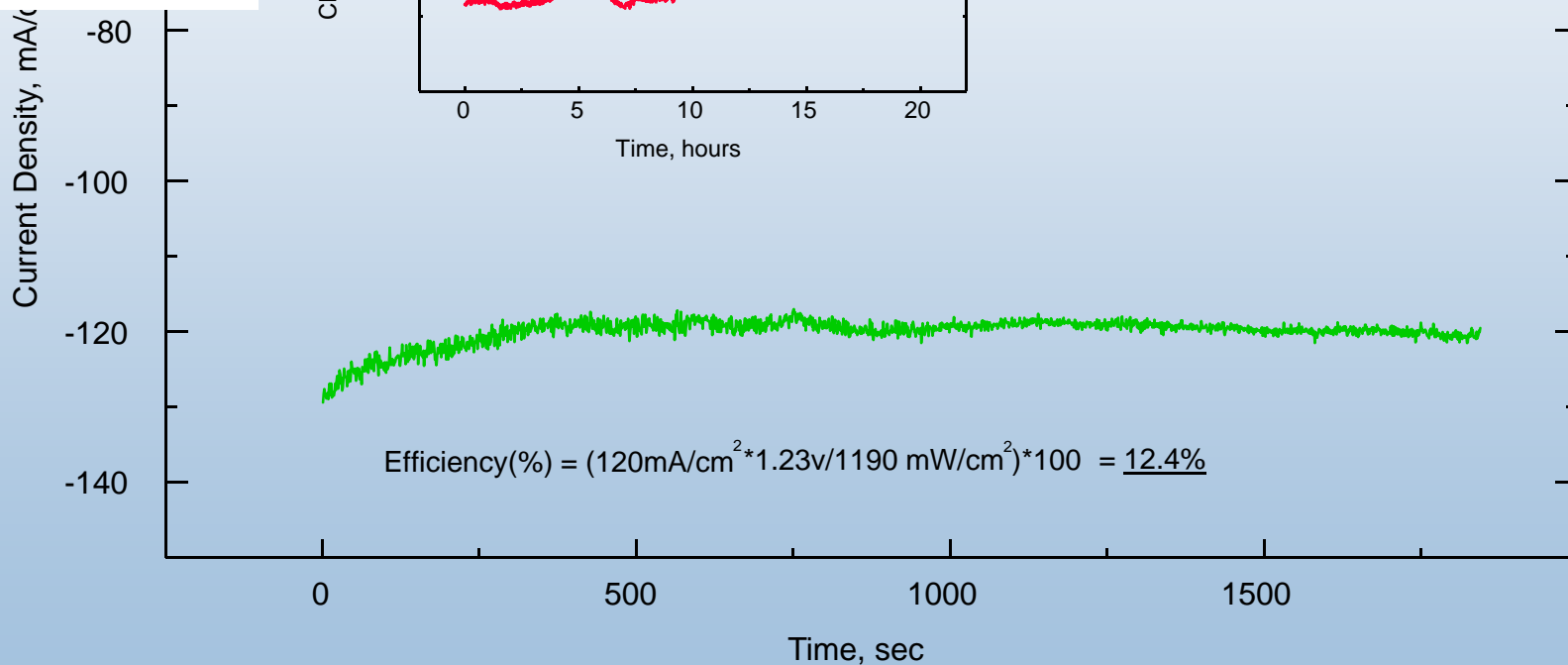
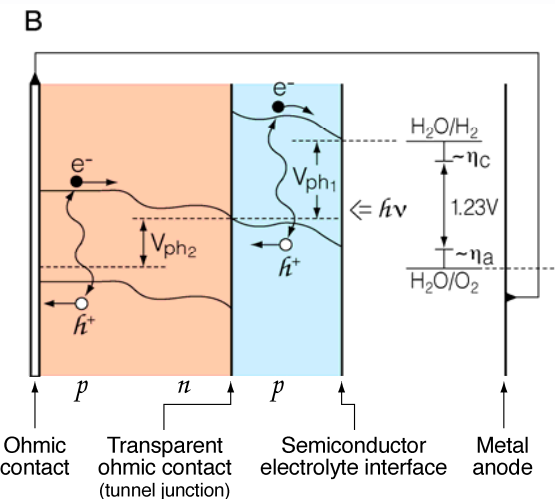
- **III-V materials have the highest solar conversion efficiency of any semiconductor material**
 - Large range of available band gaps (0.7eV – 3.4 eV)
 - Stability an issue – nitrides show promise for increased lifetime
 - Band-edge mismatch with known materials – tandems an answer
 - I-III-VI materials offer high photon conversion efficiency and possible low-cost manufacturing
 - Synthesis procedures for desired band gap unknown
 - Other thin-film materials with good characteristics
 - SiC: low-cost synthesis, stability
 - SiN: emerging material



• Mixed Metal Oxides

- Theory-DFT calculations to identify promising candidates
- Synthesis and characterization
- Cu, Bi, Sb based ternary or multinary oxides

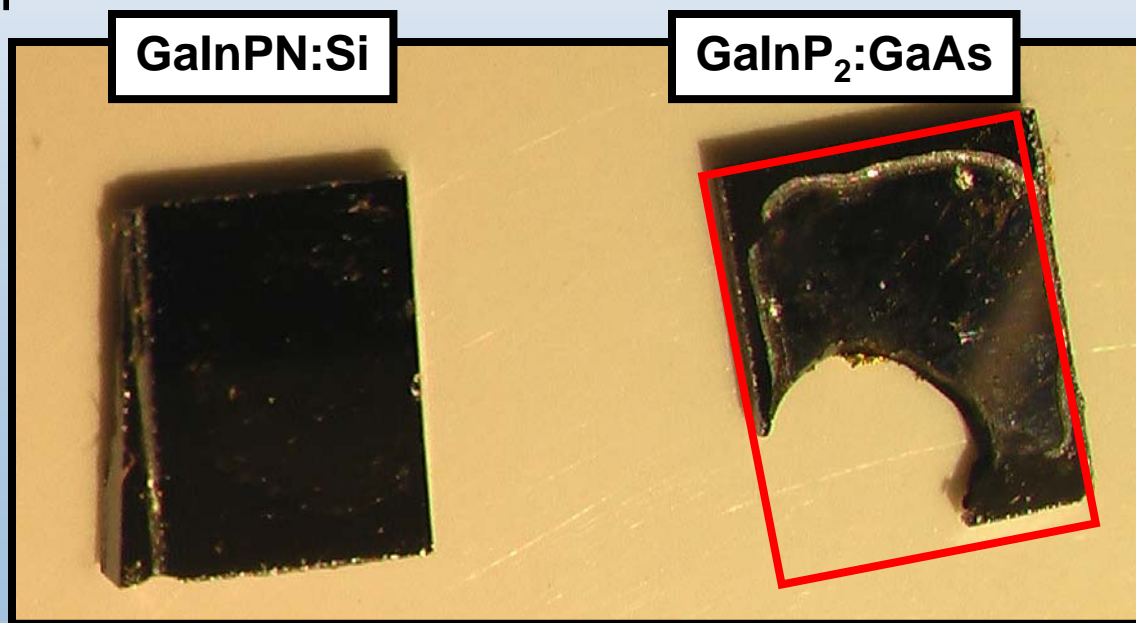
Photocurrent time profile for PEC/PV Water-Splitting device GaAs/GaInP₂



Need materials with the same efficiency, but inherently greater stability.

Small Nitrogen Addition Shows Improved Corrosion Resistance

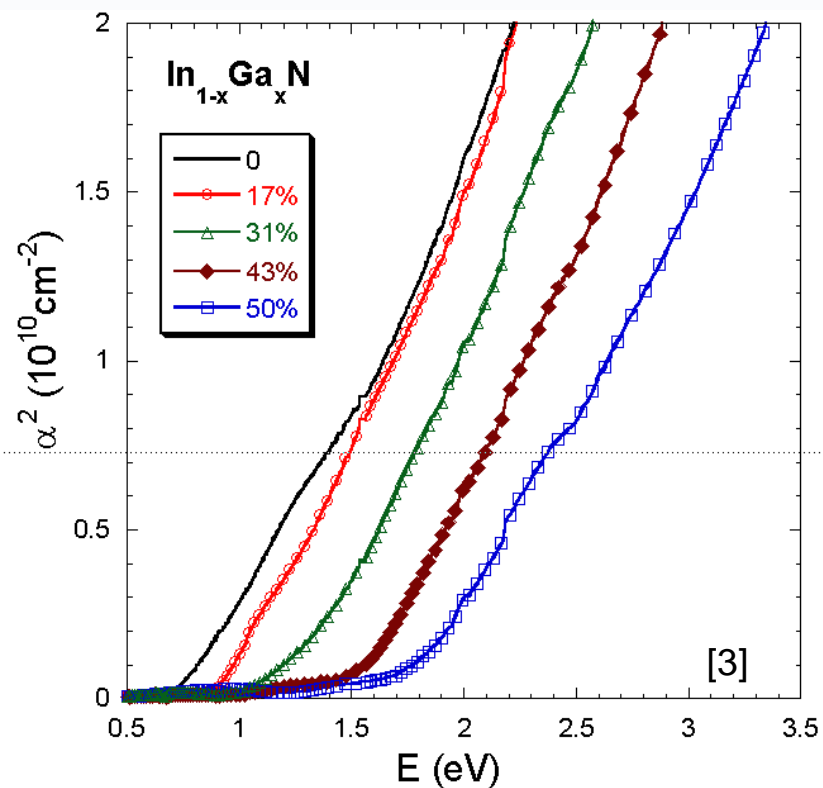
- $\text{Ga}_{.95}\text{In}_{.05}\text{N}_{.025}\text{P}_{.975}$ lattice matched to silicon
- 24-hour corrosion test
 - Constant 5 mA/cm² applied current
 - Sample illuminated at 1 sun
- Profilometry etch depth
 - 0.1 μm average



Alloy GaN with InN

Band gap for GaN: 3.44 eV
Band gap for InN: 0.7 eV¹

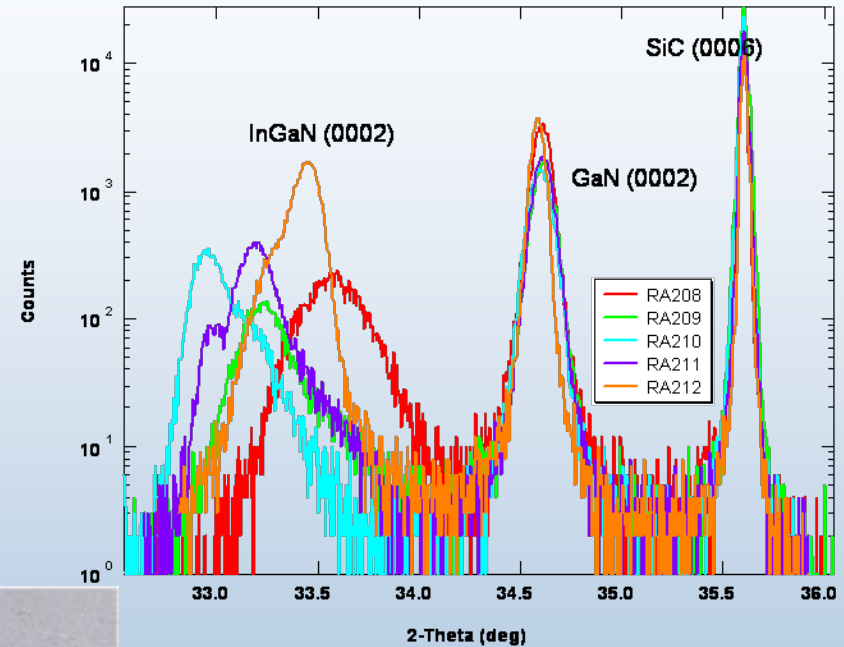
An alloy from this two
would give large
freedom to tune the band
gaps.



- (1) Inushima, T.; Vecksin, V. V.; Ivanov, S. V.; Davydov, V. Y.; Sakon, T.; Motokawa, M. *J. Cryst. Growth* **2001**, *481* (1), 227–228.
- (2) Bhuiyan, A. G.; Hashimoto, A.; Yamamoto, A. *Appl. Phys. Rev.* **2003**, *94* (5), 2779–2807.
- (3) J. Wu, W. Walukiewicz, K.M. Yu, J.W. Ager III, E.E. Haller, Hai Lu, and William J. Schaff, *APL*, 80, p4741 **2002** (<http://www.osti.gov/energycitations/purl.cover.jsp?purl=/799591-nLuLXr/>)

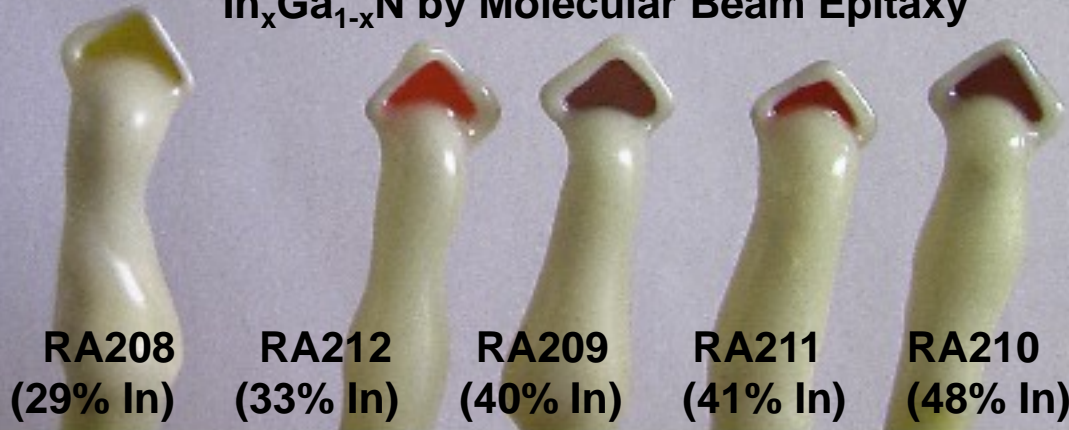
A Possible PEC Material Set

- $\text{In}_x\text{Ga}_{1-x}\text{N}$ Materials by Molecular Beam Epitaxy (MBE)
 - Higher purity (no trapped impurities)
 - Improved efficiency
 - Improved stability
 - Pure nitride (not mixed group V)
 - Improved transport properties (GaN)
 - Tunable (direct) band gap
 - Adding indium lowers E_g



XRD

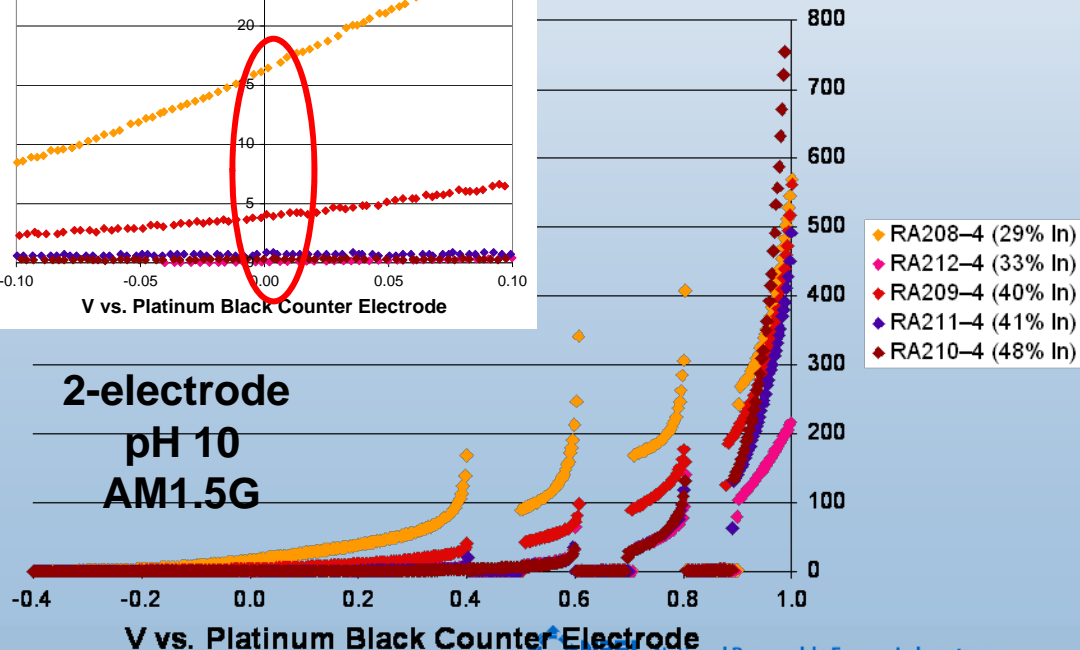
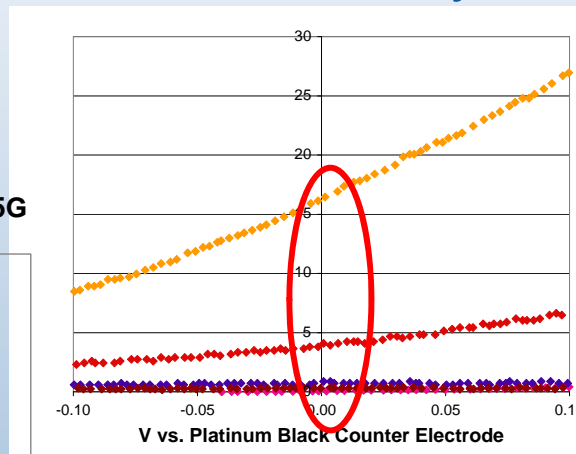
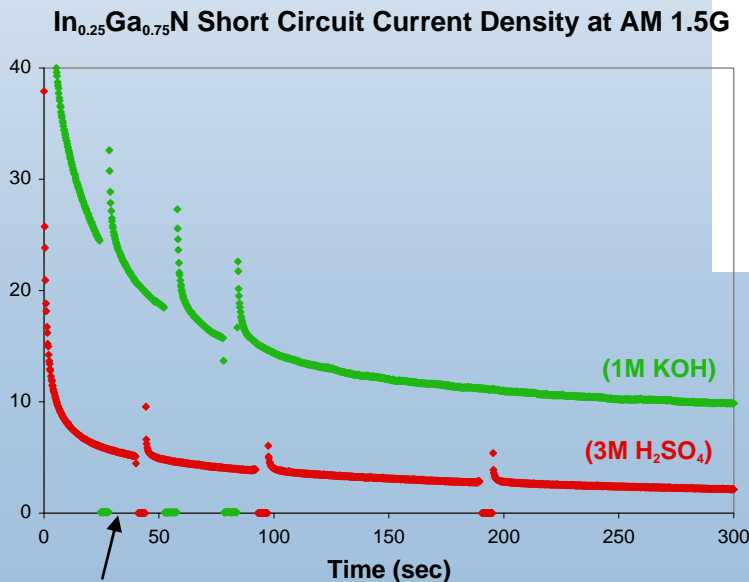
$\text{In}_x\text{Ga}_{1-x}\text{N}$ by Molecular Beam Epitaxy



Material Search: InGaN Alloys by MBE

- Tunable band gap in visible region
- Band edge alignment
 - M-S: aligned
 - OCP, PC onset: Not aligned

- Unbiased water splitting
 - Photocurrent at zero bias
 - Very low efficiency
 - Catalyzed by Pt
- Durability not yet assessed



Note: current density falls to zero when light blocked

Metal Oxides – A materials assessment

PEC devices must have the same external photon-to-electron conversion efficiency as PV devices.

- Transitions which impart color to the oxides typically involve d and f levels and are generally forbidden transitions = low absorption coefficients.
 - The low absorption coefficients result in the incident light penetrating deep into the material.
 - 100's um of material are necessary for complete adsorption.
- Carrier mobilities in oxides are very low so recombination of photogenerated carriers occurs before they can reach the semiconductor/electrolyte interface.
- Even good single crystals of metal oxides have very low energy conversion efficiencies due to inherently short diffusion lengths.

Woodhouse, Herman & Parkinson, *Chem. Mater.* 17, p4318 (2005)

However a success in this area, e.g. an oxide with good to excellent conversion properties, could revolutionize the PV industry as well as make PEC near-term.

The Status of Current Oxides

~200 oxides tested

Chem. Mater, 20, 35 (2008)

No metal oxide is even close to meeting the criteria

10's of millions of possibilities

High T_c oxides are multicomponent - ($\text{HgBa}_2\text{CaCu}_2\text{O}_6$)
Therefore many elements may be necessary to meet the required properties.

Discovering new oxide semiconductors

Combinatorial is like saying "I'm clueless", but where do you start and where to you go?

A collaboration of theory, synthesis, and characterization groups is necessary to achieve fundamental PEC goals.

Band structure calculations using Density Functional Theory can give you spectra, nature of the transition (direct, indirect) and band gap energy trends.

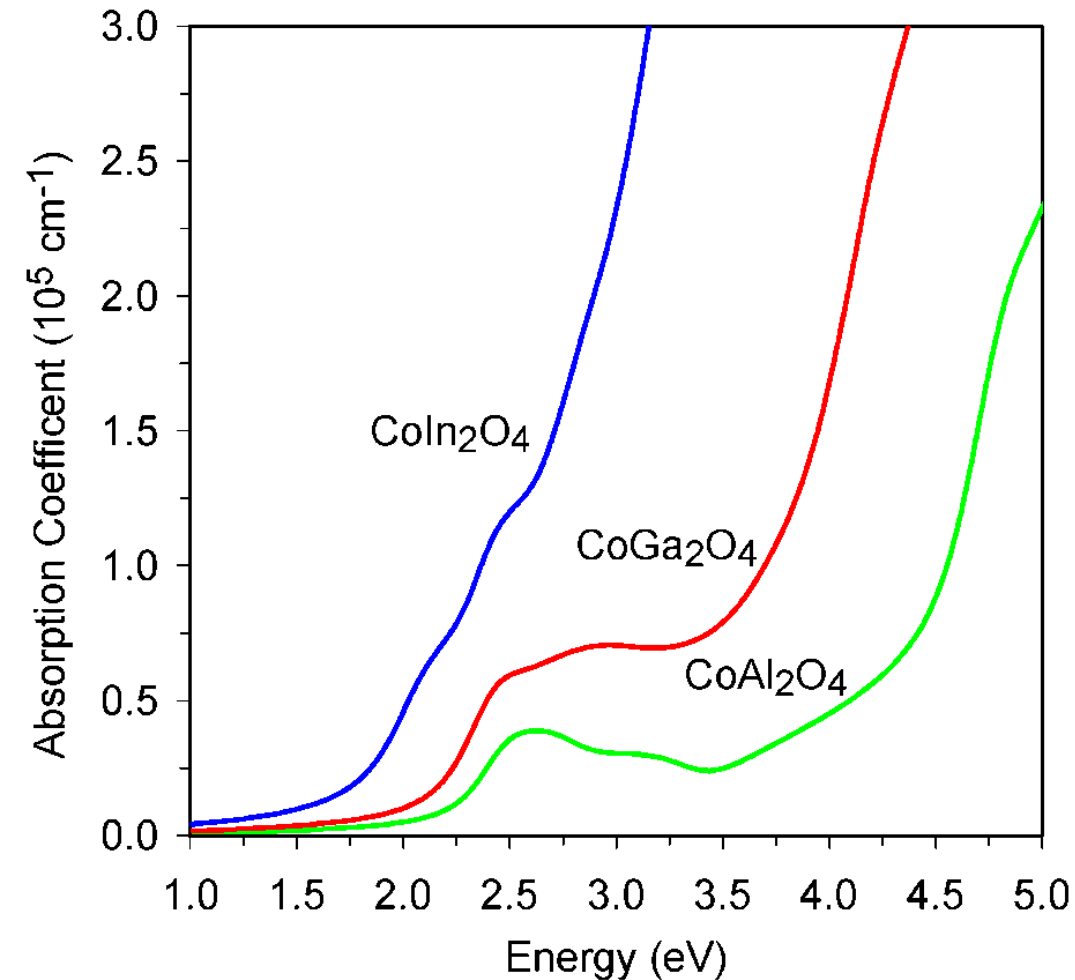
The actual band structure depends on

**Symmetry, composition, bond length
and requires**

Sophisticated DFT calculations

The key will be the predictive capability of the theory groups coupled with the synthesis capability of the growth groups.

Prediction from DFT

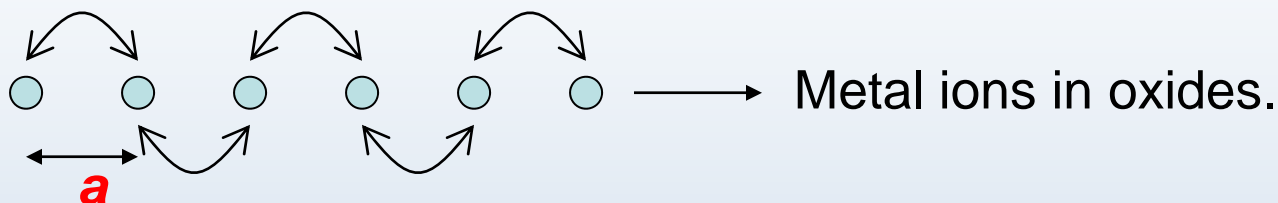


CoAl₂O₄ has poor absorption characteristics, but should improve with Ga and In.

The bandgap trend was correct, but the performance was abysmal.

Why is conduction poor in some oxides?

Electron hopping



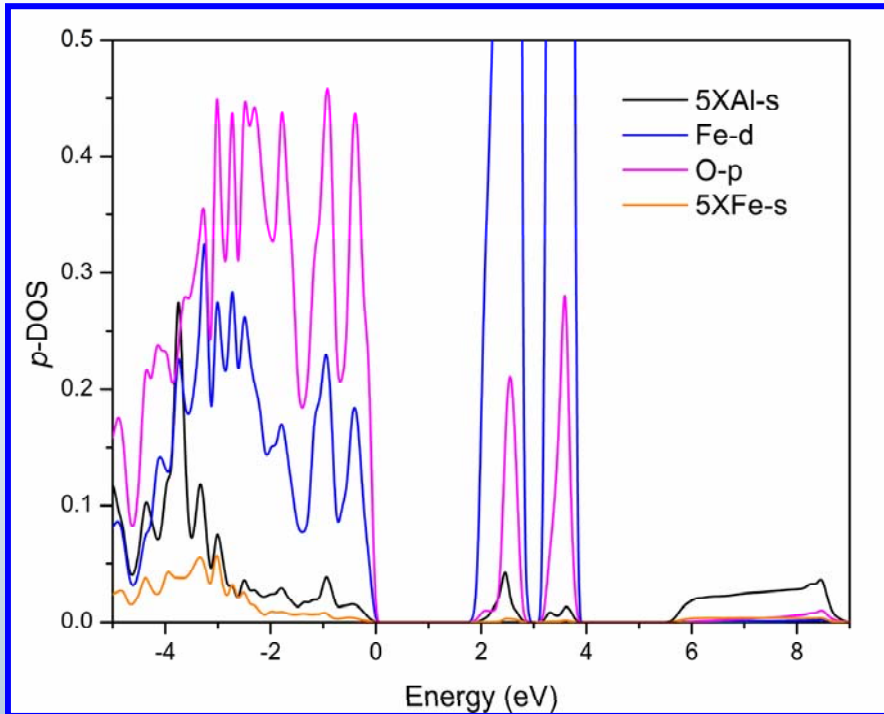
For example: $\text{Co}^{+2} \longrightarrow \text{Co}^{+3}$ in spinel structure.

And $\text{Fe}^{+2} \longrightarrow \text{Fe}^{+3}$ in Fe_2O_3

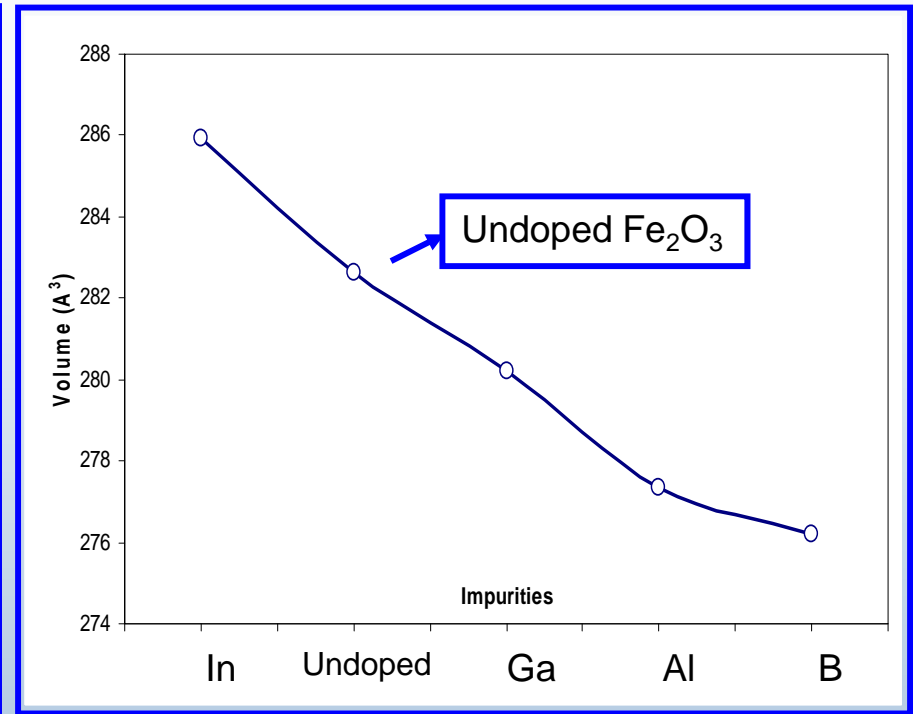
- If a increases, the charge hopping probability decreases.
- At large a the electrons are tightly bounded to the atoms.
- In general, doping will not improve the situation.

Improving current oxides

Reducing the volume increases "hopping" probability



$\text{Fe}_2\text{O}_3:\text{Al}$

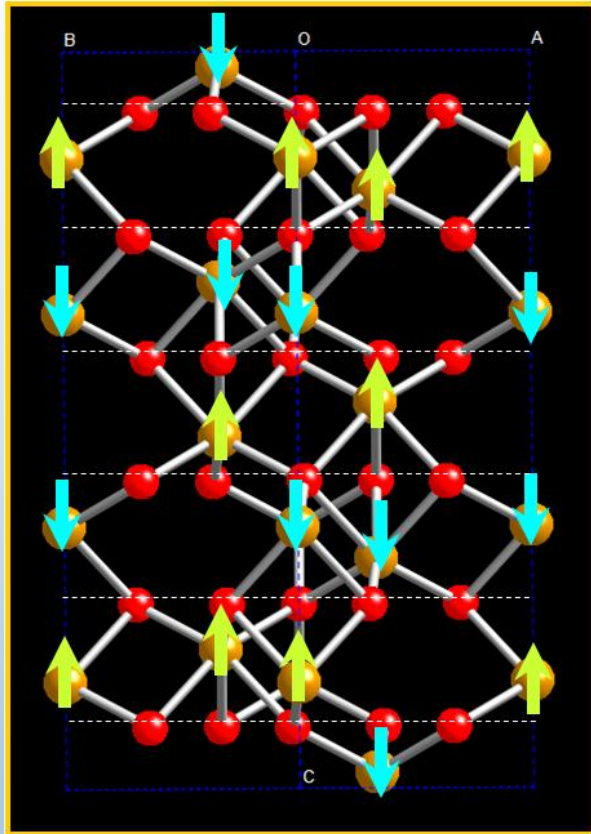


$\text{Fe}_2\text{O}_3:\text{M}^{\text{III}}$

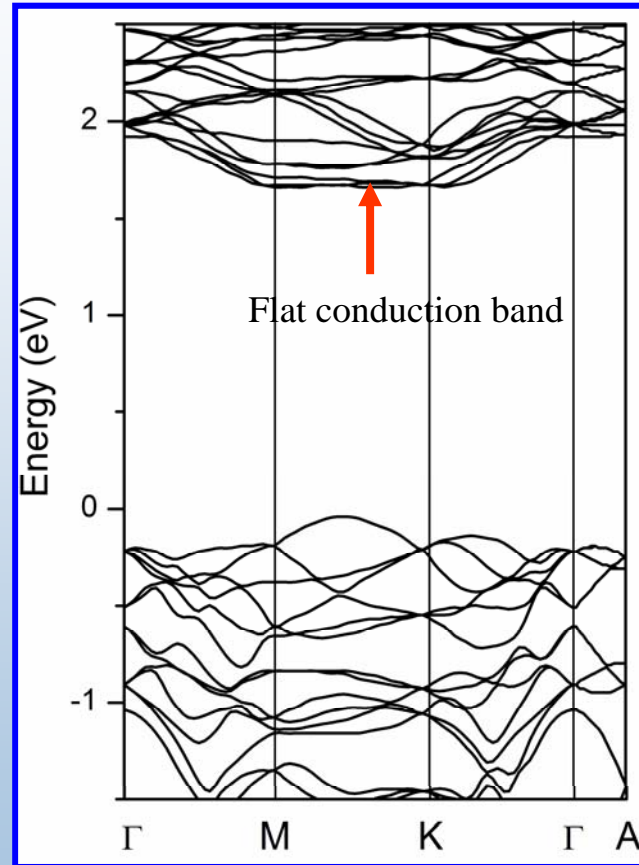
A volume compression with 50 GPa pressure is needed to break the Mott-Hubbard state for Fe_2O_3 (M.P. Pasternak, G.K. Rozenberg, G.Y. Machavariani, O. Naaman, R.D. Taylor, R. Jeanloz, Phys. Rev. Lett. 82, 4663 (1999).)

Theoretical Considerations – Localized Bands

Identifying problems for $\alpha\text{-Fe}_2\text{O}_3$ (Hematite)



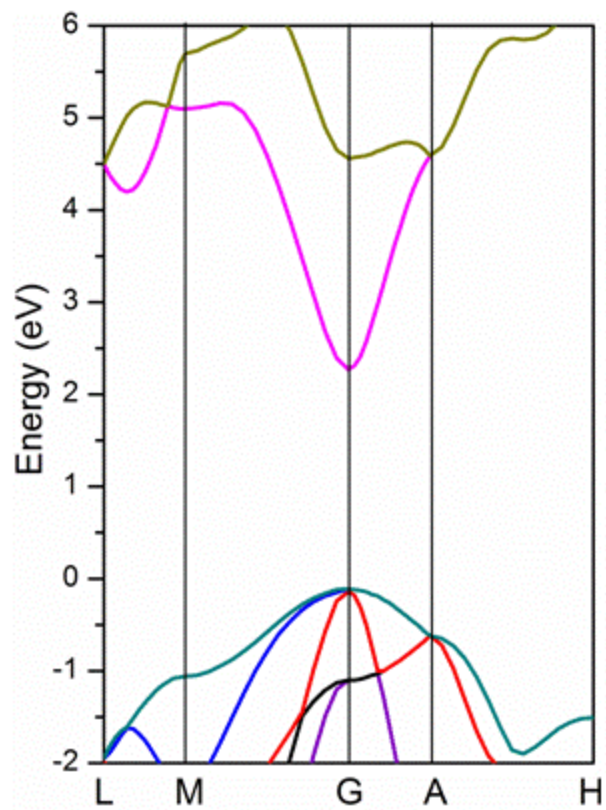
Atomic structure



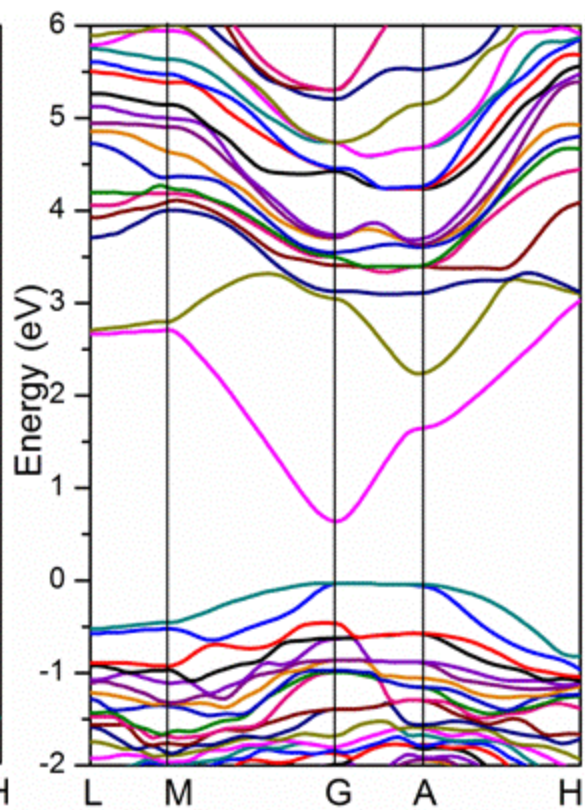
Calculated band structure

Problem: Huge electron effective mass – short carrier life time

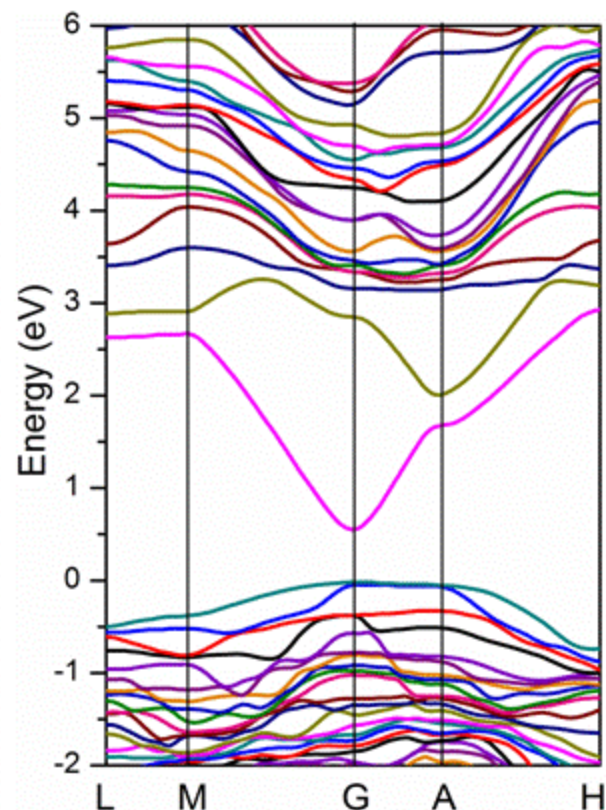
Band structure



Pure-GaN



In6-subst

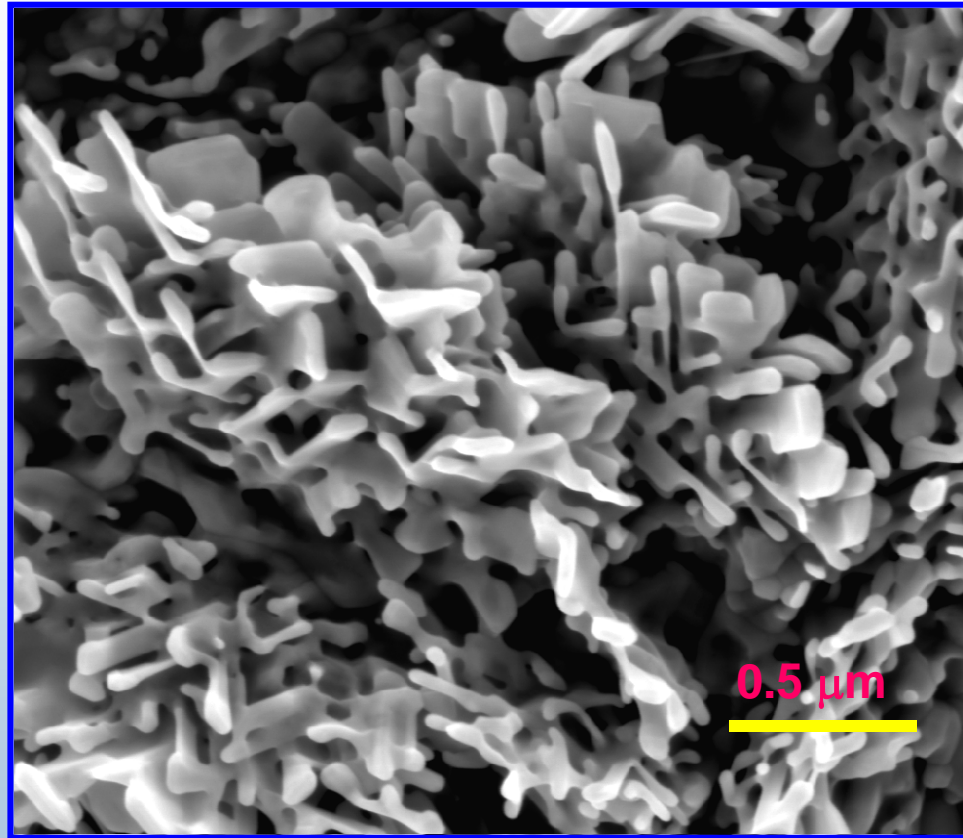


In7-subst

Nanostructure

PEC cells: Conformal S/L interface

Reduce thickness (electrode)



However, if nanostructure does not address the fundamental limitations of the electronic structure, then it is of little value.

Discovering new semiconductors

Trend of atomic orbitals – the intrinsic property

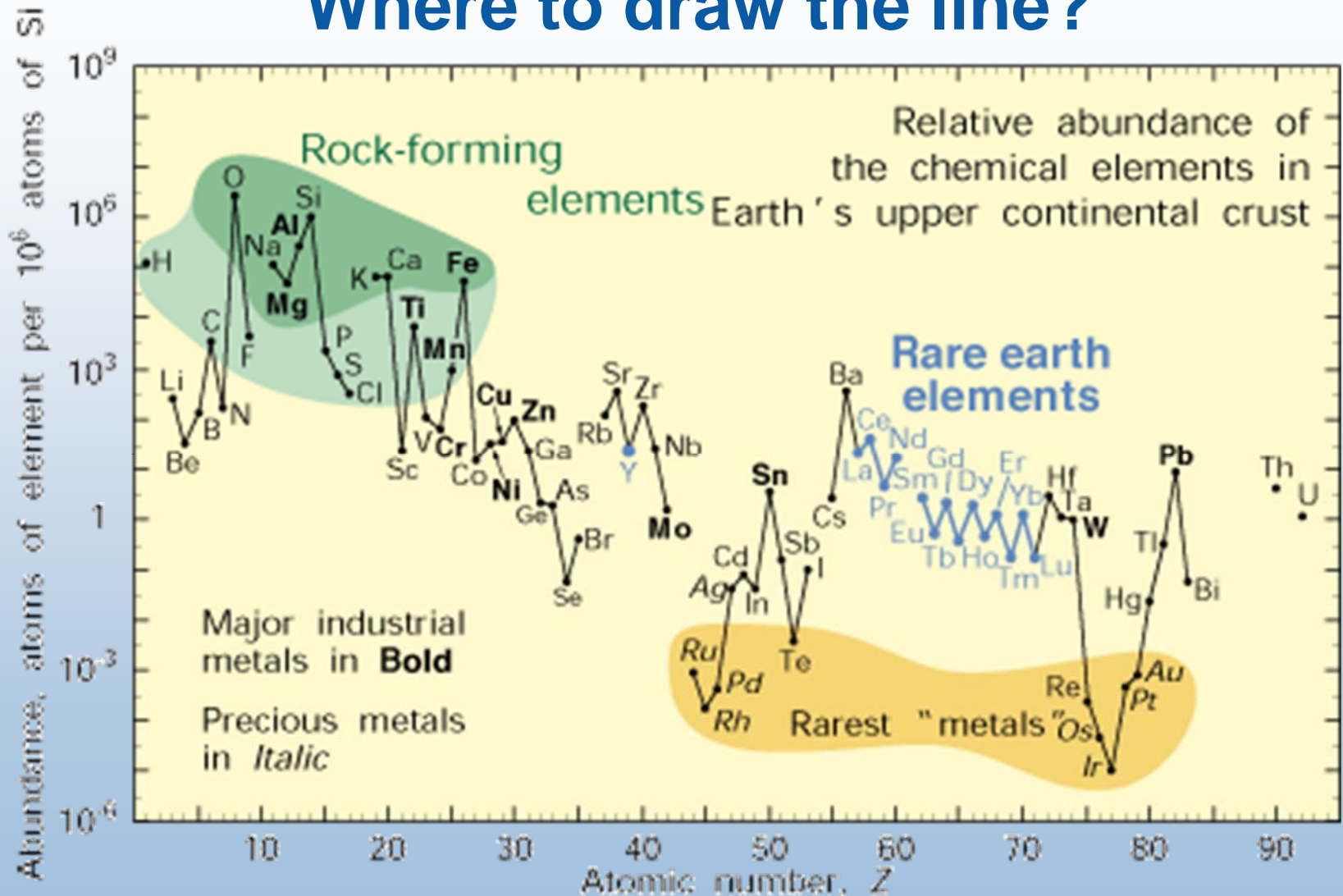
Periodic Table of the Elements

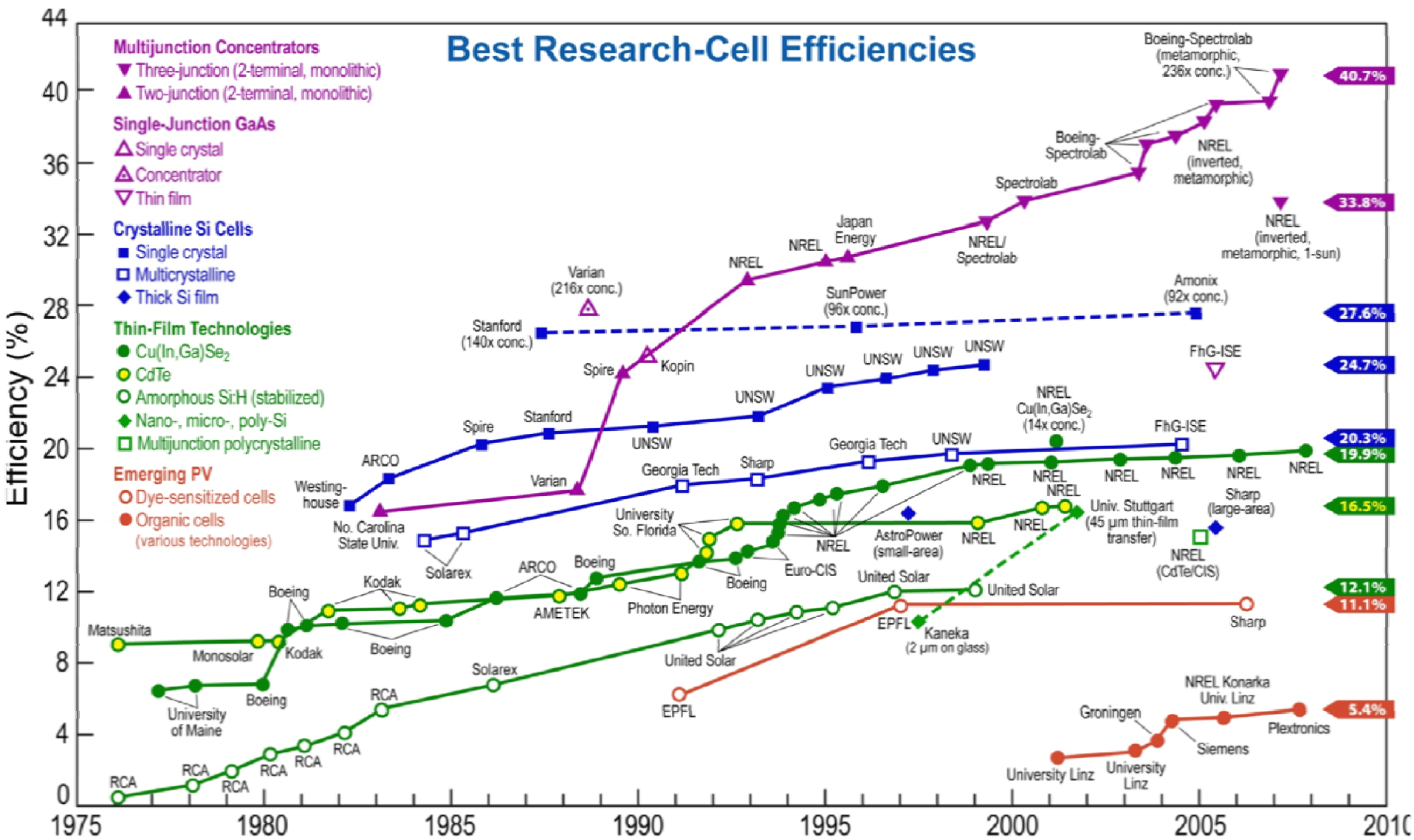
1 H																	2 He														
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne														
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar														
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr														
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe														
55 Cs	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn														
87 Fr	88 Ra	89 Ac	104 Unq	105 Unp	106 Unh	107 Uns	108 Uno	109 Une	110 Unn																						
																		58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
																		90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

- hydrogen
- alkali metals
- alkali earth metals
- transition metals
- poor metals
- nonmetals
- noble gases
- rare earth metals

Abundance

Where to draw the line?





Doc. 01.15.01

If PV is to meet its potential, it must be able to sustain a high growth rate. What technologies can do that? We need new PV materials



Combinatorial design of semiconductor chemistry for bandgap engineering: “virtual” combinatorial experimentation

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Abstract

The objective of this paper is to show how one may design combinatorial libraries a priori by integrating data mining techniques with physically robust multivariate data. It is shown that large datasets can be developed from relatively small amounts of experimental and theoretically based information. This involves a process of strategically selecting appropriate physical based parameters that can be analyzed in a multivariate manner. In this paper we identify for the first time the bandgap and lattice parameters of nearly 200 stoichiometries of new and yet to be synthesized compound chalcopyrite semiconductors. The robustness of this “virtual” combinatorial experimentation approach is demonstrated by comparison to band gap predictions from theoretical studies on a range of compositions for a selected quaternary compound semiconductor.

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JEL classification: 71.55.Cn; 71.55.Eq; 71.55.Gs

Keywords: Semiconductor compounds; Crystallographic databases; Crystal stoichiometry

1. Introduction

The field of “bandgap engineering” is in fact one of the earliest examples of combinatorial design of materials. The recognition that by matching lattice parameters of different covalently bonded semiconductors, one can engineer the bandgap of epitaxial heterostructures has been one of the success stories in integrating fundamental physics into device engineering. However, the strategy of what materials one may work with is limited to relatively few and the “discovery” of new materials with more complex chemistries is still a slow

process. Clearly high throughput experimentation techniques offer some exciting possibilities for developing such new materials. In this paper we wish to outline the use of a statistically based strategy combined with the appropriate understanding of key physical parameters to show how we can develop a computational screening tool prior to conducting combinatorial experiments. We propose the idea of “virtual” combinatorial libraries, which lay a map of suggested chemical combinations, likely to give the desired properties one is seeking. Using chalcopyrite semiconductors as a testbed, we show how such a library can be built. The formalisms of the mathematical foundations are described in Appendix A but suffice it to say that a judicious use of multivariate statistics tools serves as the means to manipulate and process the incoming data.

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URL: <http://www.rpi.edu/~rajank/materialsdiscovery>.

Table 4 (Continued)

Compound	Predicted band gap energy (eV) by PLS	Theoretical band gap energy (eV)	Nature of band gap ^a	Predicted lattice constant by PLS	Lattice constant (Å)	c/a ratio	Reference
Zn _{0.5} Si _{0.5} P	2.3591	1.56 (GW)	d	5.3759	5.262		[9]
Zn _{0.5} Si _{0.5} As	1.5299	0.68 (GW)	md	5.571	5.483		[8]
ZnSbSb ₂	-0.055	0.9		5.6125	6.077		[2]
Zn _{0.5} Si _{0.5} Sb	-0.055			5.6123	5.962		[8]
ZnSiBi ₂	-1.6445			5.9063			
ZnGeN ₂	4.9757			5.7709			
Zn _{0.5} Ge _{0.5} P	1.8692	1.15 (GW)	I	5.4837	5.382		[9]
Zn _{0.5} Ge _{0.5} As	1.04	0.23 (GW)	md	5.6789	5.597		[9]
ZnGeSb ₂	-0.5449	0.5		5.7202	6.111		[2]
ZnGeBi ₂	-2.1344			6.0141			
ZnSnN ₂	4.4468			5.8719			
ZnSnP ₂	1.3403			5.5847	5.651	2	[1,2]
Zn _{0.5} Sn _{0.5} P	1.3404	1.70 (GW)	I	5.5847	5.688		[9]
ZnSnAs ₂	0.5112			5.7799	5.851	2	[1,2]
Zn _{0.5} Sn _{0.5} As	0.5112	0.79 (GW)	md	5.7799	5.87		[9]
ZnSnSb ₂	-1.0738			5.8212	6.275	2	[1]
ZnSnBi ₂	-2.6633			6.1151			
ZnPbN ₂	3.7358			6.0915			
ZnPbP ₂	0.6293			5.8043			
ZnPbAs ₂	-0.1998			5.9994			
ZnPtSb ₂	-1.7848			6.0407			
ZnPtBi ₂	-3.3743			6.3347			
CdCN ₂	5.8097			5.9651			
CdCP ₂	2.7032			5.6779			
Cd _{0.5} C _{0.5} P	2.7032			5.6779	4.973		[8]
CdCAS ₂	1.8741			5.8731			
Cd _{0.5} C _{0.5} As	1.8741			5.8731	5.201		[8]
CdCSb ₂	0.2891			5.9143			
Cd _{0.5} C _{0.5} Sb	0.2891			5.9143	5.62		[8]
CdCBi ₂	-1.3004			6.2083			
CdSiN ₂	5.2692			5.9568			
Cd _{0.5} Si _{0.5} P	2.1627	1.22 (GW)		5.6696	5.378		[9]
Cd _{0.5} Si _{0.5} As	1.336			5.8648	5.61		[8]
CdSiSb ₂	-0.2514	0.8		5.9061	6.344		[2]
CdSiBi ₂	-1.18409			6.2			
CdGeN ₂	4.7793			6.0646			
Cd _{0.5} Ge _{0.5} P	1.6729	0.33 (GW)	d	5.7774	5.523		[9]
Cd _{0.5} Ge _{0.5} As	0.8437		Metallic	5.9726	5.755		[8]
CdGeSb ₂	-0.7412	0.2		6.0139	6.383		[2]
CdGeBi ₂	-2.3308			6.3078			
CdSnN ₂	4.2504			6.1657			
Cd _{0.5} Sn _{0.5} P	1.144			5.8785	5.797		[8]
CdSnSb ₂	-1.2701	-0.80 (FLAPW)		6.1149	6.479		[6]
CdSnBi ₂	-2.8596			6.4089			
CdPbN ₂	3.5394			6.3852			
CdPbP ₂	0.433			6.098			
CdPbAs ₂	-0.3962			6.2931			
CdPtSb ₂	-1.9811			6.3344			
CdPtBi ₂	-3.5706			6.6284			
HgCN ₂	4.5586			6.2613			
HgCP ₂	1.4522			5.9741			
HgCAS ₂	0.623			6.1693			

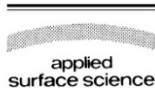
Computational approach for combinatorial design of semiconductor chemistry for bandgap engineering.



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Combinatorial design of semiconductor chemistry for bandgap engineering: “virtual” combinatorial experimentation

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Abstract

The objective of techniques with ph amounts of experit physical based para and lattice paramete The robustness of predictions from th

JEL classification: 7

Keywords: Semicond

ZnSnN₂ ~ 4.4eV

ZnSnP₂ ~ 1.3eV

?Would it be possible to grow a ZnSnPN alloy combination and tune the bandgap for PEC?

1. Introduction

The field of “bandgap engineering” is in fact one of the earliest examples of combinatorial design of materials. The recognition that by matching lattice parameters of different covalently bonded semiconductors, one can engineer the bandgap of epitaxial heterostructures has been one of the success stories in integrating fundamental physics into device engineering. However, the strategy of what materials one may work with is limited to relatively few and the “discovery” of new materials with more complex chemistries is still a slow

process. Clearly high throughput experimentation techniques offer some exciting possibilities for developing such new materials. In this paper we wish to outline the use of a statistically based strategy combined with the appropriate understanding of key physical parameters to show how we can develop a computational screening tool prior to conducting combinatorial experiments. We propose the idea of “virtual” combinatorial libraries, which lay a map of suggested chemical combinations, likely to give the desired properties one is seeking. Using chalcopyrite semiconductors as a testbed, we show how such a library can be built. The formalisms of the mathematical foundations are described in Appendix A but suffice it to say that a judicious use of multivariate statistics tools serves as the means to manipulate and process the incoming data.

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Table 4 (Continued)

Compound	Predicted band gap energy (eV) by PLS	Theoretical band gap energy (eV)	Nature of band gap ^a	Predicted lattice constant by PLS	Lattice constant (Å)	c/a ratio	Reference
Zn _{0.5} Si _{0.5} P	2.3591	1.56 (GW)	d	5.3759	5.262		[9]
Zn _{0.5} Si _{0.5} As	1.5299	0.68 (GW)	md	5.571	5.483		[8]
ZnSnSb ₂	-0.055	0.9		5.6125	6.077		[2]
Zn _{0.5} Si _{0.5} Sb	-0.055			5.6123	5.962		[8]
ZnSiBi ₂	-1.6445			5.9063			
ZnGeN ₂	4.9757			5.7709			
Zn _{0.5} Ge _{0.5} P	1.8692	1.15 (GW)	I	5.4837	5.382		[9]
Zn _{0.5} Ge _{0.5} As	1.04	0.23 (GW)	md	5.6789	5.597		[9]
ZnGeSb ₂	-0.5449	0.5		5.7202	6.111		[2]
ZnGeP ₂	2.1344			6.0141			
ZnSnN ₂	4.4468			5.8719			
ZnSnP ₂	1.3403			5.5847	5.651	2	[1,2]
Zn _{0.5} Sn _{0.5} As	1.5404	1.70 (GW)	I	5.5847	5.688		[9]
ZnSnAs ₂	0.5112			5.7799	5.851	2	[1,2]
Zn _{0.5} Si _{0.5} As	0.5112	0.79 (GW)	md	5.7799	5.87		[9]
ZnSnSb ₂	-1.0738			5.8212	6.275	2	[1]
ZnSnBi ₂	-2.6633			6.1151			
ZnPtN ₂	3.7358			6.0915			
ZnPtP ₂	0.6293			5.8043			
ZnPtAs ₂	-0.1998			5.9994			
ZnPtSb ₂	-1.7848			6.0407			
ZnPtBi ₂	-3.3743			6.3347			
CdCN ₂	5.8097			5.9651			
CdCP ₂	2.7032			5.6779			
Cd _{0.5} C _{0.5} P	2.7032			5.6779	4.973		[8]
CdCAS ₂	1.8741			5.8731			
Cd _{0.5} C _{0.5} As	1.8741			5.8731	5.201		[8]
CdCSb ₂	0.2891			5.9143			
Cd _{0.5} C _{0.5} Sb	0.2891			5.9143	5.62		[8]
CdCBi ₂	-1.3004			6.2083			
CdSiN ₂	5.2692			5.9568			
Cd _{0.5} Si _{0.5} P	2.1627	1.22 (GW)		5.6696	5.378		[9]
Cd _{0.5} Si _{0.5} As	1.336			5.8648	5.61		[8]
CdSiSb ₂	-0.2514	0.8		5.9061	6.344		[2]
CdSiBi ₂	-1.18409			6.2			
CdGeN ₂	4.7793			6.0646			
Cd _{0.5} Ge _{0.5} P	1.6729	0.33 (GW)	d	5.7774	5.523		[9]
Cd _{0.5} Ge _{0.5} As	0.8437		Metallic	5.9726	5.755		[8]
CdGeSb ₂	-0.7412	0.2		6.0139	6.383		[2]
CdGeBi ₂	-2.3308			6.3078			
CdSnN ₂	4.2504			6.1657			
Cd _{0.5} Sn _{0.5} P	1.144			5.8785	5.797		[8]
CdSnSb ₂	-1.2701	-0.80 (FLAPW)		6.1149	6.479		[6]
CdSnBi ₂	-2.8596			6.4089			
CdPtN ₂	3.5394			6.3852			
CdPtP ₂	0.433			6.098			
CdPtAs ₂	-0.3962			6.2931			
CdPtSb ₂	-1.9811			6.3344			
CdPtBi ₂	-3.5706			6.6284			
HgCN ₂	4.5586			6.2613			
HgCP ₂	1.4522			5.9741			
HgCAS ₂	0.623			6.1693			

Final Comments

- ✓ Photoelectrochemical water splitting needs new materials, our first silicon.
- ✓ This material may or may not be useful for PV, but still must have the same efficiency as commercial PV devices.
- ✓ A collaboration of theory, synthesis, and characterization groups is necessary to achieve fundamental PEC goals.
 - Any material search must rapidly achieve a fundamental understanding of the limiting factors of the current material sets and then identify alloy combinations that can address these limitations
 - The key will be the predictive capability of the theory groups coupled with the synthesis capability of the growth groups.
 - The right questions are needed, experimentalists and theorists
- ✓ Prioritize the properties to search for:
 1. Bandgap
 2. Type of transition (direct, indirect) and localized vs. delocalized bands
 3. Stability, band edges, catalysis
- ✓ PEC is a useful tool to screen possible semiconducting materials

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