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The Ecology of Energy Materials

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"The Stone Age did not end for lack of stone, and the Oil Age will end long before the world runs out of oil."

Sheikh Zaki Yamani
former Saudi Arabian Oil Minister

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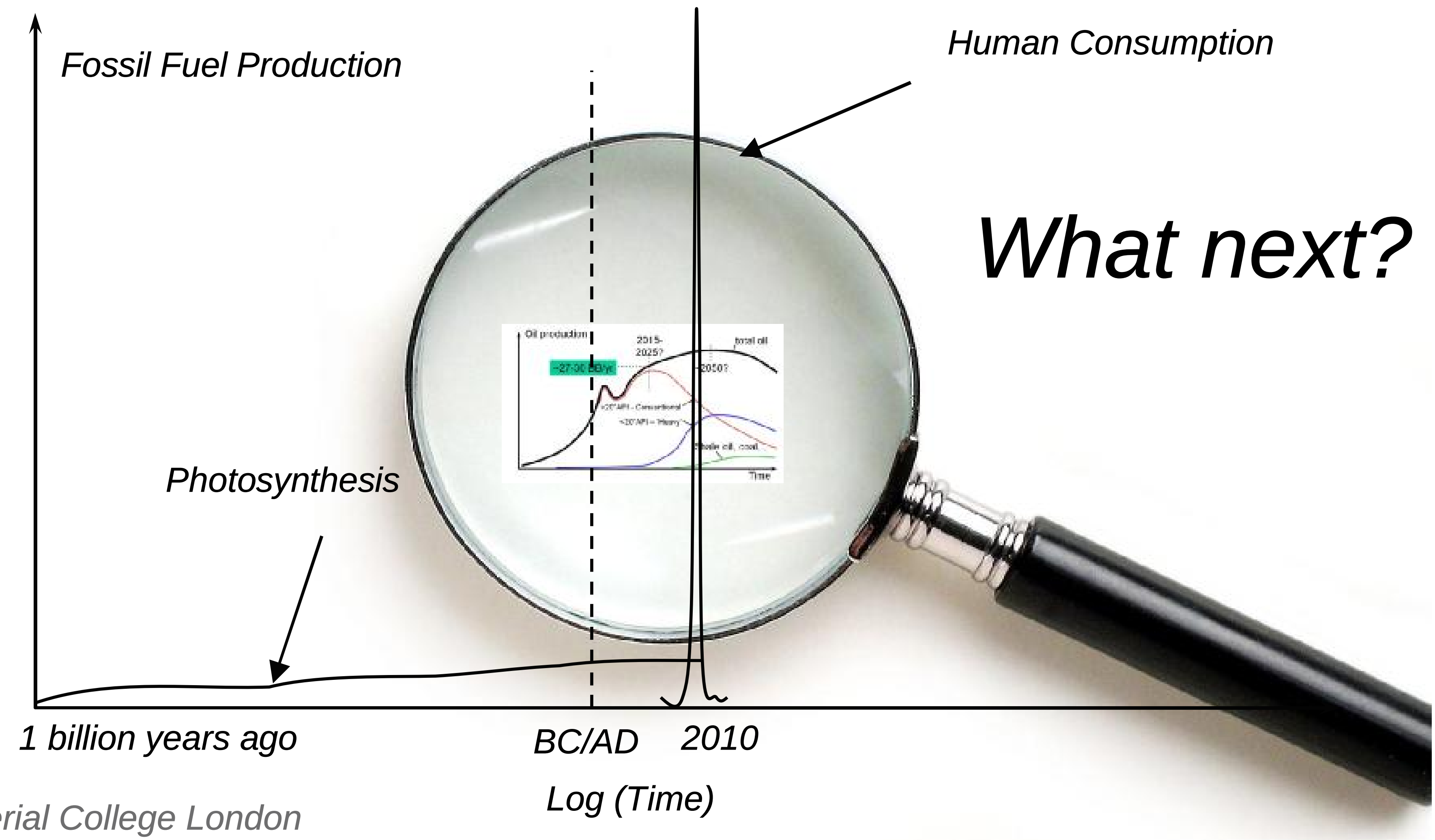
Log [Time] Graph



Ecology of Energy Materials

- Introduction and Definition
- Drivers for Innovation
- Sustainable Energy
- Hydrogen Production Pathways
- Materials Requirements
- Outlook and Final Remarks

Basic Needs and Energy Requirements

- Food
- Water
- Shelter
- Energy
- Transport
- Recreation

Energy and Transport

Means	Distance covered 1 hour	1 day	Mode Switch at GDP/person
• Foot	4 km	30 km	
• Horse	20 km	100 km	$ 500
• Car	130 km	1000 km	$ 5,000
• Aeroplane	800 km	10,000 km	$ 25,000
• Spaceship	20,000 km	200,000 km	$ 20M → $ 200k

Number of people at transition threshold

Horse (bike) → Car	~ 3Billion
Car → Aeroplane	~ 1Billion

e.g. domestic Chinese passengers: 6M (1985), 40M (1995), 146M (2007)

Role of Energy and Energy Materials

- All materials require energy input for transformation (reaction) and/or separation e.g. fuel, fertiliser, cement, desalinated water

- Energy materials directly or indirectly involved in production of energy vectors e.g. fossil fuels, hydrogen

- Range of energy materials, e.g.:
  - catalysts (HDS)
  - materials of constructions (reformer tubes, reactors)
  - photovoltaic cells (semiconductors)

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Drivers for Materials Innovation

- Necessity e.g. apartheid, CO_2 reduction
- Enhancement e.g. carbon fibre
- Desire e.g. titanium, eco products, energy/fuels
- Conflict e.g. Manhattan Project
- Cost e.g. polymers

Major factor: mostly involving reduction in energy requirements per unit mass/volume as well a reduction in time

Renewable Fuels

- Biofuels
  - 1^{st}, 2^{nd}, 3^{rd}, "4^{th}" generation
  - insufficient quantity
- All electrical society?
  - requires step change in e.g. battery research (materials)
  - not all uses can be substituted (e.g. air traffic)
  - where do the electrons come from?
- Hydrogen economy:
  - sustainable production, storage, distribution network
- Synthetic hydrocarbon based fuels (from CO_2?)
  - existing infrastructure
  - need a sustainable source of hydrogen or electrons!

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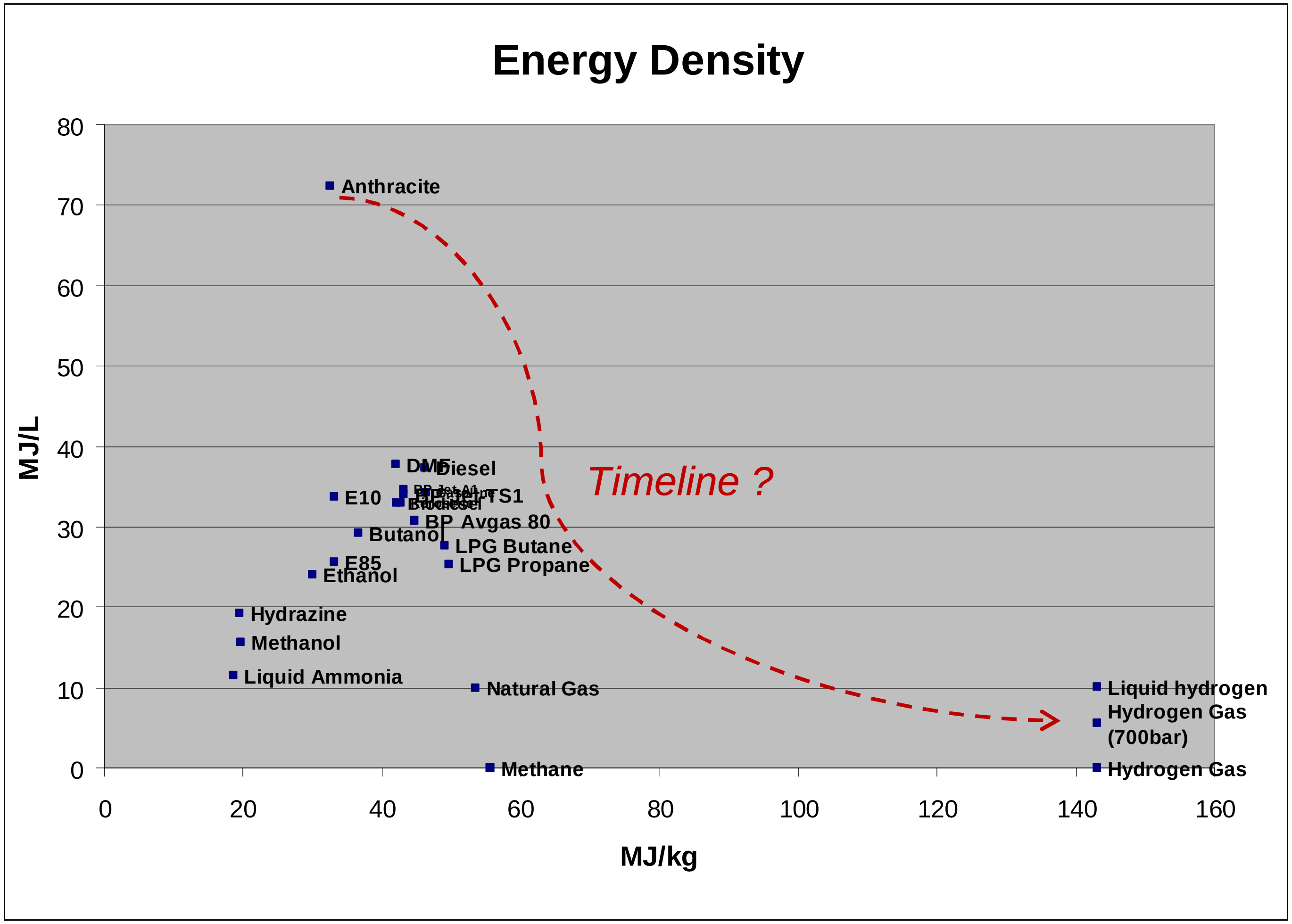
Energy Density of Materials



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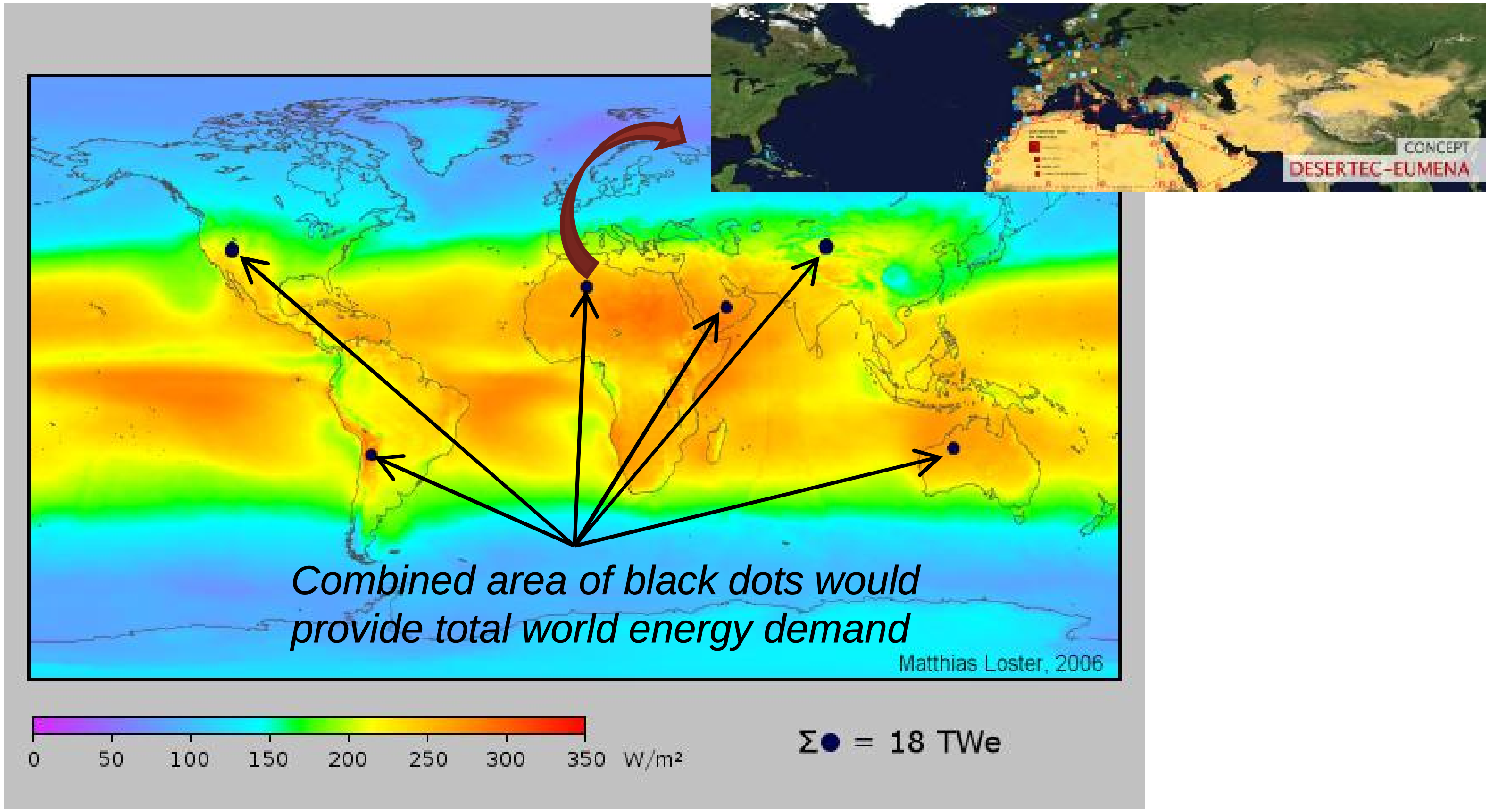
Cost of Renewable Electricity and Fuels

- Wind electricity (2m 1MW windmills [50x current] replacing coal)
- Photovoltaic electricity (2000 GW-peak PV [700x current] on $2x10^6$ ha)
- Renewable hydrogen via wind, solar (4m 1MW-peak windmills for fuel cell cars, displacing petrol-diesel)
- Biofuels for fossil fuels (add 100x current Brazil or US EtOH on $250x10^6$ ha = 16% agricultural land)

- Cost:
  - $10-20 trillion capital investment by 2030 (IEA est.)
    …not such a big number anymore…
  - 1% of world GDP (inactivity 5% of GDP) (Stern report)

See: S Pacala and R Socolow, Science, **305**, 968-972 (2004)

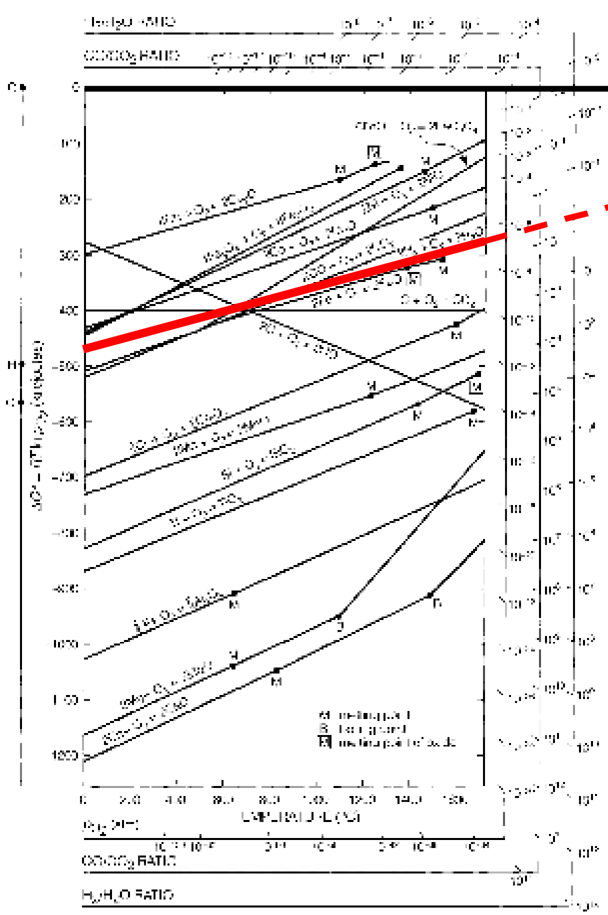
Energy Gap of 16TW by 2050



Solar
36,000 TW on land (world)

All other renewables
36 TW on land (world)

Thermodynamics



$$2H_2O \longrightarrow 2H_2 + O_2$$

$T_c = 3917\ K$

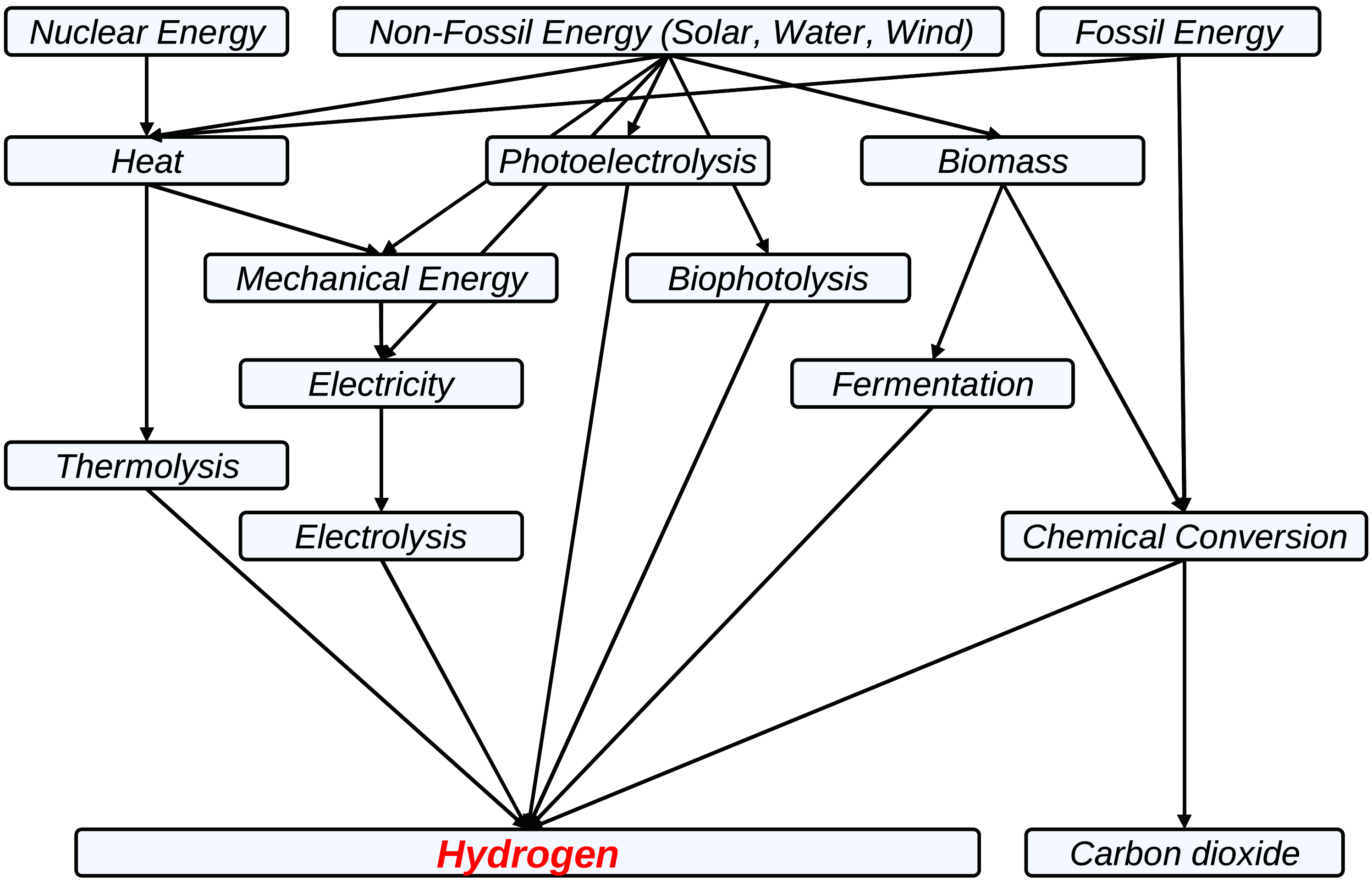
$$2H_2O \longleftarrow 2H_2 + O_2$$

$$\Delta G_T^0 \ \ / \ \mathrm{J\ (mol\ H_2)^{-1}} = -238915 + 61T = -2F \cdot E_T^0$$

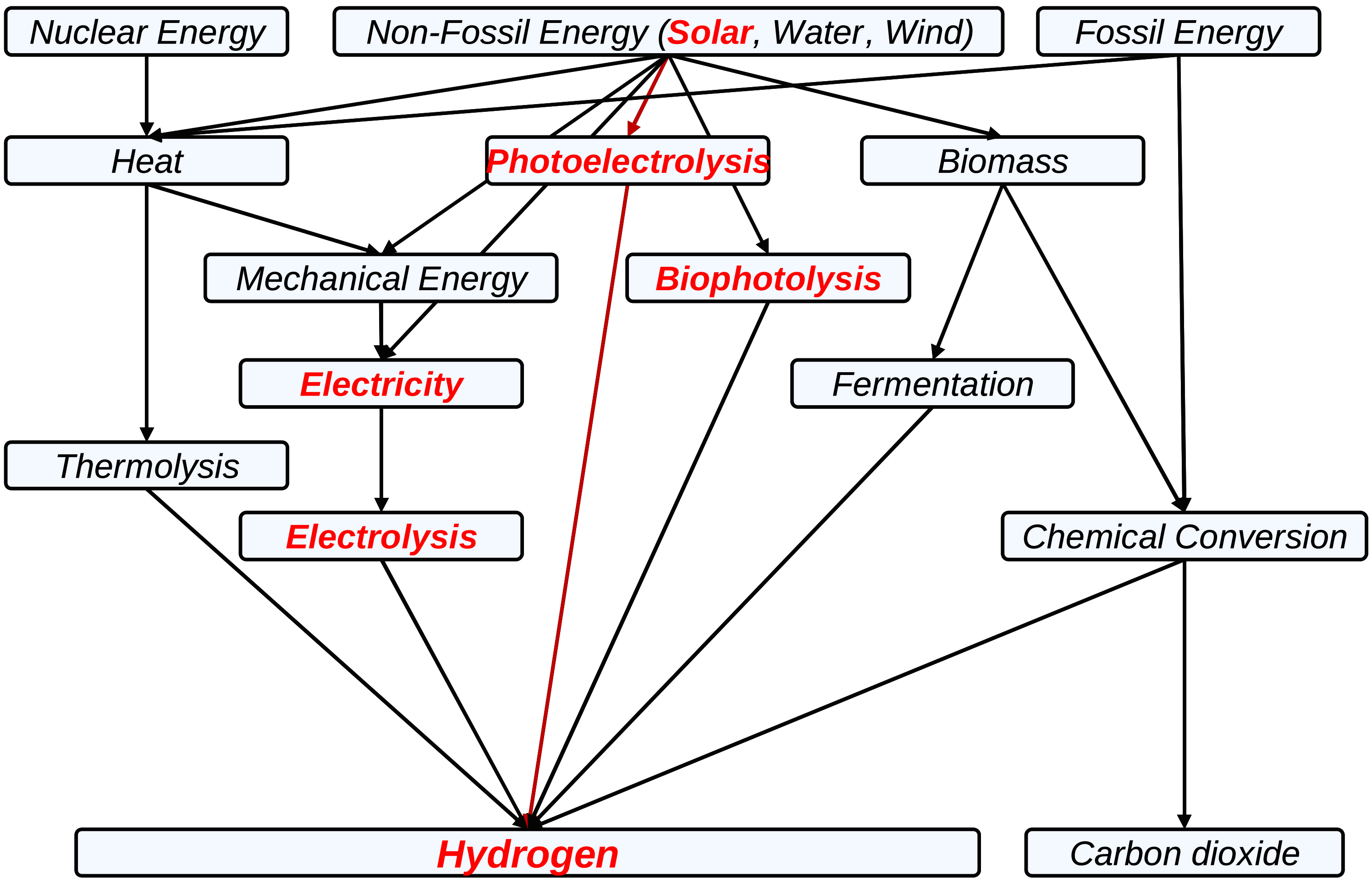
$$\Delta G_T^0 \ \ / \ \mathrm{J\ (mol\ O_2)^{-1}} = -RT \ln\left\{\frac{p_{H_2O}^2}{p_{H_2}^2 \, p_{O_2}}\right\} = -494000 + 112T$$

Obvious need for catalytic materials here!

Routes to Hydrogen



Direct Solar Hydrogen



Hydrogen Production using Electrolysis

Overall Reaction : $2H_2O \rightarrow 2H_2 \uparrow + O_2 \uparrow$

$2H_2O + 4e^- \rightarrow 4OH^- + 2H_2 \uparrow$

$4OH^- \rightarrow 4e^- + 2H_2O + O_2 \uparrow$

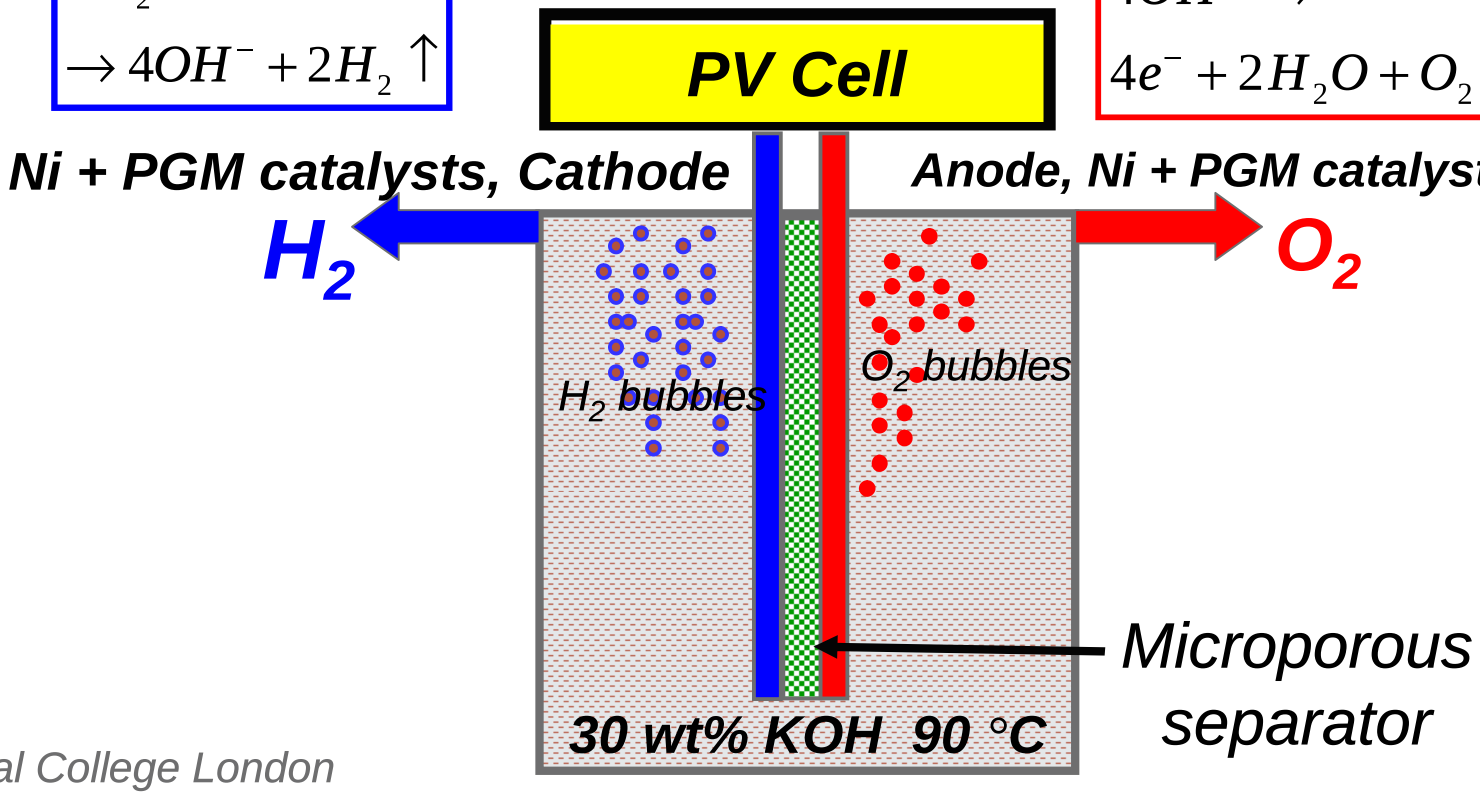
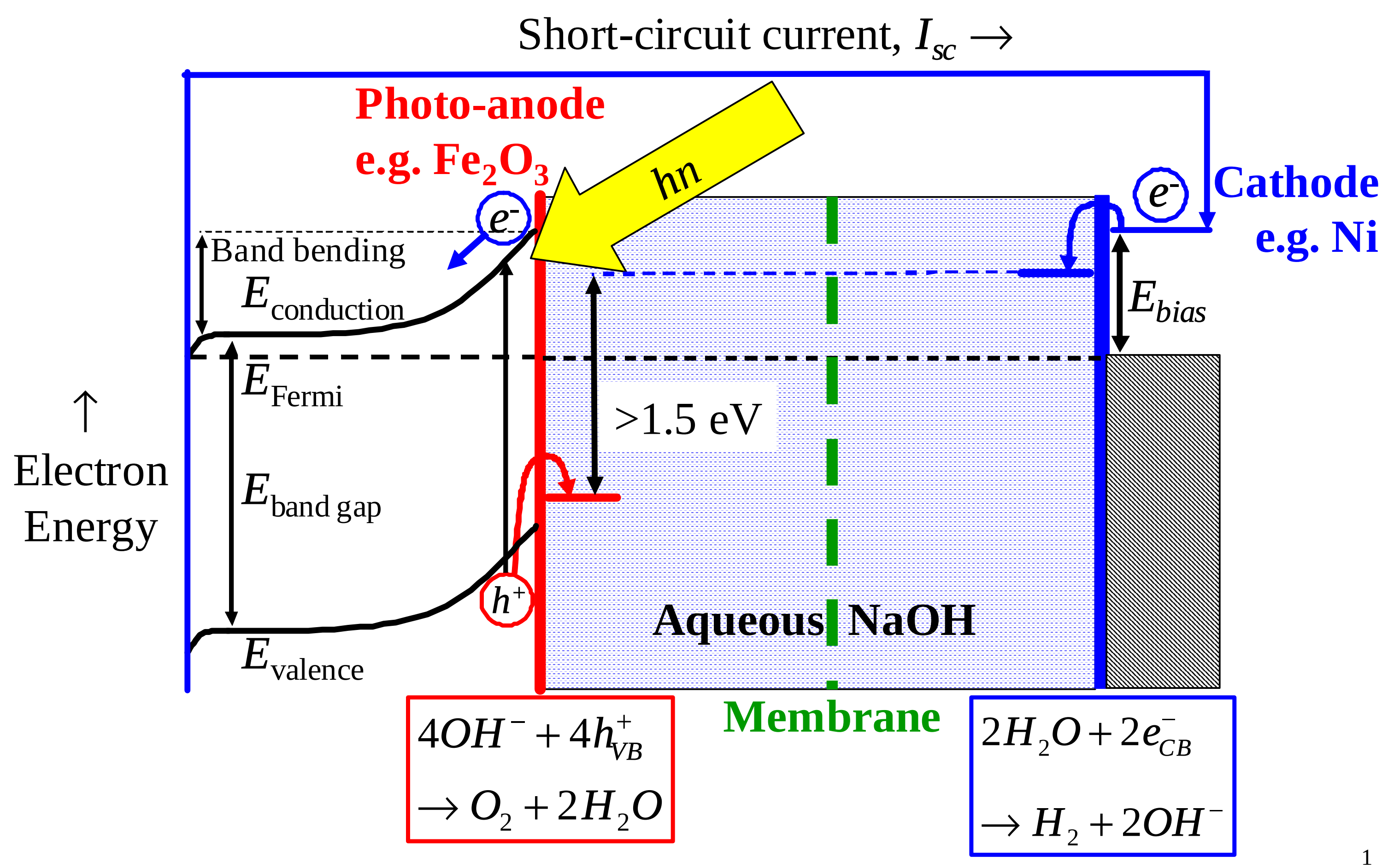


Photo-electrolytic Hydrogen



Materials Requirements

- Actually Required Band Gap ~2.4eV (520nm VIS)
  - overpotential (activation) for oxygen (0.4eV) evolution needs to be reduced (catalysts)
- Band Edges must straddle H_2O redox potentials
- Fast charge transfer/separation
- Must be stable in aqueous solutions (pH)
- Must be reasonable electron conductor
  - doping (n-type)
- Cheap and easy to prepare
- Theoretical Efficiency limit: 32%
- GaAsInP based systems 12.4% efficiency but expensive

Oxide Semiconductors

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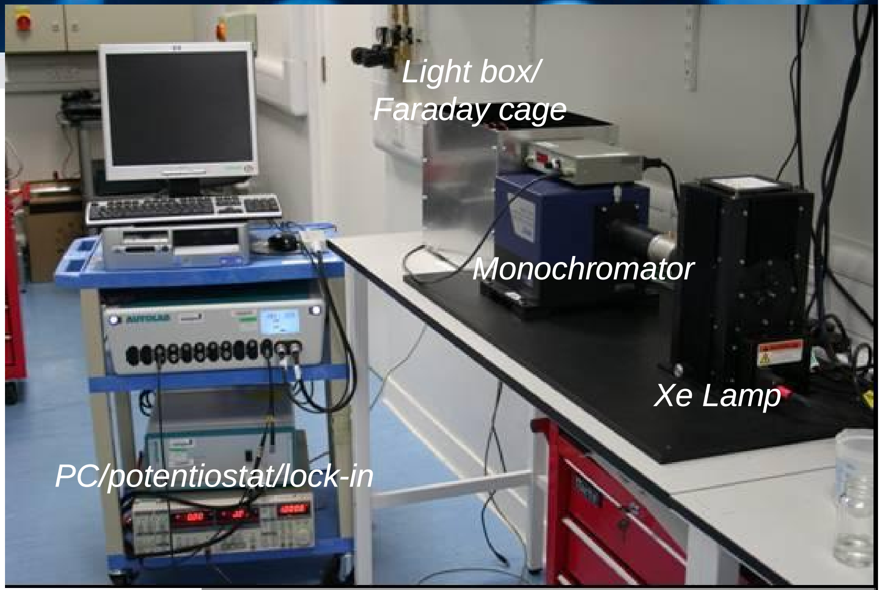
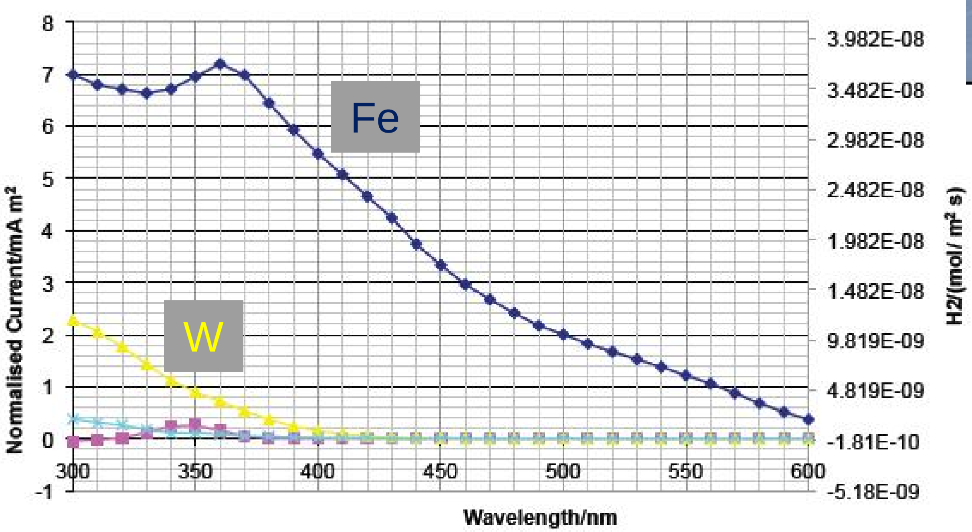
Materials Performance

- § Photo-electrochemical activity of photo-anodes based on cheap transition metal oxides (Fe, W, Ti)
- § Fe, perhaps W based system requires bias but otherwise most promising (cheap/response)





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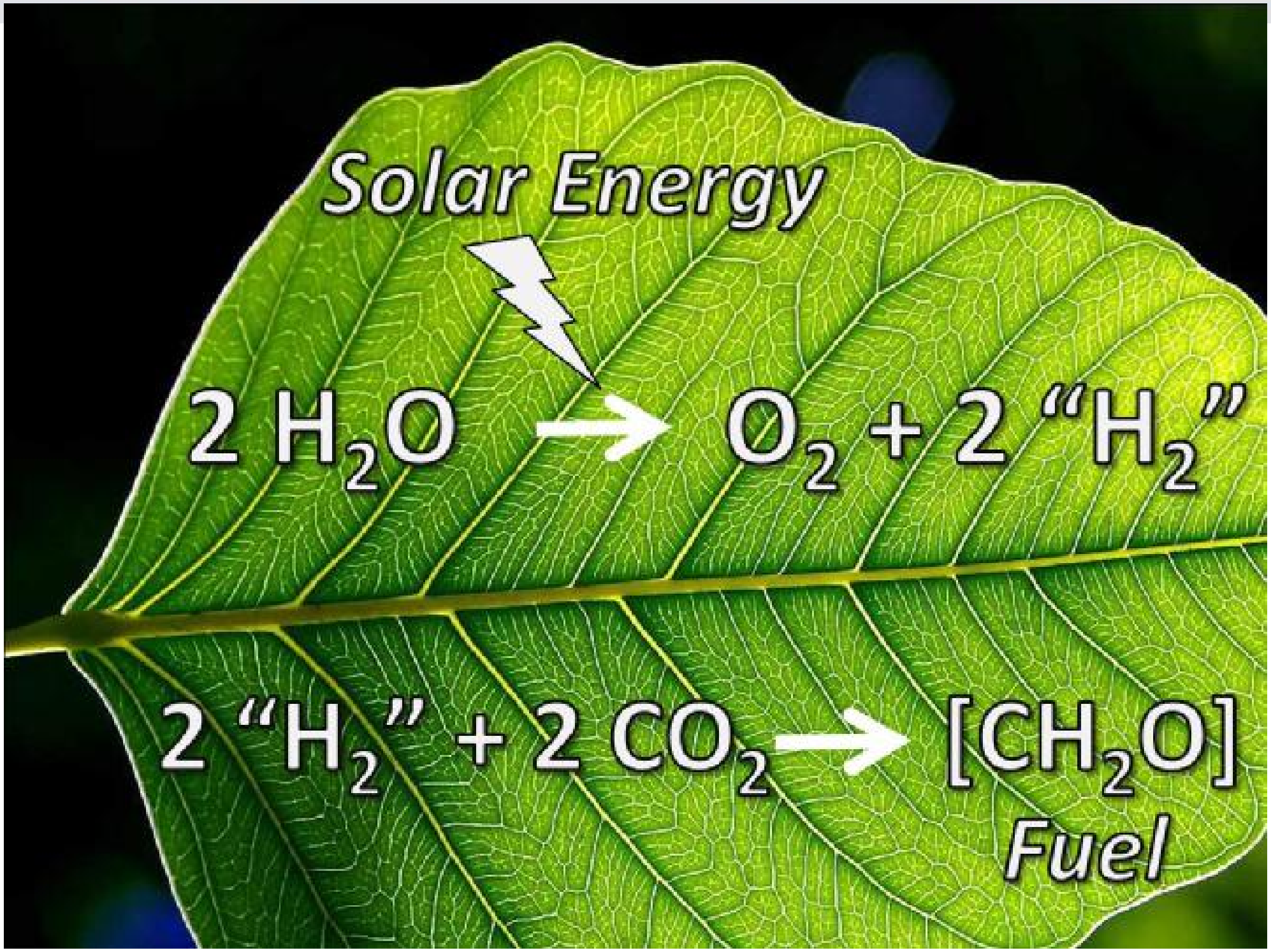
Plants can do it !



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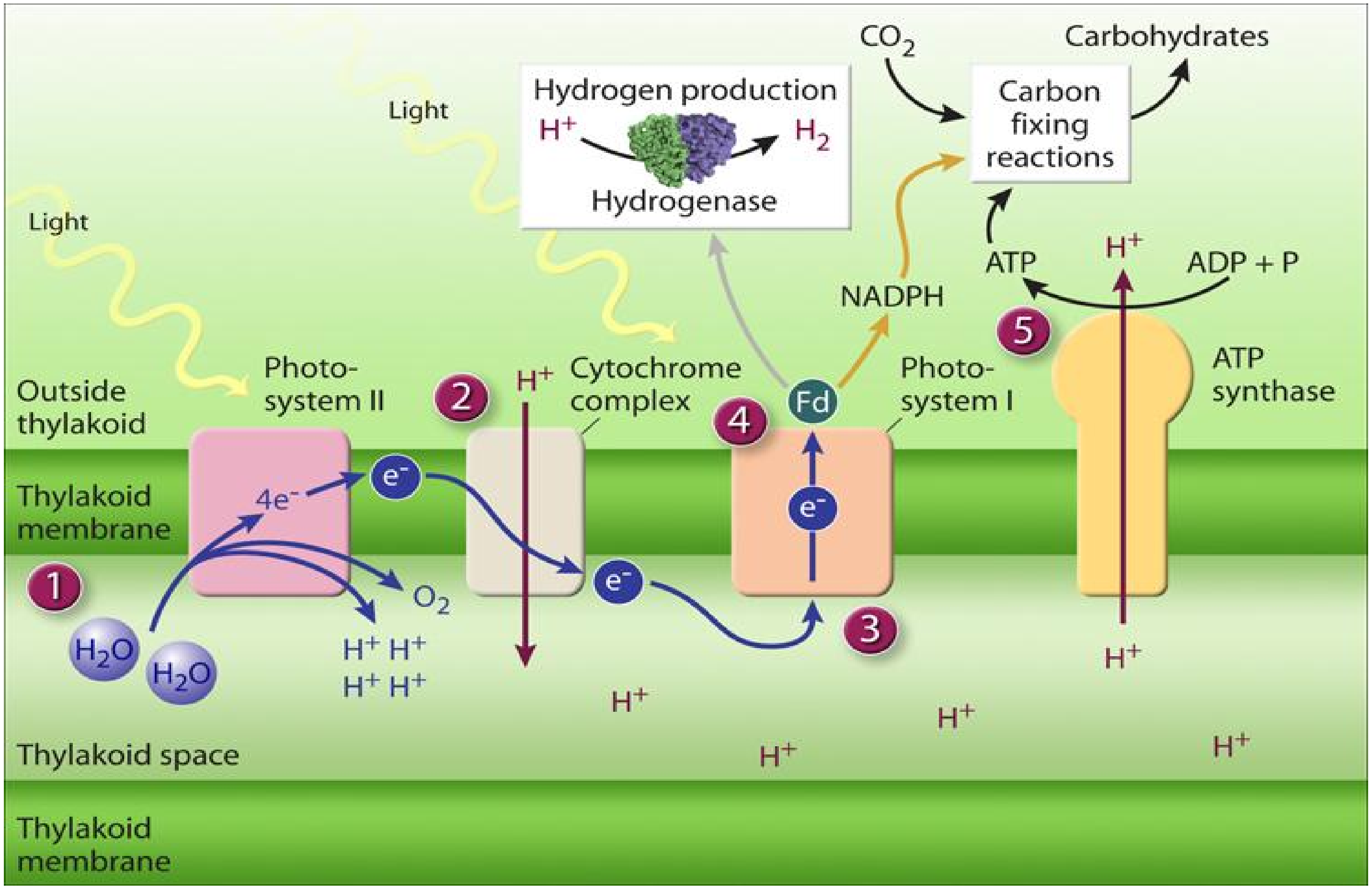
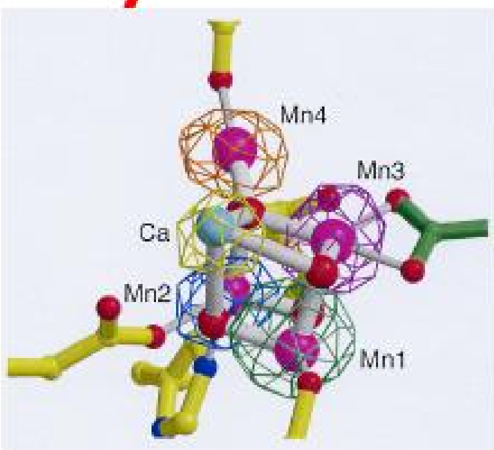
Bio-photolytic Pathway

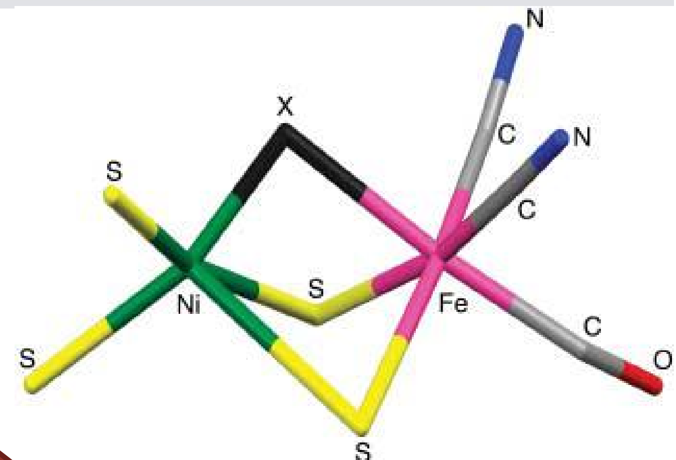


Towards an Artificial Leaf

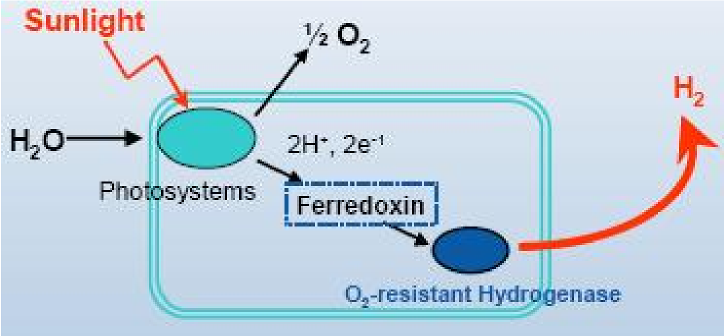


Structure of the PS II water oxidation catalyst
Barber et al. *Science* 2004

Artificial Chloroplast/ Cell Factory using Biomimetic Catalysts



Core structure of the resting form of [NiFe]hydrogenase from D. gigas, determined by x-ray analysis Ogo et al. *Science* 2007



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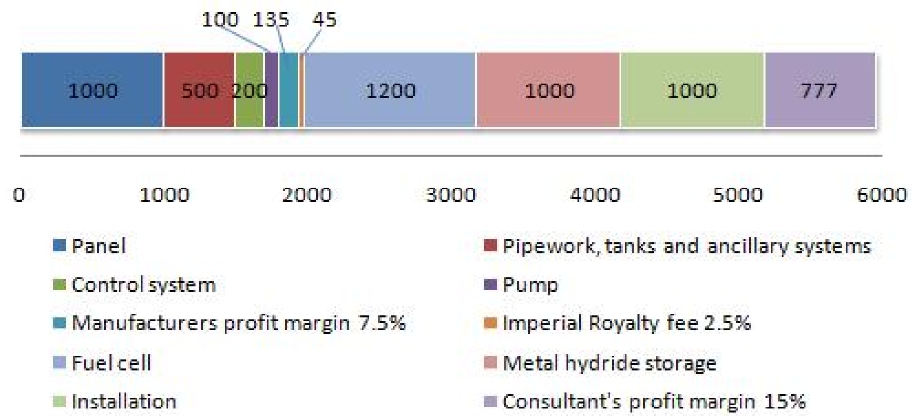
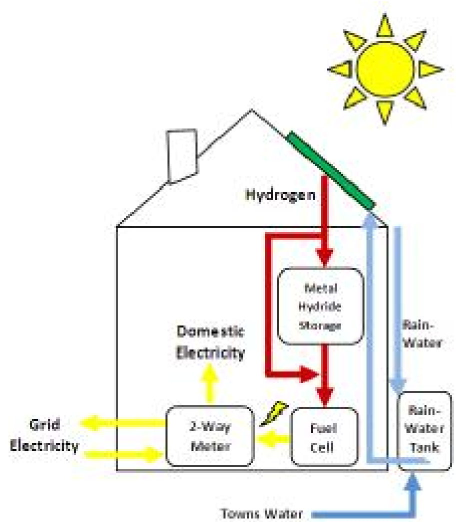
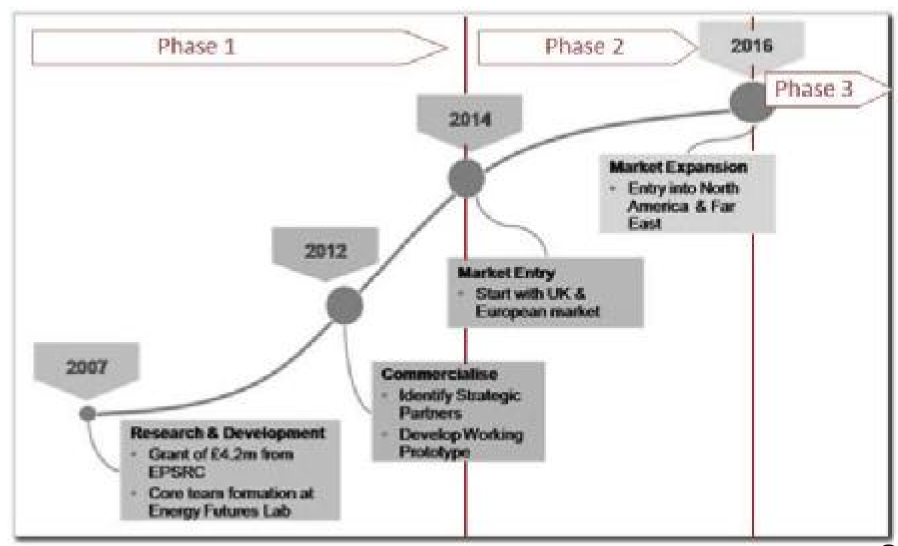
Commercialisation

- *Targets:*
  - *Photoelectrolytic H_2: £2.50/kg*
  - *Biophotolytic H_2: £5.00/kg;*
- ***Concurrent development of materials and systems !***
- *Combined with fuel cell operation*
- *Distributed market*







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Final Remarks

- Step changes in materials required for paradigm shift
- Trade-off between efficiency and cost
- Materials development should not occur in isolation – systems approach
- Solar energy is a widespread open access resource, which has implications for its governance
- Solar energy conversion technologies (direct or indirect) are the *only* sustainable option on a global scale; alternatives being fission and fusion
- CO_2 reduction technologies exist, but current policies do not offer significant economic incentives; radical new policy framework is required to facilitate solar energy innovation
- Fossil fuels will probably remain dominant for the next 100 years

"*Water will be the coal of the future*."

Jules Verne, 1874, *The Mysterious Island*

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Solar - Hydrogen Efficiency

$h_{electrolyser}$ = 80% only valid for very large systems at low current density; domestic systems ~ 40-50%

q *New generation Stirling Energy Systems – Suncatcher*

$h_{solar\text{-}electrical} = 31.25\%$ (inlc. h_{Aux})

$h_{solar\text{-}H_2} = 31.25\% \cdot 80\%$ ($h_{electrolyser}$) = 25%

q *New world record triple junction PV – Spectrolab*

$h_{solar\text{-}H_2} = 41.6\% \cdot 80\%$ ($h_{electrolyser}$) = 33.3%

q *Polycrystalline Si – Suntech*

$h_{solar\text{-}H_2} = 15.4\% \cdot 80\%$ ($h_{electrolyser}$) = 12.3%

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without electrolyzer

q *Thermal Dissociation (glow discharge) – H-Ion*

$h_{solar\text{-}H_2}$ = 2.1%

q *Direct Solar - Hydrogen (photocathode) – NREL*

$h_{solar\text{-}H_2}$ = 12.4%

q *Direct Solar – Hydrogen (photoanode) – Fe_2O_3*

$h_{solar\text{-}H_2}$ = ca. 10% (theoretical 32%)

Long term
NREL goal = 25%

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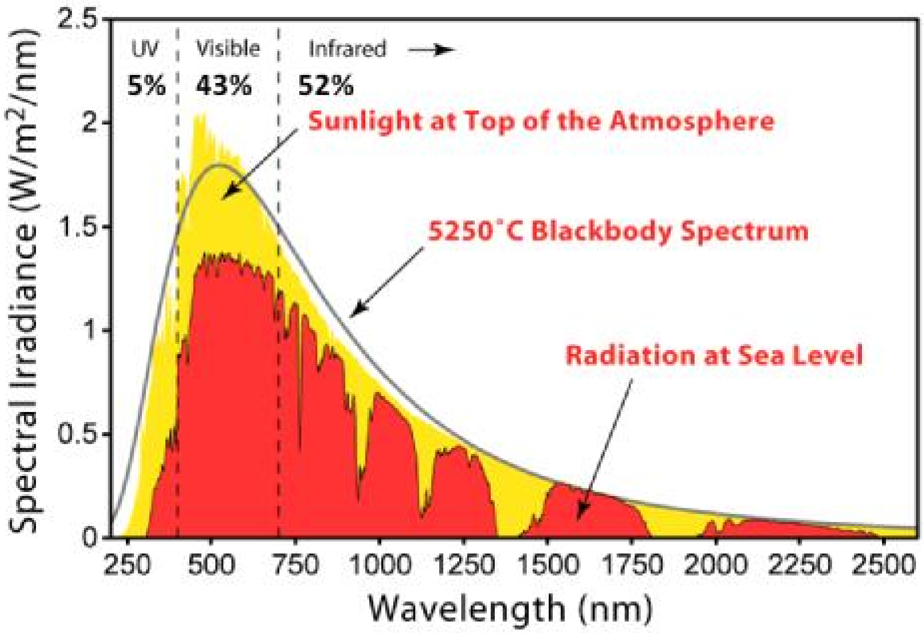
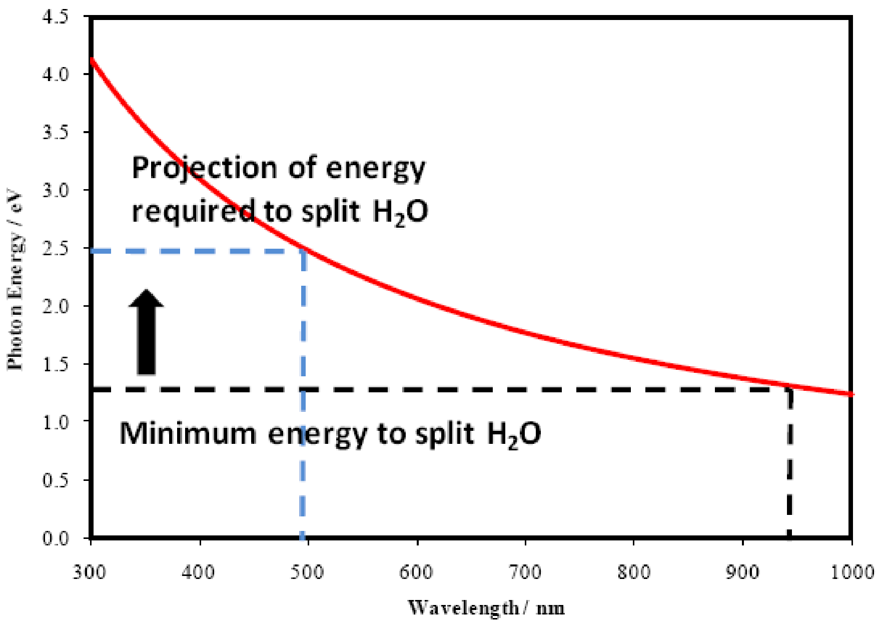
Materials Requirements



Dios, A.C.d. *Chemistry of the Environment (Greenhouse Effect)*. Available from: http://bouman.chem.georgetown.edu/S02/lect23/lect23green.html.



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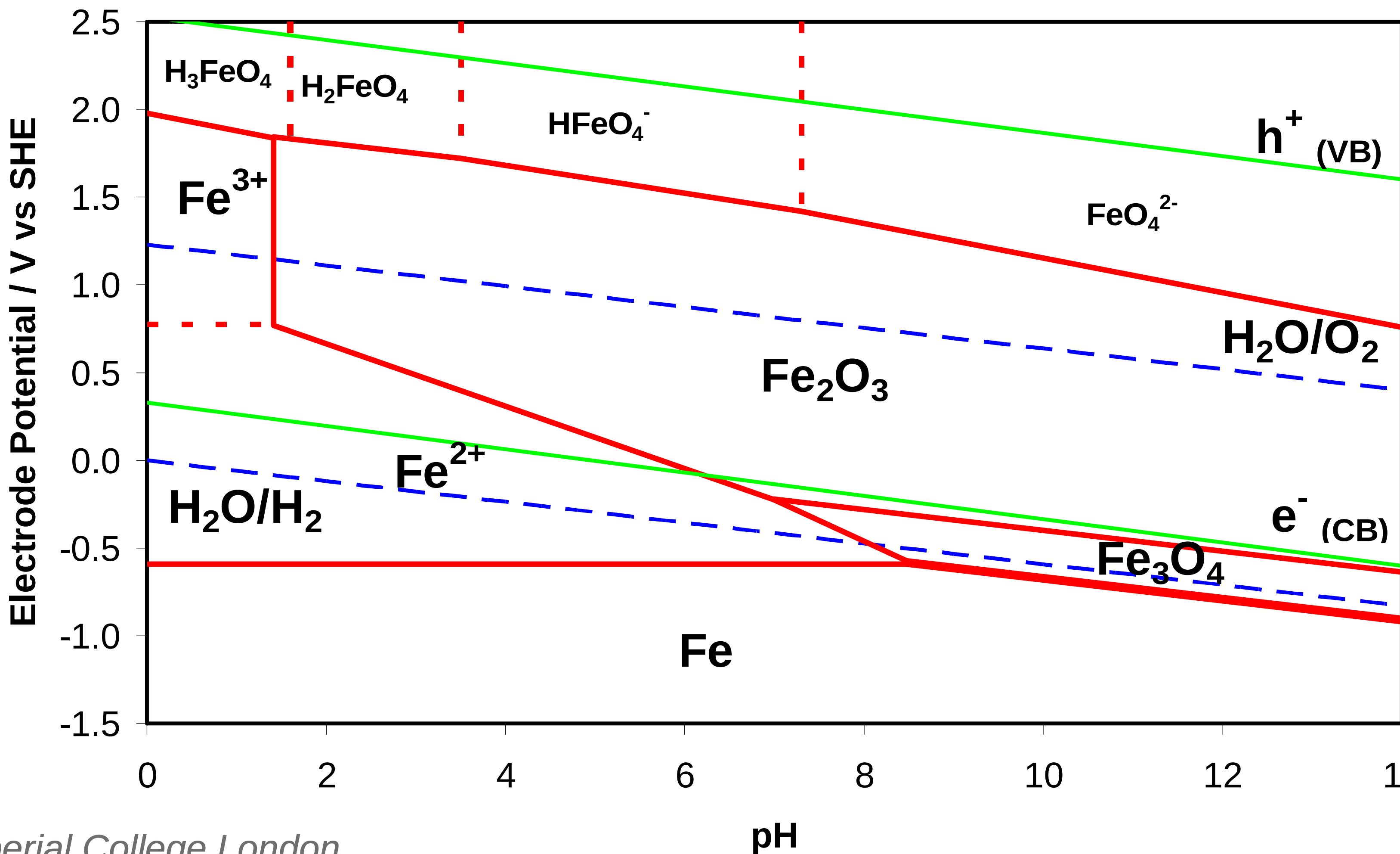
Materials Requirements



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Simulation and System Integration