

# The Ecology of Energy Materials

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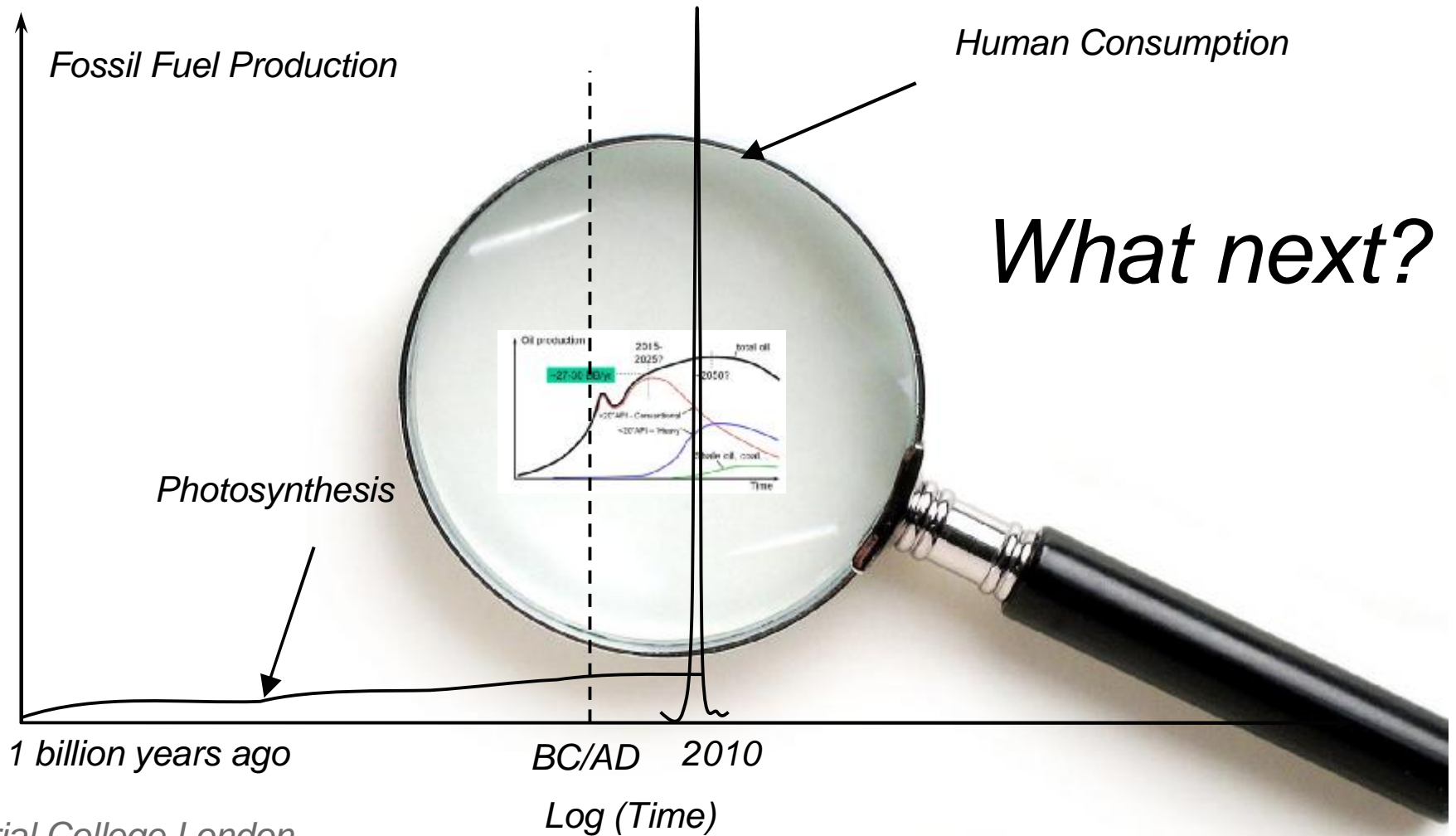
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*“The Stone Age did not end for lack of stone,  
and the Oil Age will end long before the world  
runs out of oil.”*

Sheikh Zaki Yamani  
former Saudi Arabian Oil Minister

# 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		Mode Switch at GDP/person
	1 hour	1 day	
• 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**)

# Drivers for Materials Innovation

- § Necessity e.g. apartheid, CO<sub>2</sub> 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<sup>st</sup>, 2<sup>nd</sup>, 3<sup>rd</sup>, “4<sup>th</sup>” 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?

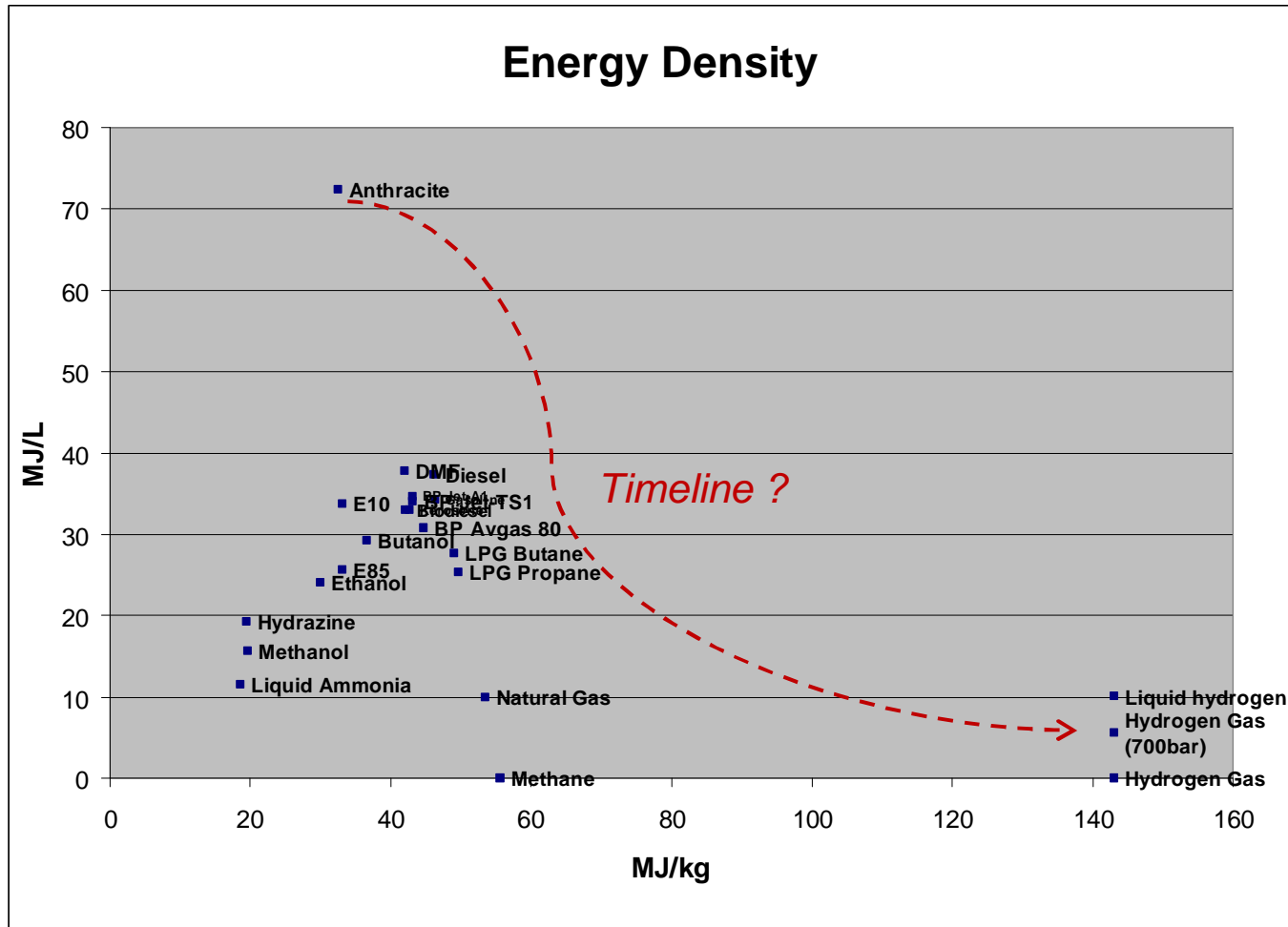
## § Hydrogen economy:

- sustainable production, storage, distribution network

## § Synthetic hydrocarbon based fuels (from CO<sub>2</sub>?)

- existing infrastructure
- need a sustainable source of hydrogen or electrons!

# Energy Density of Materials

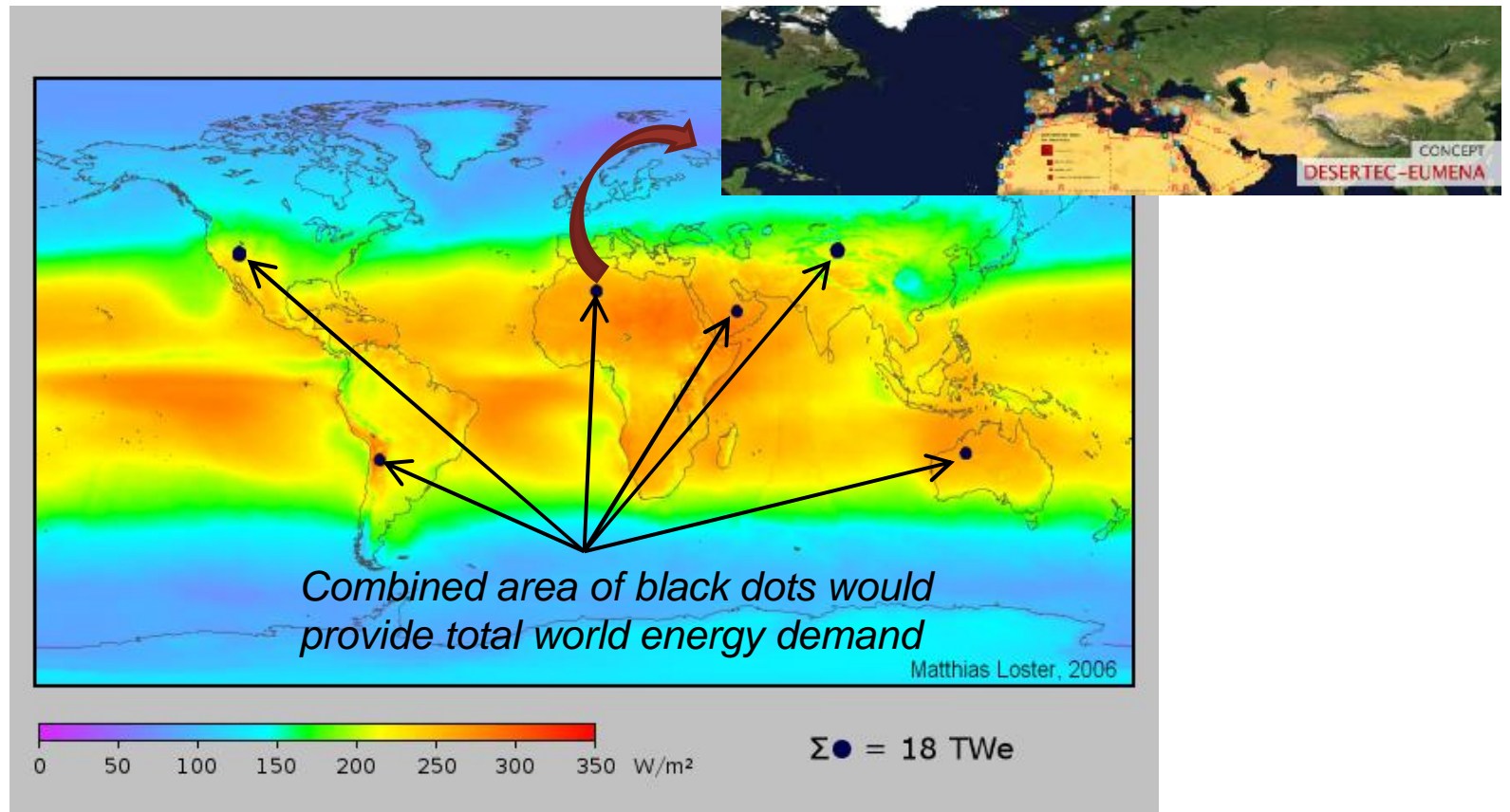


# Cost of Renewable Electricity and Fuels

- § Wind electricity (2m 1MW windmills [50x current] replacing coal)
- § Photovoltaic electricity (2000 GW-peak PV [700x current] on  $2 \times 10^6$  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  $250 \times 10^6$  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

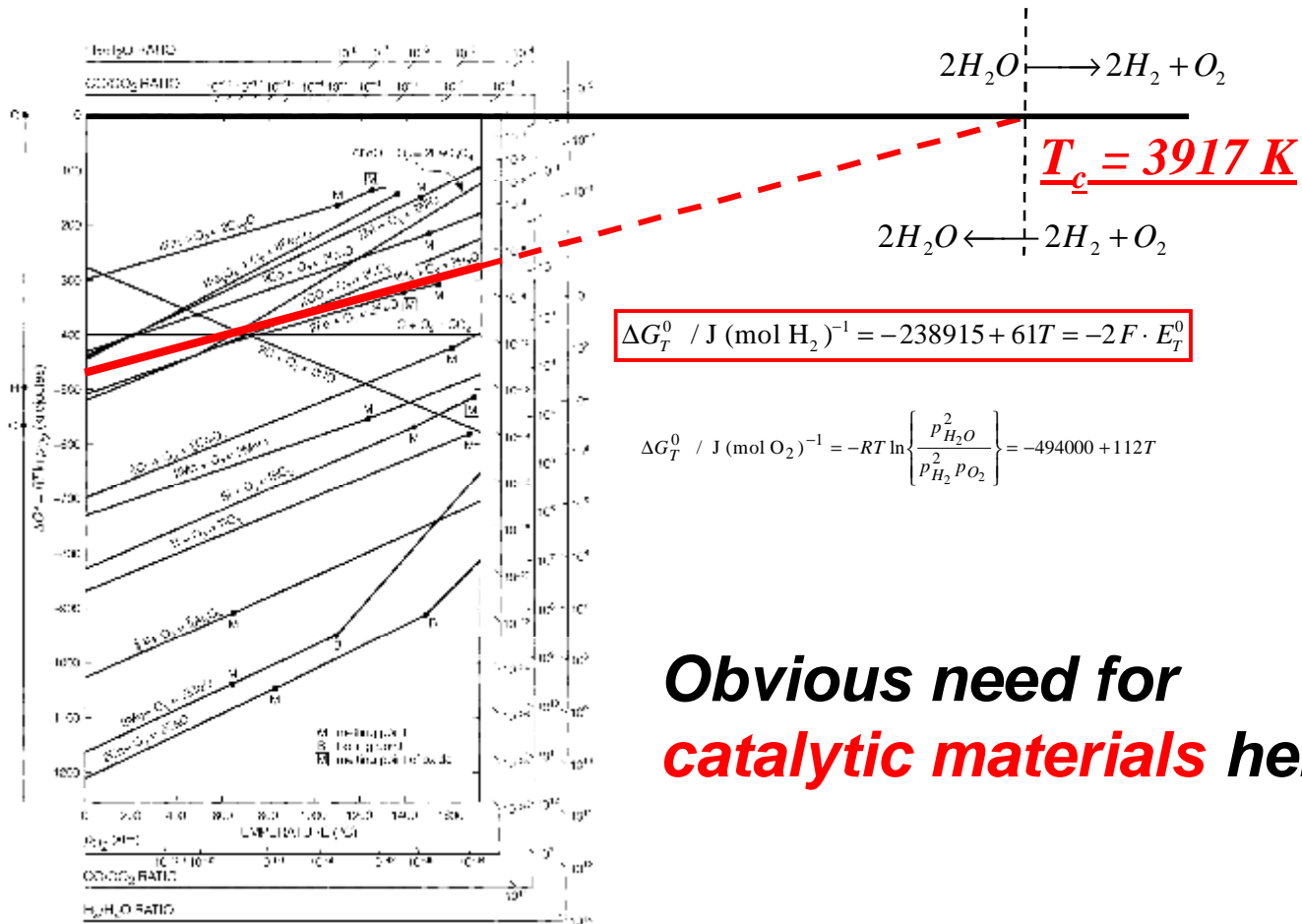
36,000 TW on land (world)



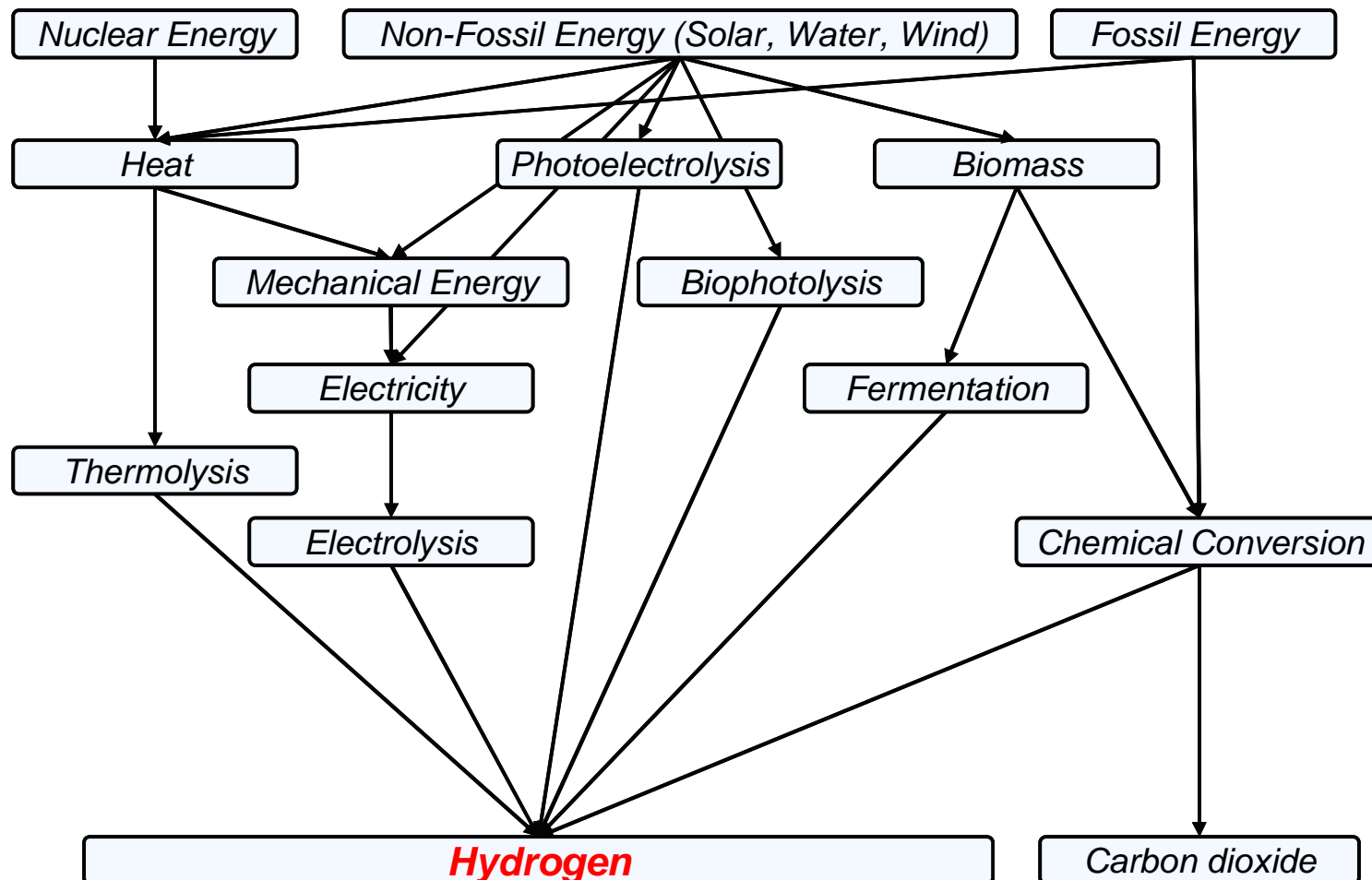
All other renewables

36 TW on land (world)

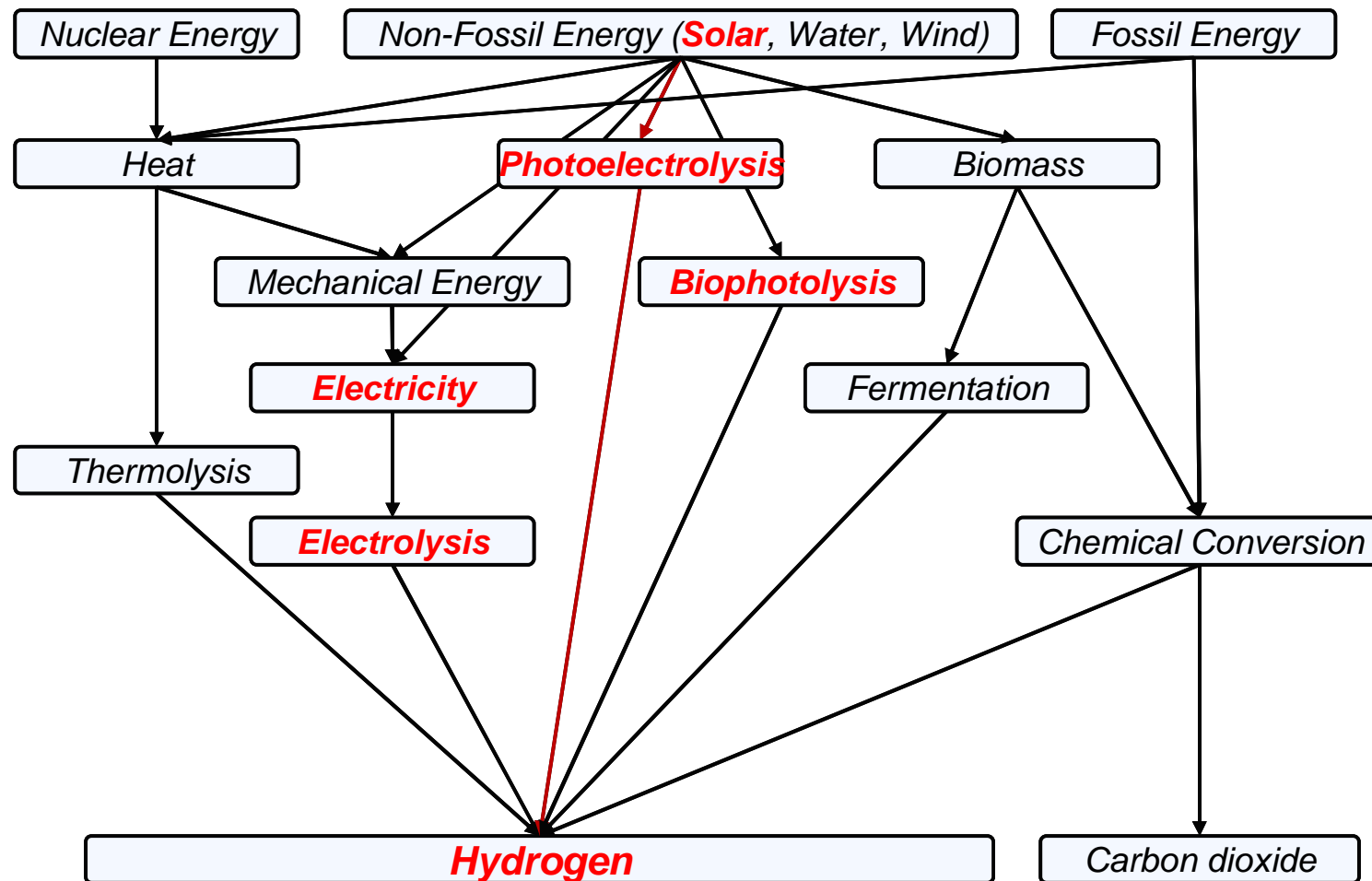
# Thermodynamics



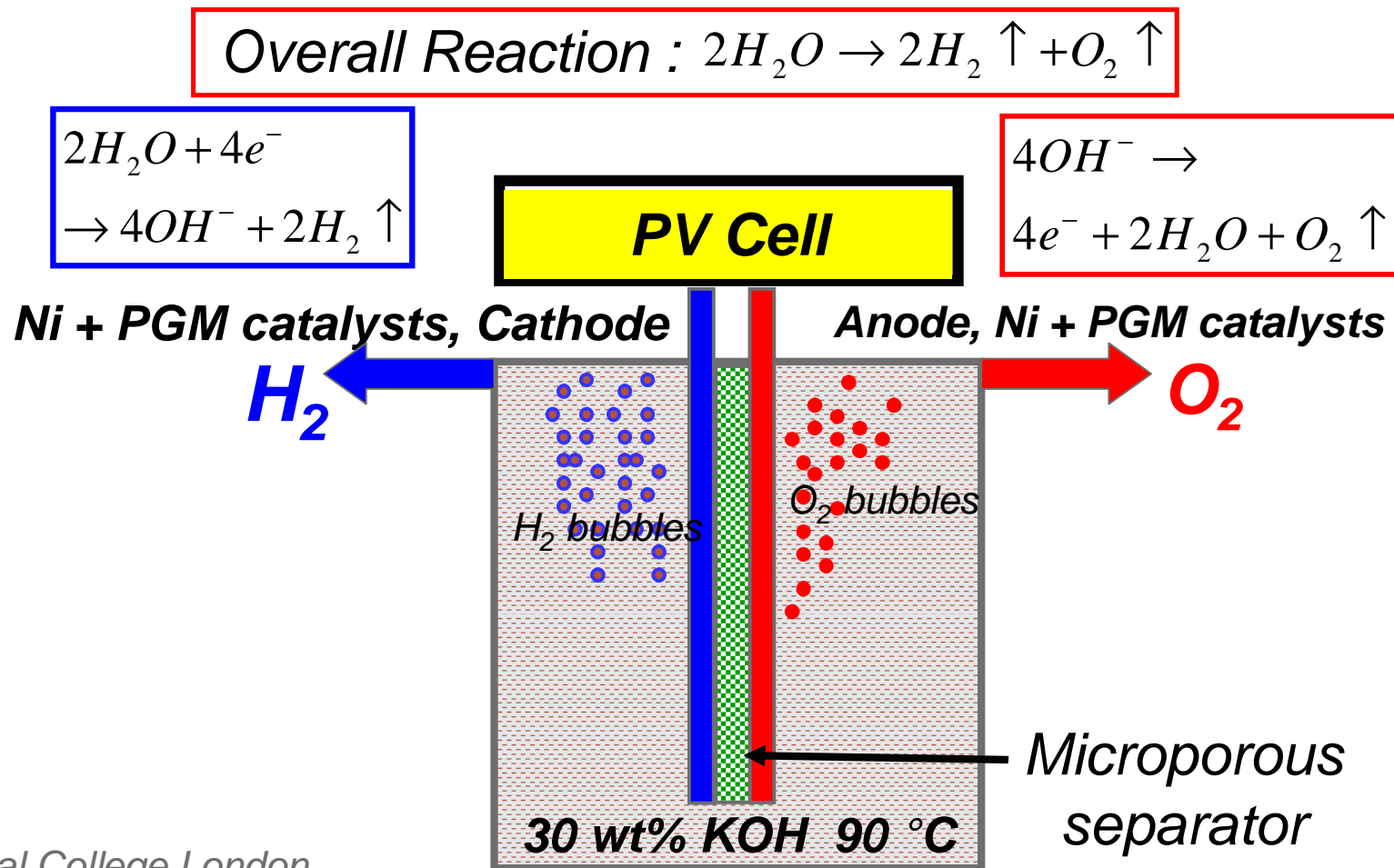
# Routes to Hydrogen



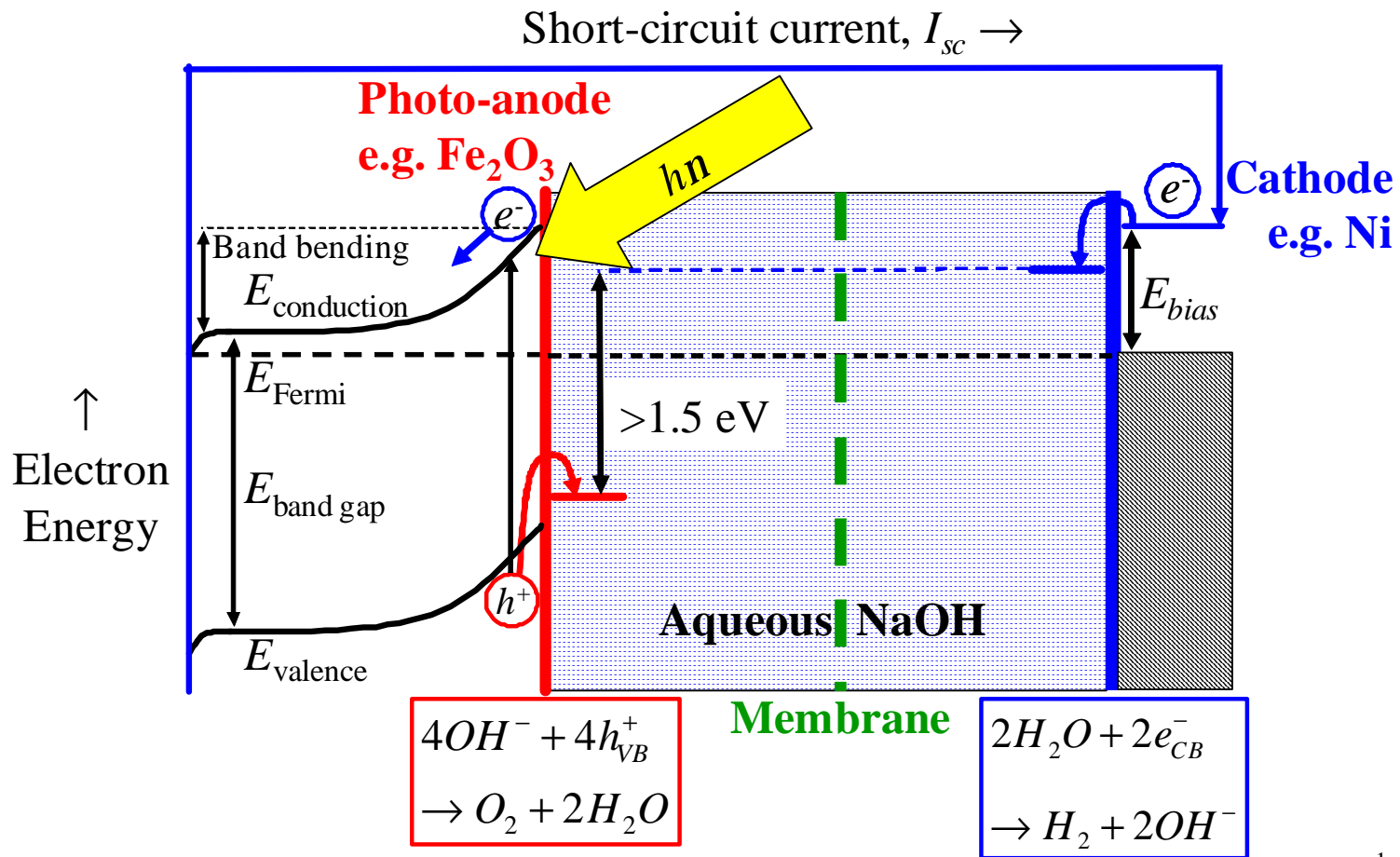
# Direct Solar Hydrogen



# Hydrogen Production using Electrolysis



# Photo-electrolytic Hydrogen



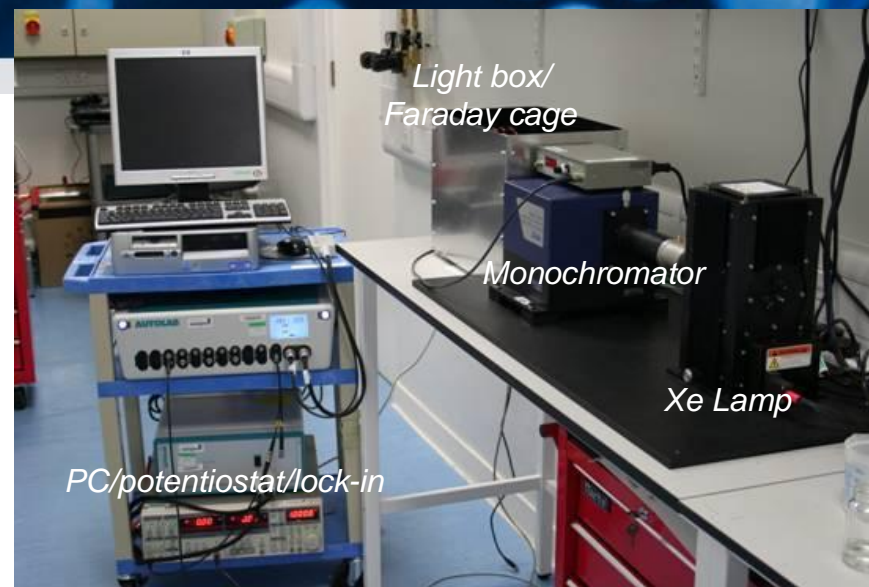
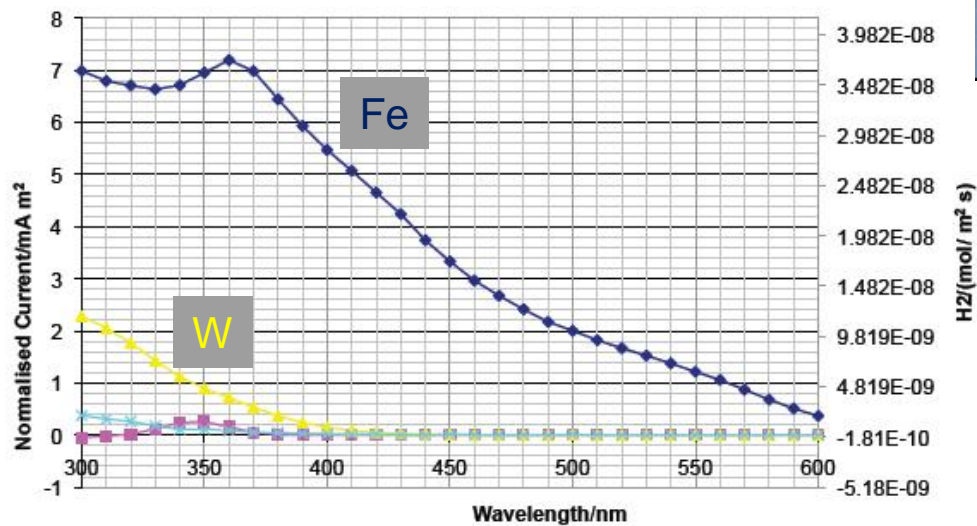
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# Materials Requirements

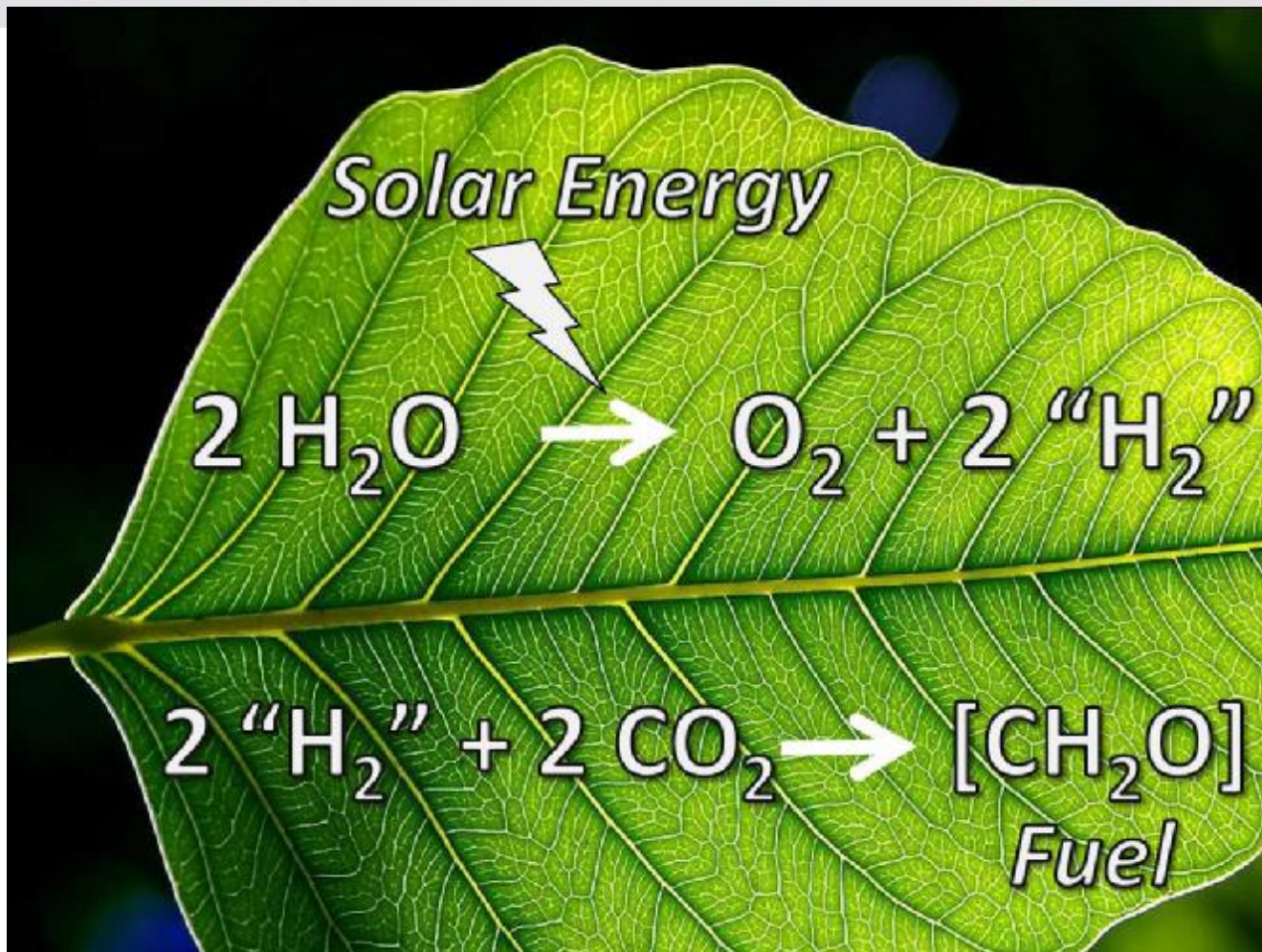
- § Actually Required Band Gap  $\sim 2.4\text{eV}$  (520nm VIS)
  - § overpotential (activation) for oxygen (0.4eV) evolution needs to be reduced (catalysts)
- § Band Edges must straddle  $\text{H}_2\text{O}$  redox potentials
- § Fast charge transfer/separation
- § Must be stable in aqueous solutions (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

# Materials Performance

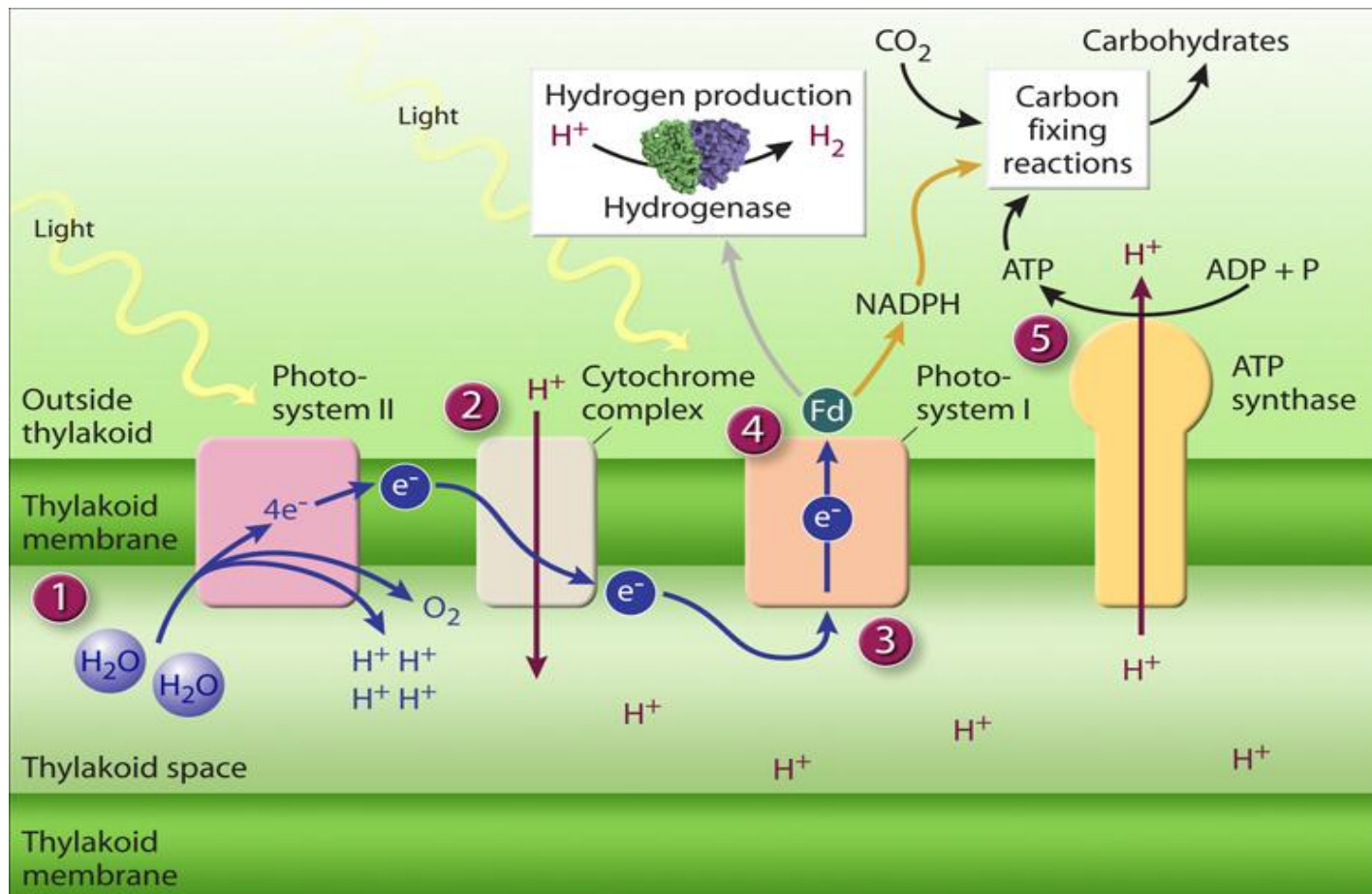
- § Photo-electrochemical activity of photo-anodes based on cheap transition metal oxides (Fe, W, Ti)
- § Fe, perhaps W based system requires bias but otherwise most promising (cheap/response)



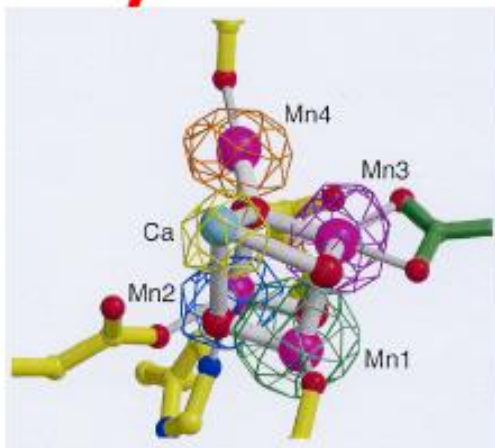
# Plants can do it !



# Bio-photolytic Pathway

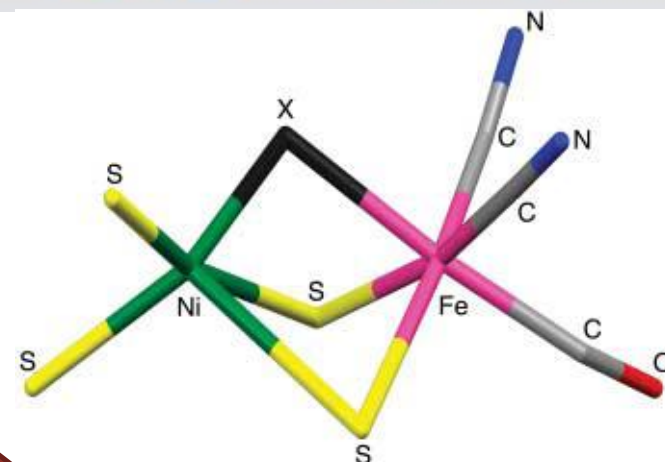


# Towards an Artificial Leaf

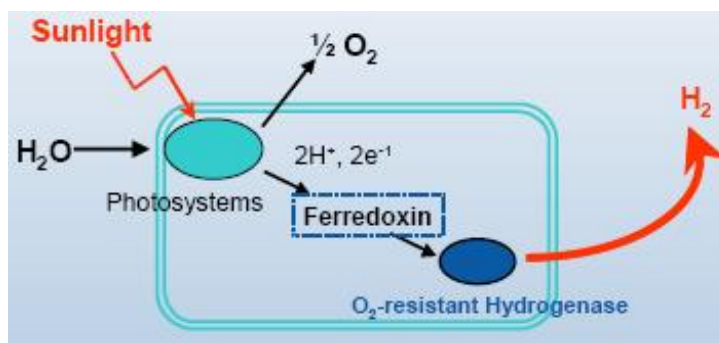


Structure of the PS II  
water oxidation catalyst  
Barber et al. *Science* 2004

## 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



## Commercialisation



### § Targets:

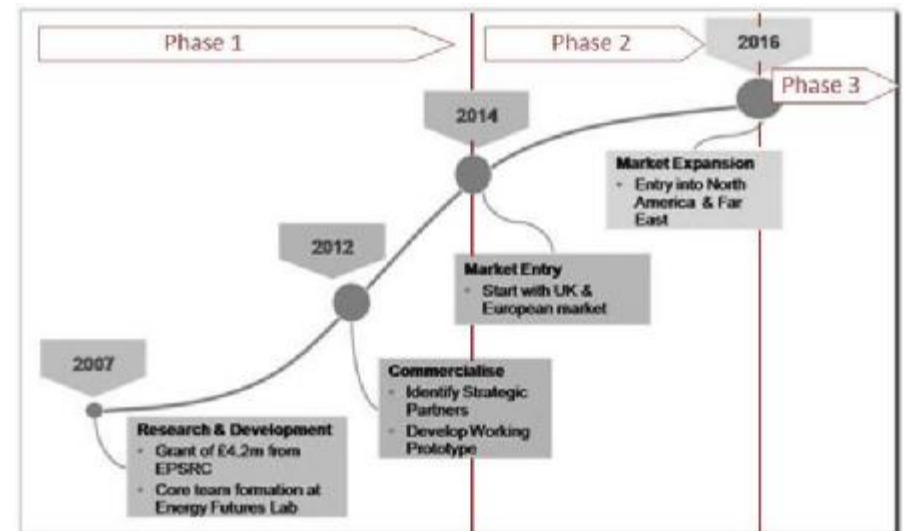
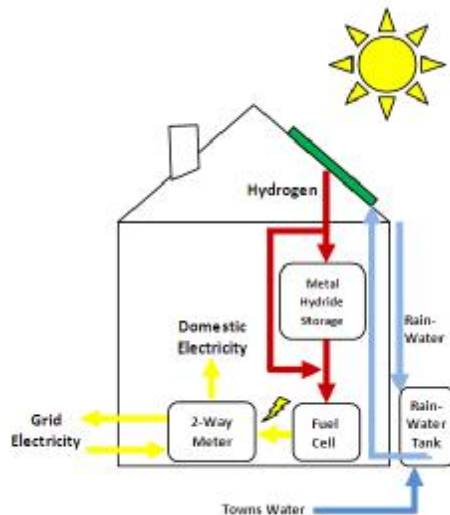
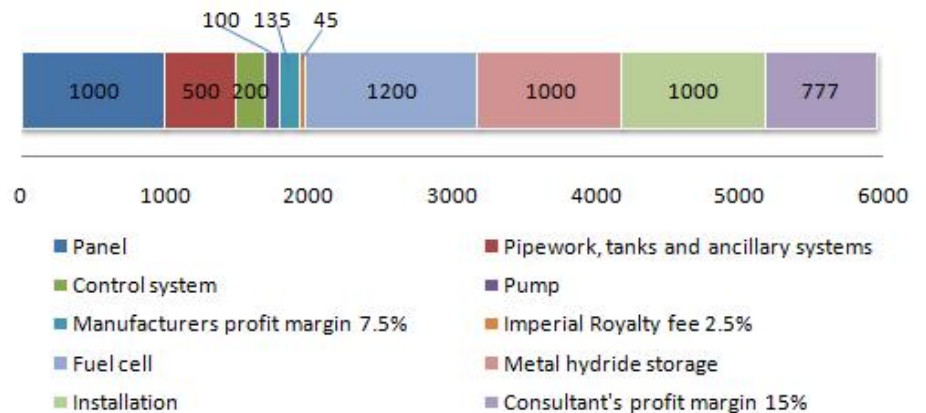
§ Photoelectrolytic  $H_2$ : £2.50/kg

§ Biophotolytic  $H_2$ : £5.00/kg;

### § Concurrent development of materials and systems !

§ Combined with fuel cell operation

§ Distributed market



## 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<sub>2</sub> 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*



# Solar - Hydrogen Efficiency

q New generation Stirling Energy Systems – Suncatcher

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

$$h_{\text{solar-H}_2} = 31.25\% \cdot 80\% (h_{\text{electrolyser}}) = 25\%$$

q New world record triple junction PV – Spectrolab

$$h_{\text{solar-H}_2} = 41.6\% \cdot 80\% (h_{\text{electrolyser}}) = 33.3\%$$

q Polycrystalline Si – Suntech

$$h_{\text{solar-H}_2} = 15.4\% \cdot 80\% (h_{\text{electrolyser}}) = 12.3\%$$

q Thermal Dissociation (glow discharge) – H-Ion

$$h_{\text{solar-H}_2} = 2.1\%$$

q Direct Solar - Hydrogen (photocathode) – NREL

$$h_{\text{solar-H}_2} = 12.4\%$$

q Direct Solar – Hydrogen (photoanode) –  $\text{Fe}_2\text{O}_3$

$$h_{\text{solar-H}_2} = \text{ca. } 10\% \text{ (theoretical } 32\%)$$

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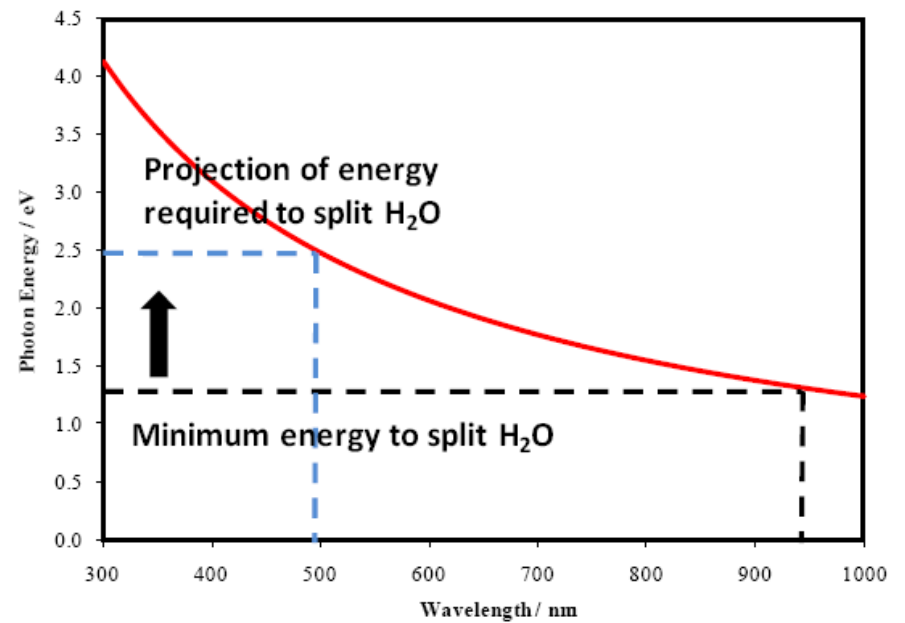
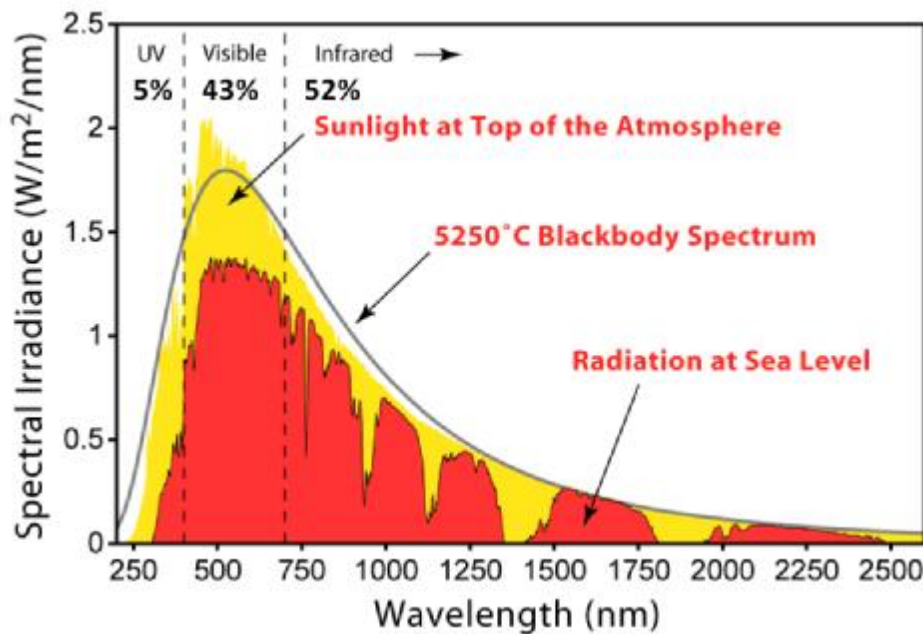
$h_{\text{electrolyser}} = 80\%$  only valid  
for very large systems at low  
current density; domestic  
systems ~ 40-50%

without electrolyzer

Long term  
NREL goal = 25%

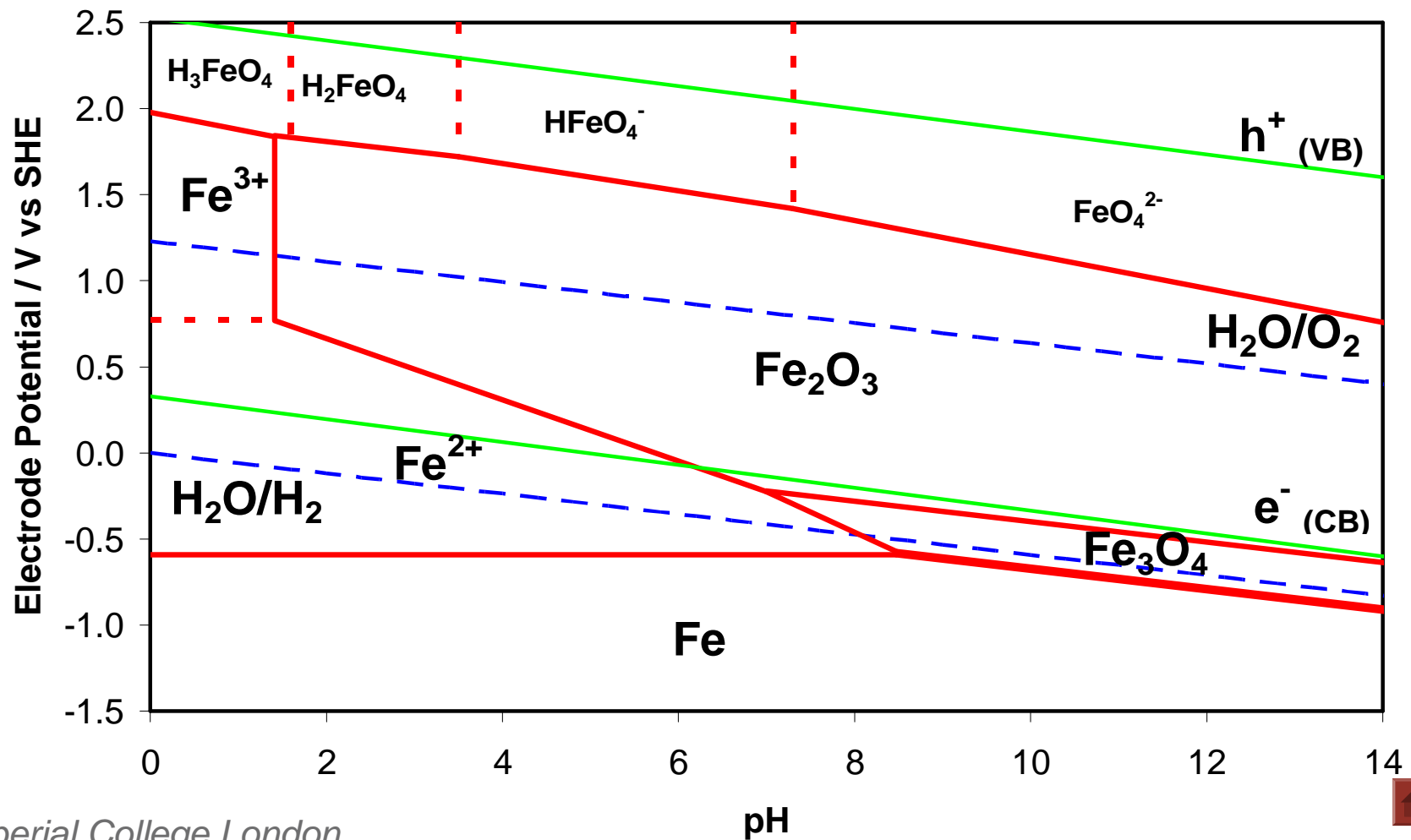


# Materials Requirements



Dios, A.C.d. *Chemistry of the Environment (Greenhouse Effect)*. Available from: <http://bouman.chem.georgetown.edu/s02/lect23/lect23green.html>.

# Materials Requirements



# Simulation and System Integration

