Breakout Session I
Photon Capture &
Charge Separation B

Wednesday, October 21, 2009
Solar Fuels by Photoelectrochemistry (PEC)

Zhebo Chen, Thomas F. Jaramillo
Stanford University
PEC processes, materials, and challenges

Many materials “issues” to consider...

- Absorbance........... dictated by bandgap → 1.23 eV < $E_g$ < 2.5 eV
- Charge Transport... dictated by crystallinity, doping, and morphology
- Band Structure Energetics.... sufficient to split water ($E_g > 1.23$ eV) and must have appropriate redox potentials for $H_2$ & $O_2$ evolution
- Surface electrocatalysis... must maximize interfacial charge transfer.
- Stability, Cost, Non-toxicity.


Nowotny, J.; Sorrell, C.C.; Bak T.; Sheppard, L.R. Solar Energy 2005, 78, 593-602
What are the most promising approaches to high efficiency photon energy capture that use earth-abundant elements? You should consider both efficiency (i.e. photon energy in to useable energy out) as well as deployability (resistant to photobleaching, oxygen degradation, water sensitivity, catalyst poisoning, etc).

There is not widespread agreement on the best assembly of components for artificial direct solar water splitting.

That means it is difficult to identify a “virtual device” target for e.g. water splitting.

Whatever the target, it must absorb visible light, separate charge long enough for using them in catalytic reactions to oxidize water and reduce protons.

The “comparison” of any direct solar system is to make H2 by water hydrolysis using electrical energy from photovoltaics. H2 is a high-value feedstock.

Can we do the light absorption and charge separation part artificially as well as biological systems do it?

Do we make a “simple” fuel as input to selective biofuels generation of higher value chemicals. It’s hard to go beyond C1 products artificially.
What are the most promising energy outputs from artificial photon capturing systems? Here, “most promising” means both highest efficiency (i.e. fraction of photon energy in delivered as useable energy out) and most likely to be integrated with a biological system.

Artificial approach can use p-type semiconductor photocathode to reduce CO2 (Bocarsley).

Can also make higher hydrocarbons with semiconductors with large overpotential.

It is not clear how to couple to biological system apart from some intermediate solar-produced fuel.

Maybe look at the reverse process: engineer a cell to emulate a semiconductor junction as in PV systems. Separate the band gaps of PSI and PSII to use blue light.

Is an artificial or hybrid artificial-biological potentially realizable in a 5-year time horizon?