Energy optimization and the design of photosynthesis

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B10NUMB3R5

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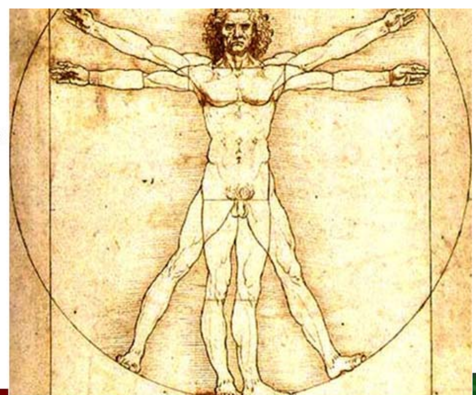
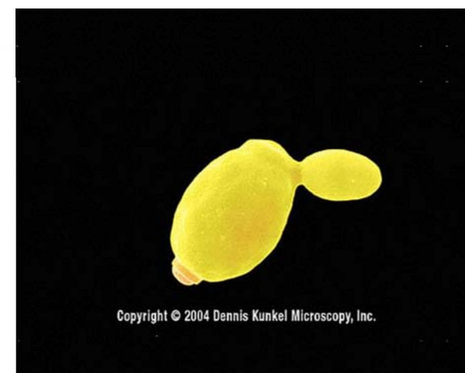
Total number of taste buds: 10,000
Weight of skin: 4.1 Kg
Average time between blinks: 2.8 Sec
Cell divisions in a life-time: 10^17
Abundance of p53: ~160000
Average brain weight: ~1350g
Eye blink duration: .1-.4 seconds
Diameter of erythrocytes: 7.5µm



Median cell (n) vol: 42 micron^3
Number of ribosomes: 200,000
Nucleus volume: 7% of cell
mRNA out of total RNA: 5%
mRNA in cell: 15,000
Nuclear/Cell volume ratio: 0.07
Cell diameter: 5µm
RNA to DNA ratio: 50



Cells in an adult male: 1031
Generation time: 4 days
Number of genes: 20621
Eggs laid during lifetime: 300
Size of Genome: 100291840bp
Life span: 2-3 weeks
Run speed at 20°C: .129mm/sec
Cells in hatched larvae: 556

ATP to make one cell: 55 billion
Volume occupied by RNA: 6 Percent
Number of tRNA/cell: 200,000
Speed: 50 micron/sec
Ribosomes: ~3000
Proteins: 3.6x10^6
Translation rate: 20aa/sec
Volume occupied by water: 70%

How long does it take a protein to diffuse from one end of prochlorococcus to the other?

A) ~100 microsec

B) ~10 msec

C) ~1 sec

D) ~1 minute

How many mRNA are in a prochlorococcus cell?

A) ~1,000

B) ~10,000

C) ~100,000

D) ~1,000,000

How much does a post-doc make per year?

A) $4,000

B) $40,000

C) $400,000

D) $4,000,000

At what rate does a chlorophyll pigment absorbs a photon under full sun illumination?

A) Every picosecond

B) Every nanosecond

B) Every microsecond

D) Every second

Systems biology requires a new tool

- In systems biology we try to go from a **qualitative** to a **quantitative** understanding of biology
- But where would the numbers come from?
- Currently searching the literature for numbers is ***very*** time-consuming and frustrating

BioNumbers – the database of useful biological numbers

- bioNumbers will enable you to find any useful biological number in a minute with full reference
- a collaborative community (wiki) effort
- Volumes, Concentrations, absolute numbers, rates, fluxes and much more
- All entries contain a reference to data source.
- Users can contribute, edit and comment
- Currently over 1500 properties at www.bionumbers.org

Up and running at www.bioNumbers.org

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More details on BioNumbers can be found at http://openwetware.org/wiki/BioNumbers. Also check out: bioNumbers clip .

Welcome to BioNumbers

Welcome to the beta version of BioNumbers!

Bionumbers is a collaborative community effort to establish a database of useful biological numbers. Search for a value you need for your research or out of curiosity. Enter Bionumbers that you want to keep track of and help others on the way. As an easily searchable and permanent database, Bionumbers is superior to napkins, post-its, and notebooks. Your colleagues will benefit from your numbers and you from theirs.

The Bionumbers database contains 1437 numbers, and it's growing every day!
More details and future directions for BioNumbers can be found at http://openwetware.org/wiki/BioNumbers.
We welcome all suggestions to improving Bionumbers. Please send suggestions to bioNumbers@gmail.com.

Best wishes,
Ron Milo, Paul Jorgensen, Michael Springer & Griffin Weber
Departments of Systems Biology & Information Technology
Harvard Medical School

Find Terms:
e.g., ribosome, p53, glucose, CO2
Organism: (all)

search reset

Below are 10 random bionumbers. Click a row for more details

ID	Property	Organism	Value	Range	Units
100955	Kcat values of UDPG pyrophosphorylase in E.coli	Bacteria Escherichia coli	21600		1/min
101317	asparagine pool size	Bacteria Escherichia coli	2.02	+-.46	umol/g
100565	ATP demand for urea synthesis in hepatocyte cell as percent of total consumption	Turtle	3		Percent
100797	Radius of aorta	Human Homo sapiens	1.5		cm
100025	Average MW of single DNA	Bacteria Escherichia coli	3e+6		kDalton
100238	Leaf area index	Biosphere	4.3		unitless
100758	Beef production efficiency	Unspecified	0	5-10	Percent
100311	Nucleolar rDNA weight	African clawed frog Xenopus laevis	25		pg
100727	Humankind total energy usage in 2005	Generic	1.1e+10		kWatt
101042	Kcat values of F1,6-biphosphatase B in Spinach leaf	Spinach Spinacia oleracea	17400		1/min

Most Popular BioNumbers Most Recent BioNumbers Random BioNumbers

Searching: ribosome

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More details on BioNumbers can be found at http://openwetware.org/wiki/BioNumbers.

Search

Find Terms: ribosome

e.g., ribosomes, p53, transcription

Organism: (all)

search reset

Click a row for more details.

ID	Property	Organism	Value	Range	Units
196	Available ribosomes	Bacteria Escherichia coli	500		nM
92	Average distance between ribosomes on mRNA	Bacteria Escherichia coli	60	41-79	nucleotides
122	Diameter of ribosome	Bacteria Escherichia coli	20		nm
343	Elongation rate of ribosomes in Xenopus laevis stage VI oocytes	African clawed frog Xenopus laevis	3		nucleotides/s
119	MW of ribosome	Bacteria Escherichia coli	2700		kDalton
112	Number of protein types to make ribosome	Bacteria Escherichia coli	55		Unitless
268	Number of ribosomes	Budding yeast Saccharomyces cerevisiae	200000		Unitless
111	Number of ribosomes/cell	Bacteria Escherichia coli	18000		Unitless
113	Number rRNA types to make ribosome	Bacteria Escherichia coli	3		Unitless
253	Percent of total transcription devoted to ribosomal RNA	Yeast	60		Percent
198	Ribosome + RNAn --> Ribosome·RNAn+1	Bacteria Escherichia coli	100		bp/sec
484	Ribosome diameter	Generic	30		nm
483	Ribosome volume	Generic	1.4e-5		um3
396	Ribosomes	African clawed frog Xenopus laevis	10e+11		ribosomes
51	Volume occupied by ribosomes	Bacteria Escherichia coli	8		Percent
123	Volume of ribosome	Bacteria Escherichia coli	4.2e-6		um3

What do you need to do ?

- Use, enjoy and tell others: www.bioNumbers.org

- Add bioNumbers as you read papers - QuickSubmit.

- Tell us what would make you use bioNumbers

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Why are biological systems built the way they are?

- In biology we usually ask (and answer) questions about:
  - **what** are the processes? **how** are they functioning?
  - **who** are the molecular players? **when** and **where** are they expressed?

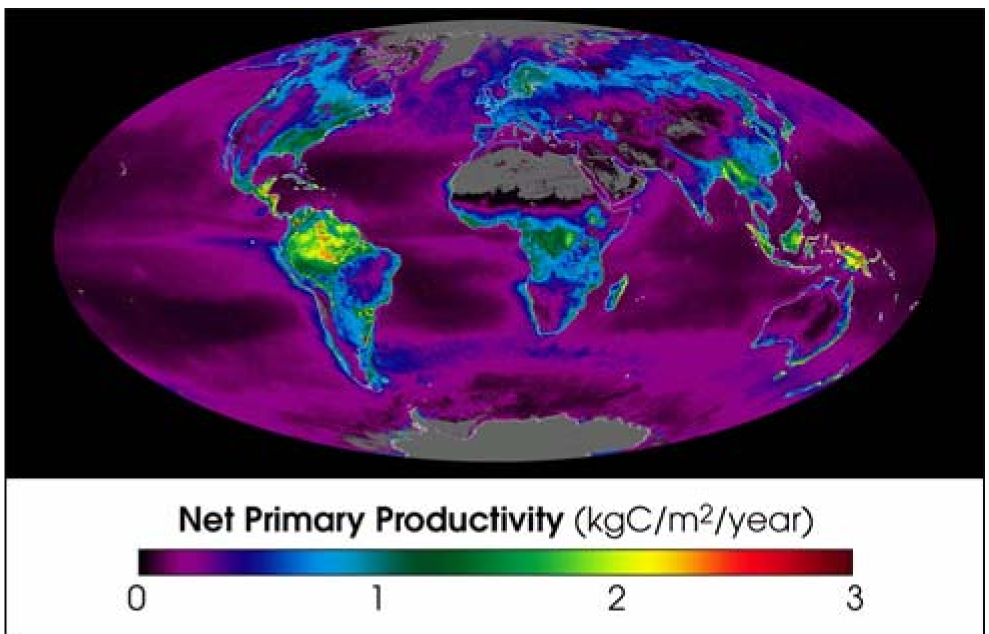
Optimality analysis helps to sharpen our understanding

- Chemotaxis, gene expression, metabolic networks and fluxes, age of reproductive maturity, number of eggs in a clutch, foraging strategy etc. (http://openwetware.org/wiki/Optimality_In_Biology)

- "**Optimization models help us to test our insight into the biological constraints that influence the outcome of evolution. They serve to improve our understanding about adaptations, rather than to demonstrate that natural selection produces optimal solutions.** " (Parker & Maynard-Smith, Nature 1990)

Why is photosynthesis built the way it is? What limits productivity?

- What is the maximal possible productivity?
- Is the limit reached? If not, what limits it and can it be overcome? (nutrients & water, light variability, competition)
- Relevant to biodiversity, biofuels, agriculture



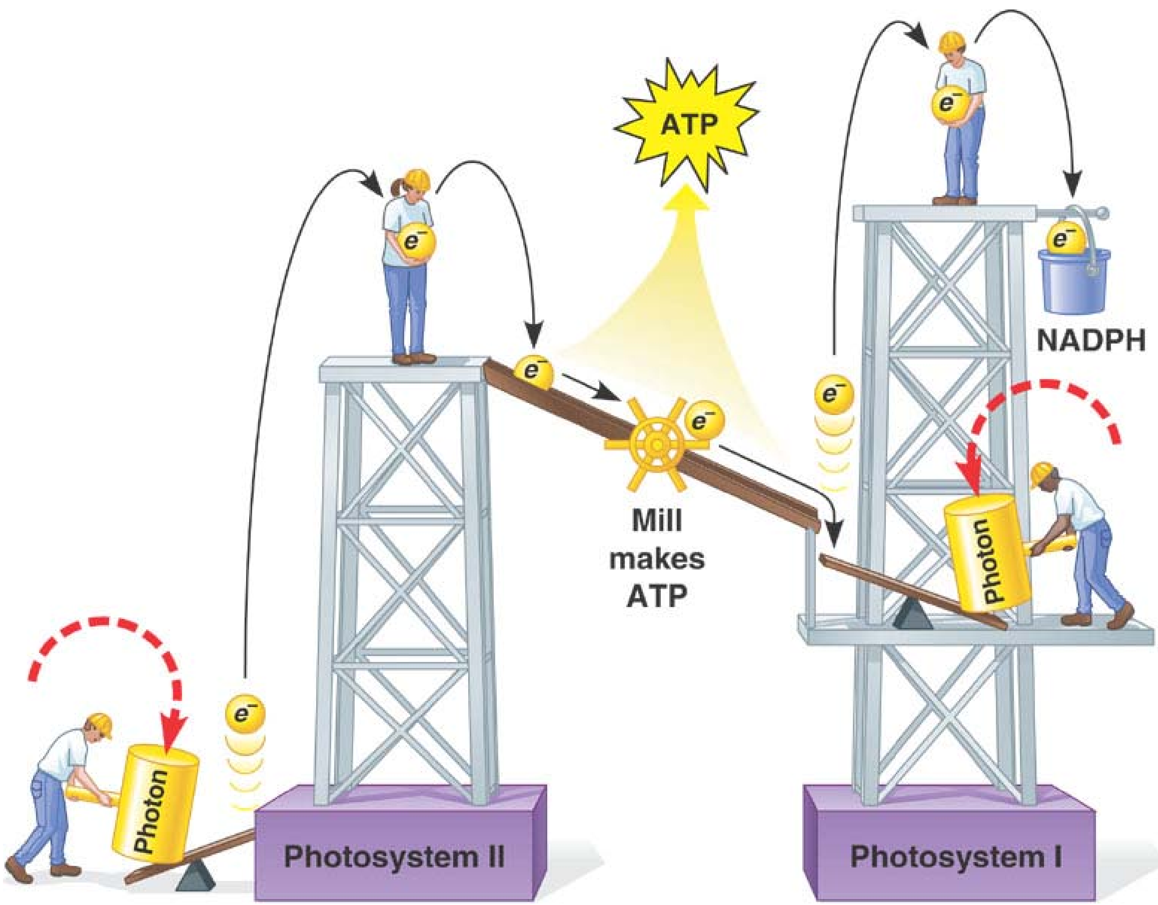
Photosynthesis is the primary biological process on earth

- Converts solar energy into utilizable chemical energy

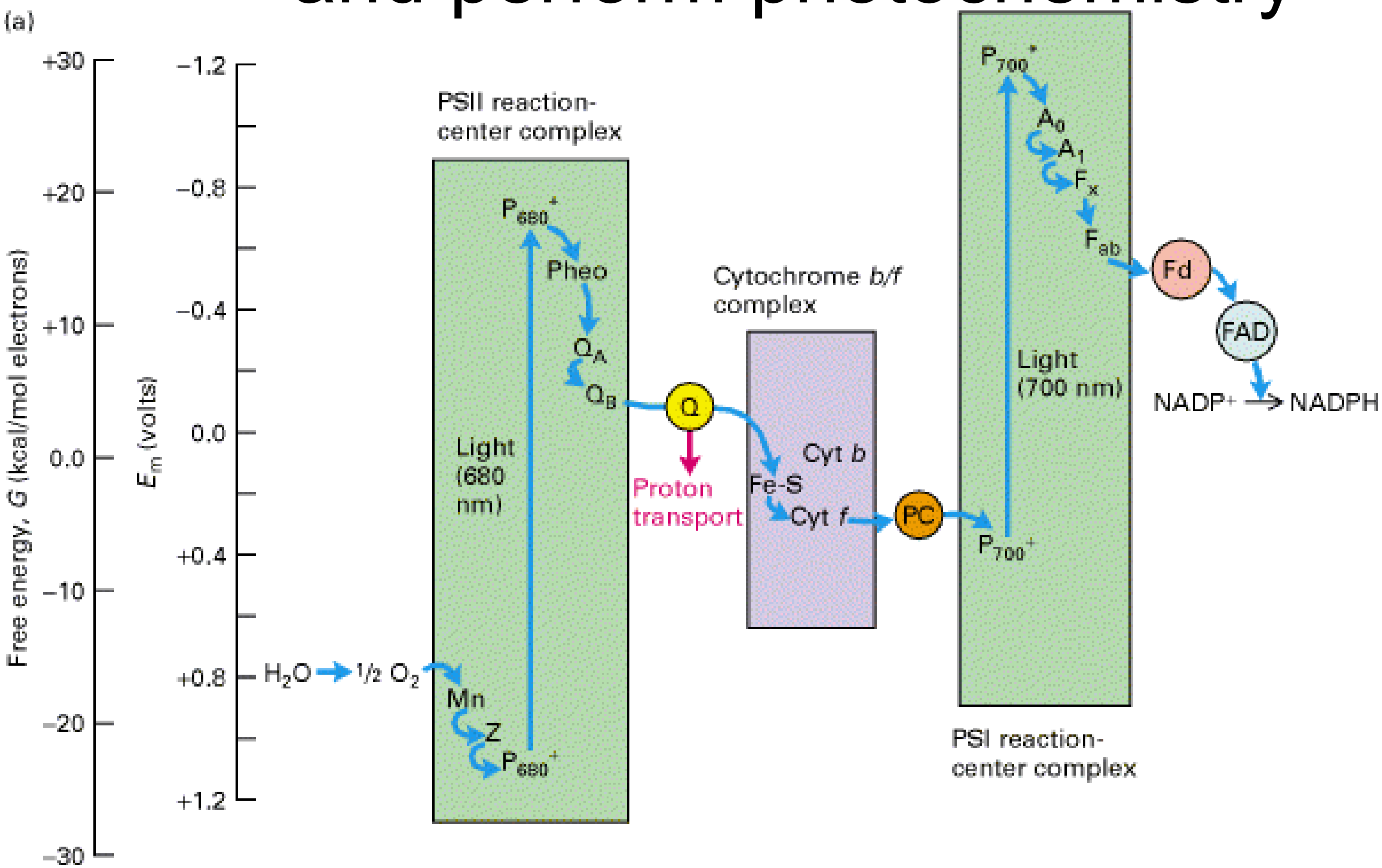
$$6CO_2 + 12\ H_2O + \mathbf{48}\boldsymbol{hv} \longrightarrow \mathbf{C_6H_{12}O_6} + 6O_2 + 6H_2O$$

- Responsible for removal of ~300 billion tons of CO_2 from the atmosphere yearly (humans emit ~30 billion tons from fossil fuels)

Reminder - Turning radiation energy into chemical energy



An intricate machinery to store redox potential and perform photochemistry



Lodish *et.al.*

Conserved in all green plants, algae and cyanobacteria

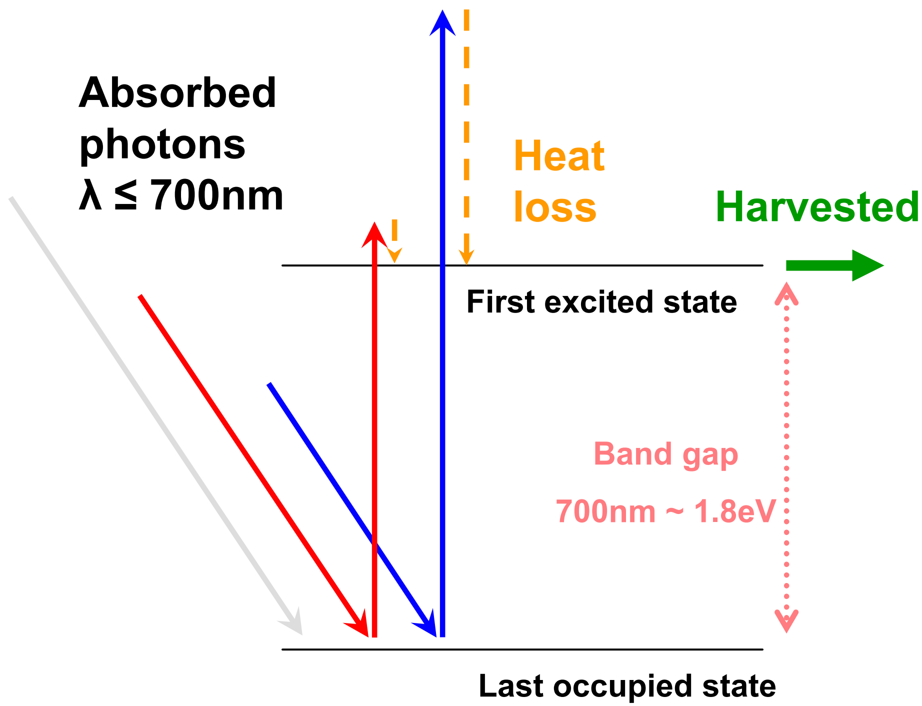
Why does photosynthesis happen at 680-700nm ?

Photosynthesis is an ideal model system for optimality analysis

- Photosynthesis has unique advantages as model system:
  - Input (sun's spectrum) well defined
  - Alternative possible realizations are clear (other wavelengths of operation)
  - Biophysical properties well understood

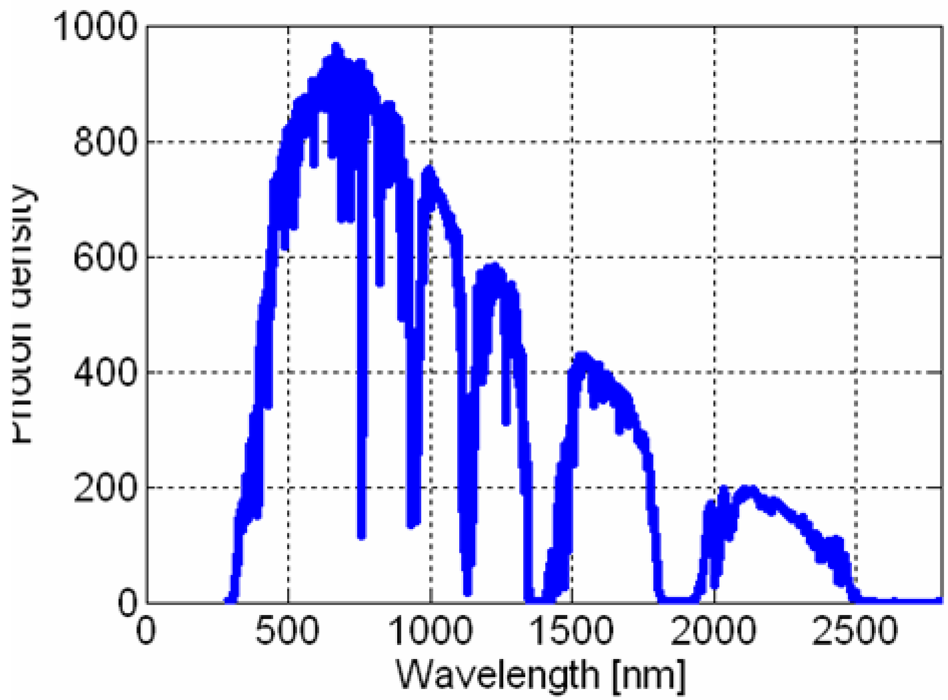
Basic physics of photon harvesting

- Reaction center is a band gap → energy difference
- Photons with less energy than the band gap are not absorbed ("wasted").
- Photons with more energy are absorbed but only the band gap energy is chemically utilized



The sun’s spectrum at sea level is the input for calculating the efficiency

- The physics of photon harvesting implies a tradeoff:
  - Longer wavelength → More photons, less energy per photon
  - Shorter wavelength → Less photons, more energy per photon



700nm

ASTM G173-03e1 Standard Tables for Reference Solar Spectral Irradiances: Direct Normal and Hemispherical on 37° Tilted Surface

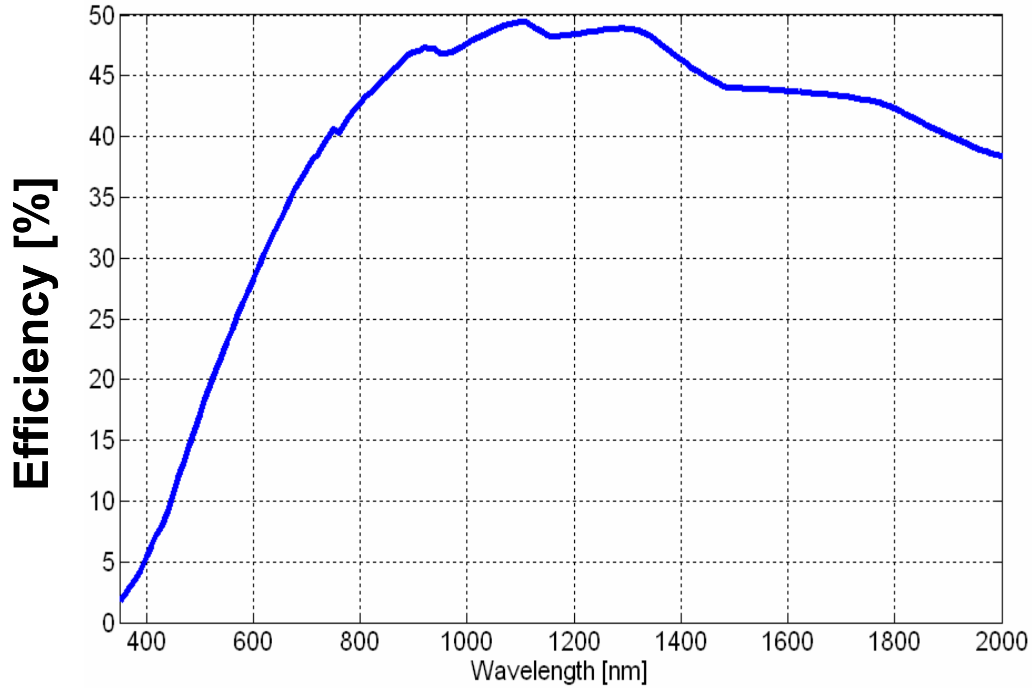
How efficient is the photosystem in utilizing the sun's energy?

- The photosystem utilizes about 37% percent of the sun's energy.
- Can one do any better at a different wavelength?

$$\eta_{light} = \frac{\int_{\lambda=0}^{700nm} I_{sun}(\lambda)E(\lambda = 700nm)d\lambda}{\int_{\lambda=0}^{\infty} I_{sun}(\lambda)E(\lambda)d\lambda} = 0.37$$

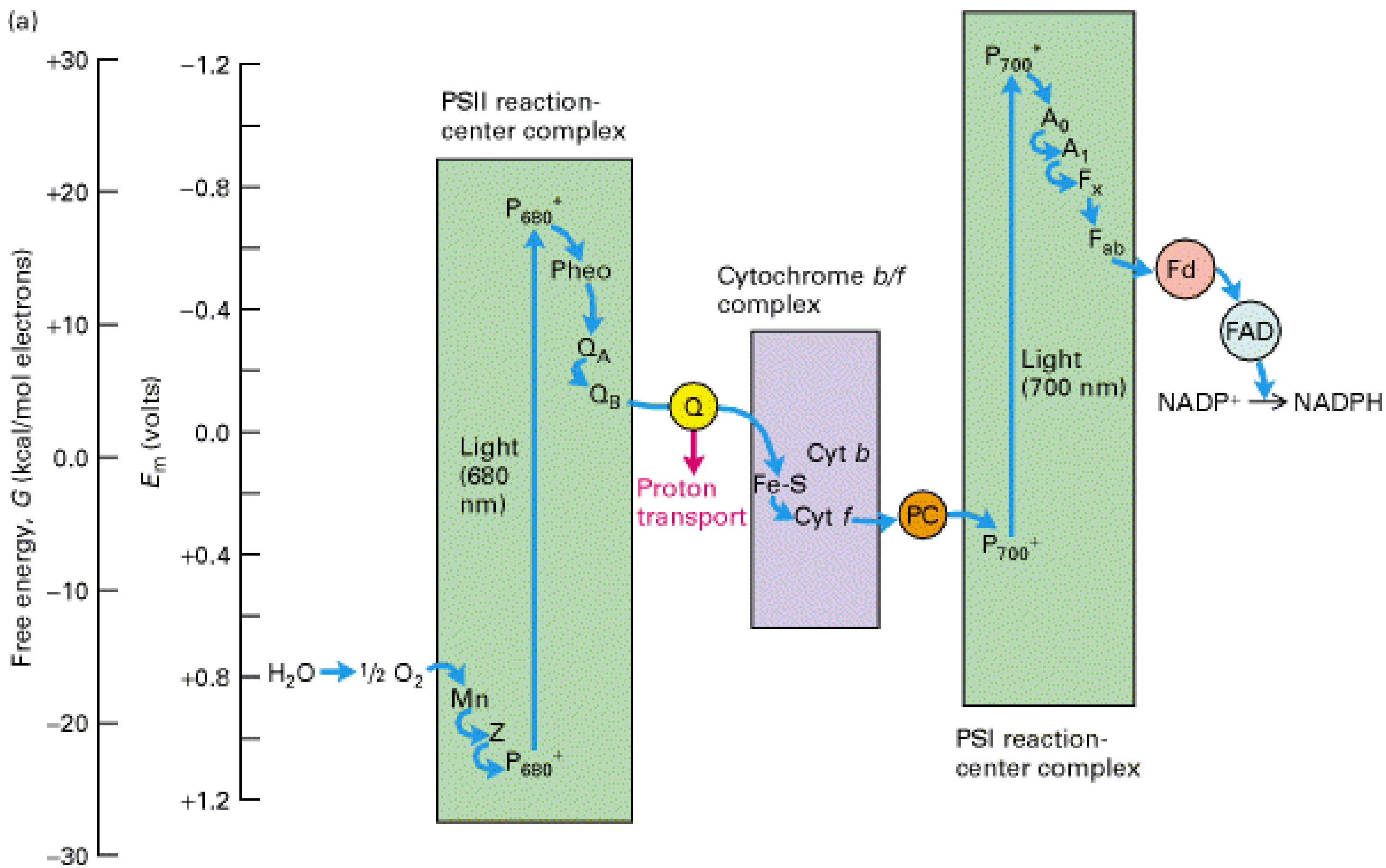
Duysens 1958; Shockley & Queisser, 1961; Ross & Calvin 1967; Knox 1969; Parson 1978; Bolton 1985; Lavergne & Joliot 1996

Efficiency as a function of the reaction center wavelength



- Maximum in the near IR (~1100nm)

Thermo-kinetic cost - energy “wasted” in charge separation, stabilizing against back reactions and insuring reaction rate



All steps are “downhill” – need to “waste” energy

Lodish *et.al.*

Extensive measurements indicate how much energy is wasted

Energy invested:

– E(eV) = hc / λ → (1240/680)+(1240/700) =~ **3.6 eV**

Energy Harvested:

- Redox potential storage:
  – H_2O→1/2 O_2 E_m=0.82V; $NADP^+$→NADPH E_m=-0.32V → 1.14 eV
- ATP formation:
  – 3 H^+ pumped, ~4 protons drive ADP→ATP, ΔG = -50 KJ/Mole → 0.37 eV
- In total **1.5 eV** gained (from two photons)

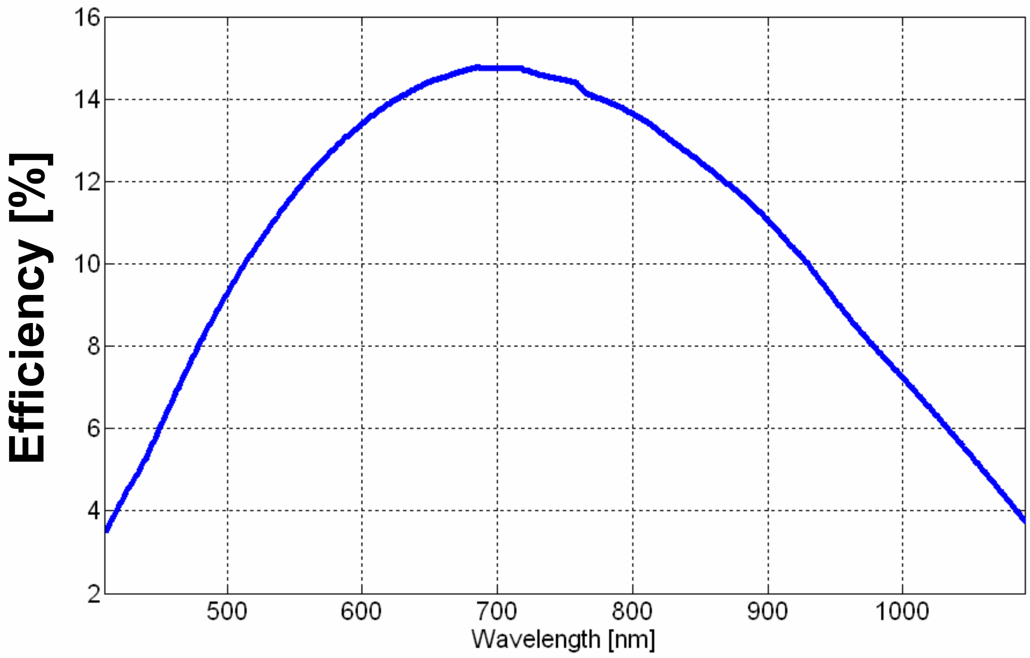
→ Thermo-kinetic cost C_{TK}=(3.6-1.5)/2=**1.05 eV** per photon

I assume this is an inescapable thermo-kinetic cost

Efficiency calculation taking into account the thermo-kinetic cost

$$\eta(\lambda = \lambda_{RC}) = \frac{\int_{\lambda=0}^{\lambda_{RC}} I_{sun}(\lambda)(E(\lambda_{RC}) - C_{TK})d\lambda}{\int_{\lambda=0}^{\infty} I_{sun}(\lambda)E(\lambda)d\lambda}$$

Efficiency of photosystem accounting for charge separation cost



- **Broad maximum in the range 684-716nm**

Assuming that 1.05eV is a constant thermo-kinetic cost necessary for performing the photochemistry

R. Milo, Manuscript in preparation

Suggestion: Wavelength utilized in PSI/II reaction centers maximizes sun energy harvesting given constraints

Alternative formulation

- We are testing our understanding of what shaped photosynthesis band gap energy
- Possible hypothesis:
  - Not optimized for energy
  - Energy optimized, no constraints
  - Energy optimized, constant thermo-kinetic cost constraint
  - Energy optimized, variable thermo-kinetic cost constraint
  - Energy optimized, constant energy harvested constraint

Arising questions

- Analysis for photosynthetic bacteria with other photosystems (purple bacteria, green sulfur bacteria, heliobacteria).
- Effect of water column
- What if the sensitivity if thermo-kinetic cost is not constant ?
- Does energy from photosynthesis ever limits growth?

Summary

- Wavelength utilized in PSI/II reaction centers maximizes sun energy harvesting given constraints
- Energy output was a selection force in shaping the photosynthetic wavelength parameter.
- Future challenges:
  - Investigate the constancy of the thermo-kinetic cost
  - Analyze a framework that incorporates carbon fixation

SOM figures

Examples of things to optimize for

- Reproductive success / Fecundity: The expected number of surviving offspring produced by an individual over a generation time
  - Maximum energy utilization
  - Minimal energy expenditure
  - Accuracy/minimal error rate
  - Robustness
  - Maximal sensitivity
  - Minimal cross talk

Acknowledgements

- ***Marc Kirschner***
- ***Michael Brenner***
- ***Mike Springer***
- ***Eran Bouchbinder***

Some bacteria have different absorption wavelengths → different electron donors - prediction suggests different charge separation cost

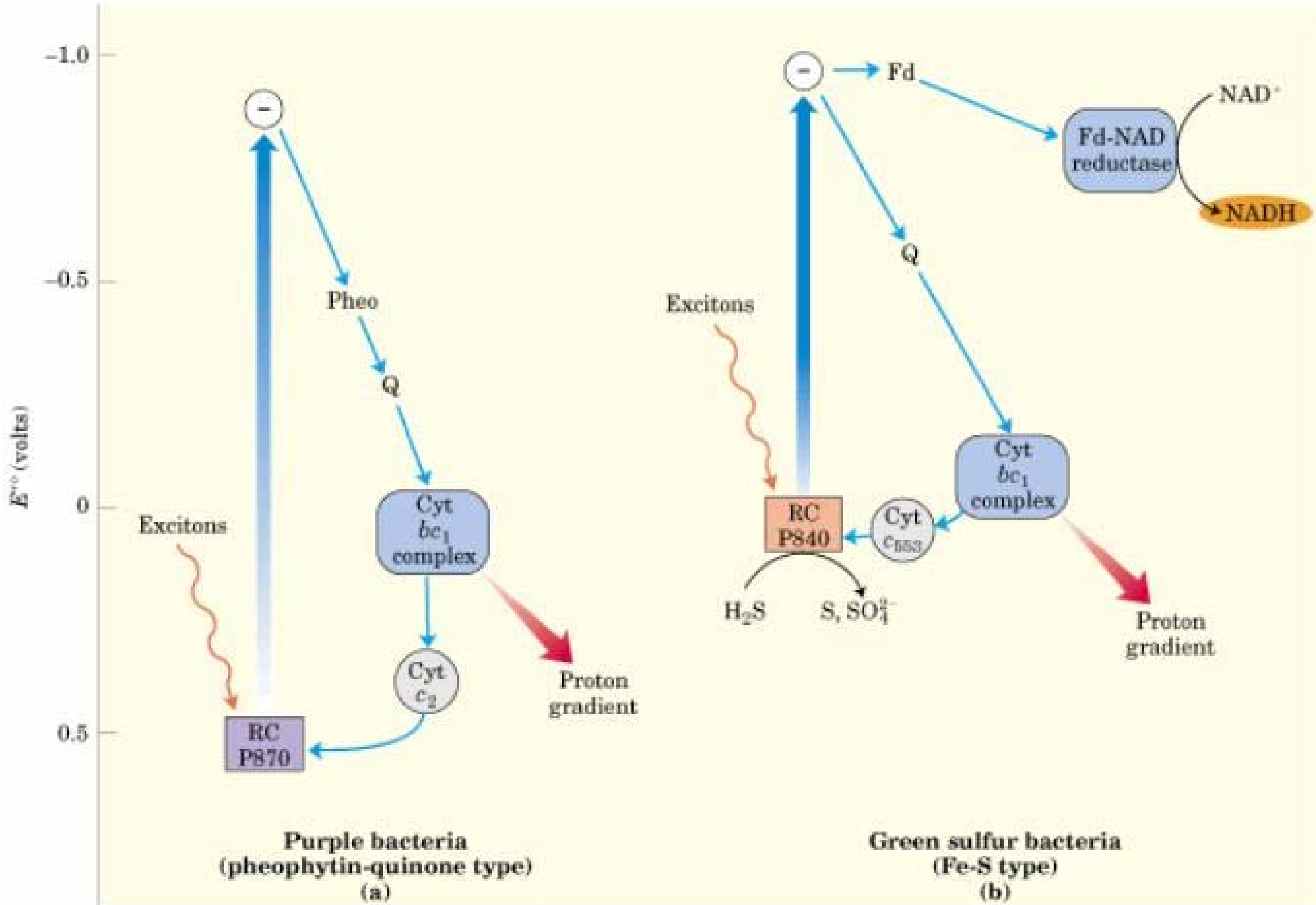
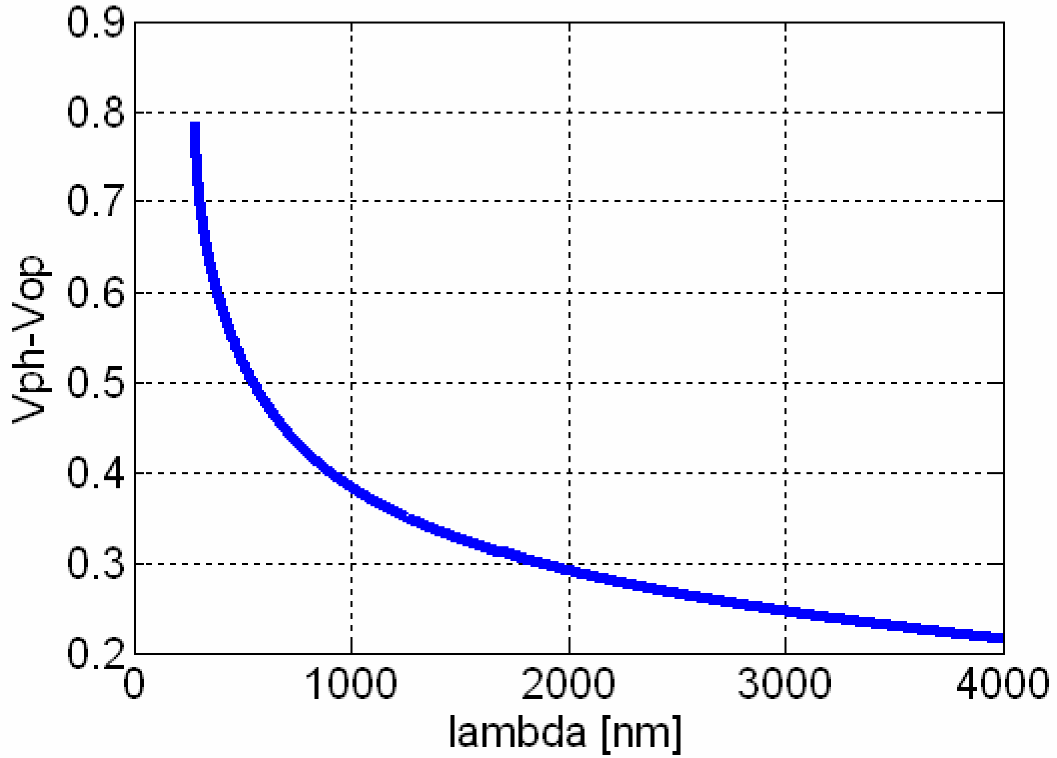


Fig. S1: **SQ or detailed balance limit thermodynamic cost as a function of wavelength.** The associated cost in units of eV. [PSOptimalitySQ1.m]



Effect of effective value of thermodynamic cost on optimal wavelength of the reaction center.

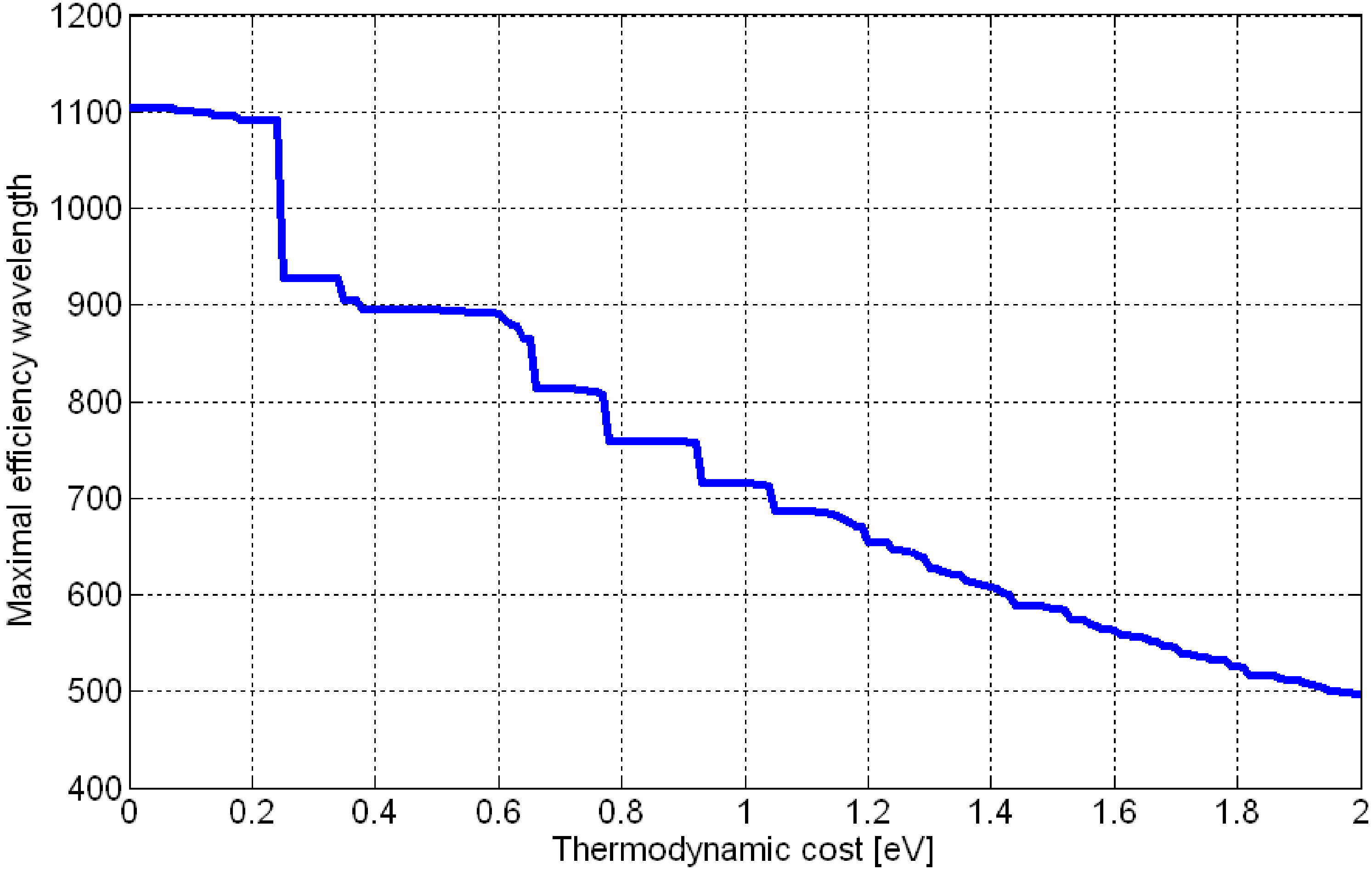


Fig.S2: **Effect of effective value of thermodynamic cost on optimal wavelength of the reaction center.** Assuming [PSOptimalityThermo2.m]

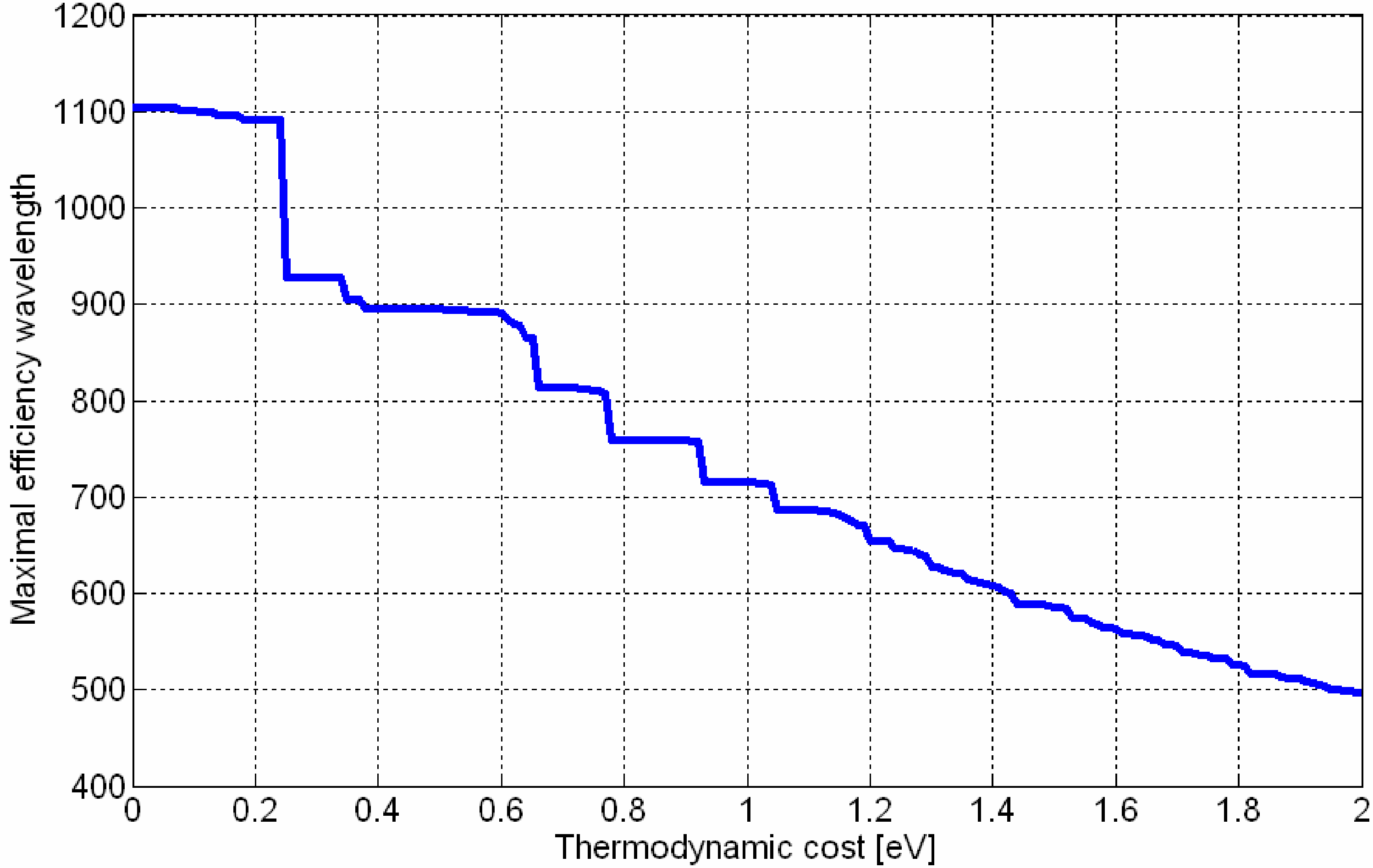


Fig.S3: **Effect of thermodynamic cost dependence on wavelength on optimal wavelength of the reaction center.**
Assuming [PSOptimalityCostslope4.m]

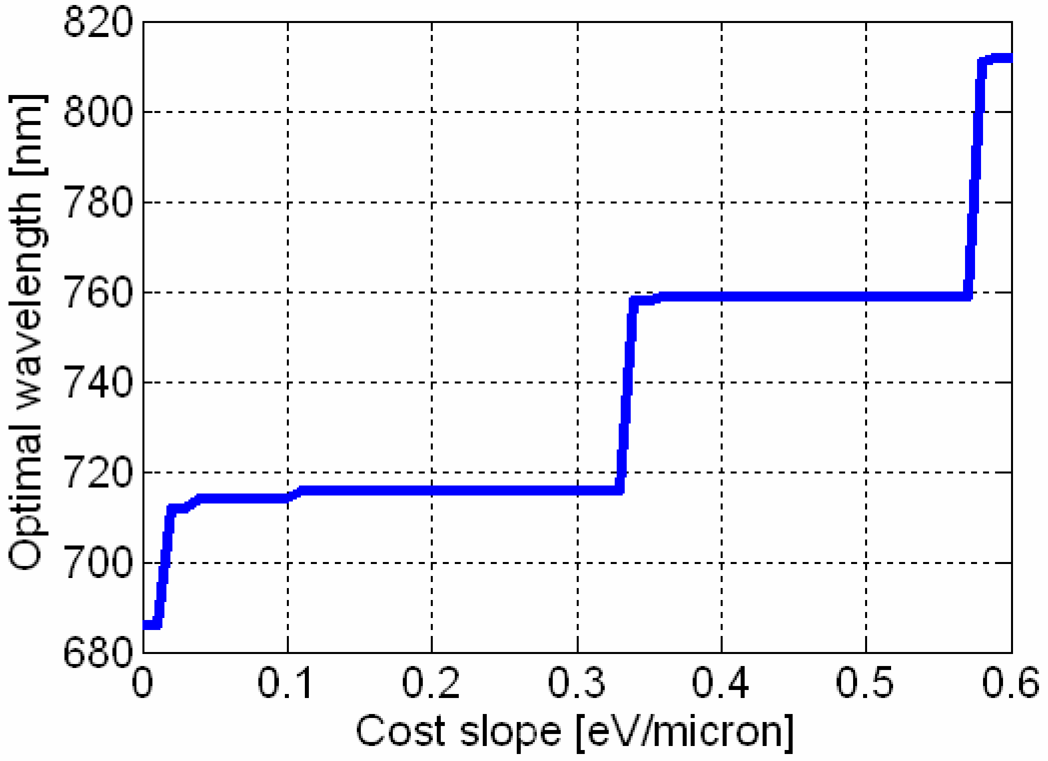


Fig.S4: **The sun's spectrum at sea level for a colder sun as it was 3 billion years ago is the input for calculating the efficiency of photosynthesis.** The physics of photon harvesting implies a tradeoff where a shorter wavelength for the band gap energy will harvest more photons but with less energy per photon. Whereas, longer wavelength will imply that less photons will be harvested but more energy will be gained per photon.[PSOptimalityBB3]

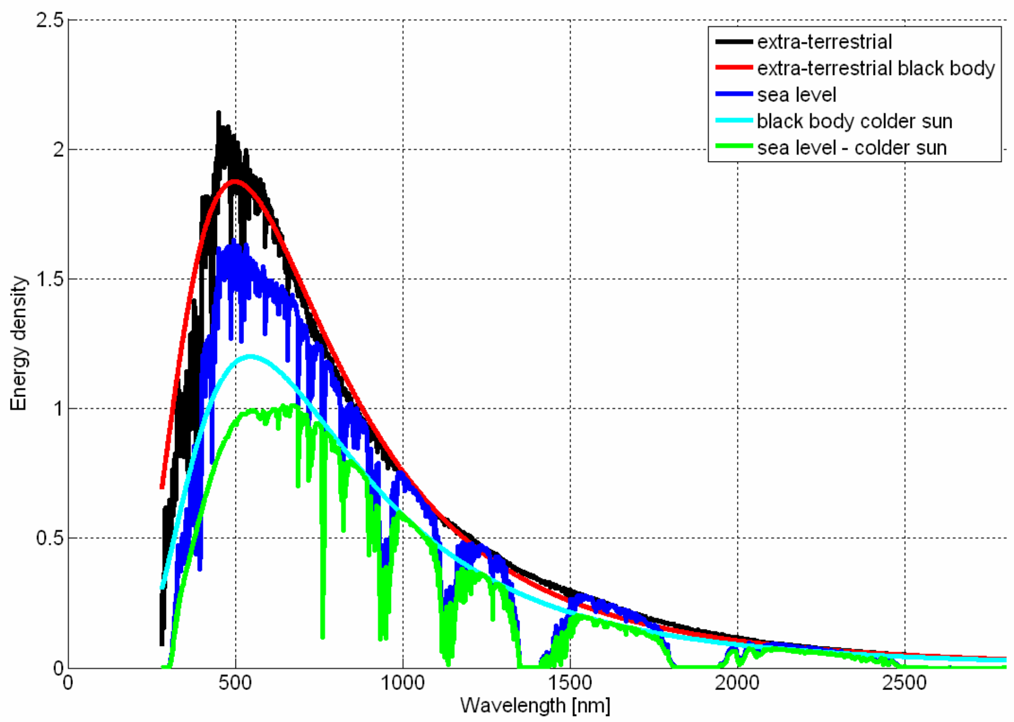


Fig.S5: **Geometrical interpretation of optimality condition.** The condition for maximal harvesting of the sun's spectrum can be understood geometrically. The x axis represents the energy of the band gap in the reaction center and the y axis is the cumulative number of photons with energy larger than the given energy. The area of a rectangle within the curve is proportional to the overall energy harvested. An optimal wavelength for the reaction center is an energy value where the corresponding rectangle will have the largest area (red rectangle). Inclusion of the thermodynamic cost is equivalent to a shifting of the reference point for the area (black dotted vertical line). In this case the optimal energy value has the corresponding green rectangle. [PSOptimalityGeo2.m]

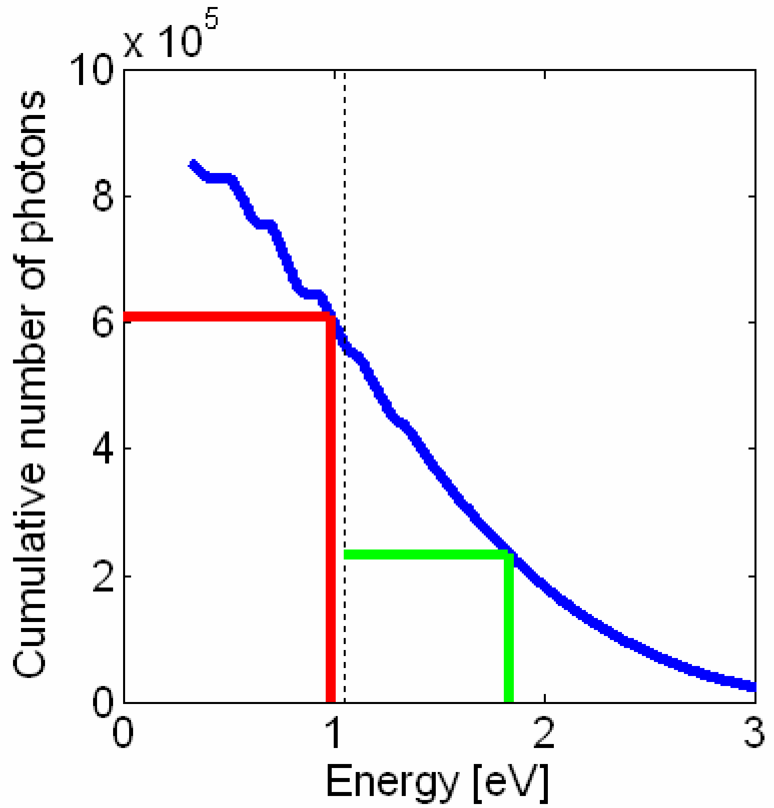


Fig.S6: **Efficiency of photosystem accounting for charge separation cost and assuming a colder sun.** Assuming that 1.05eV is a constant cost necessary for running the energy transformation and that the sun's output is 30% lower than it is today. Maximum efficiency is achieved at 716nm. [PSOptimalityBBColderSun2]

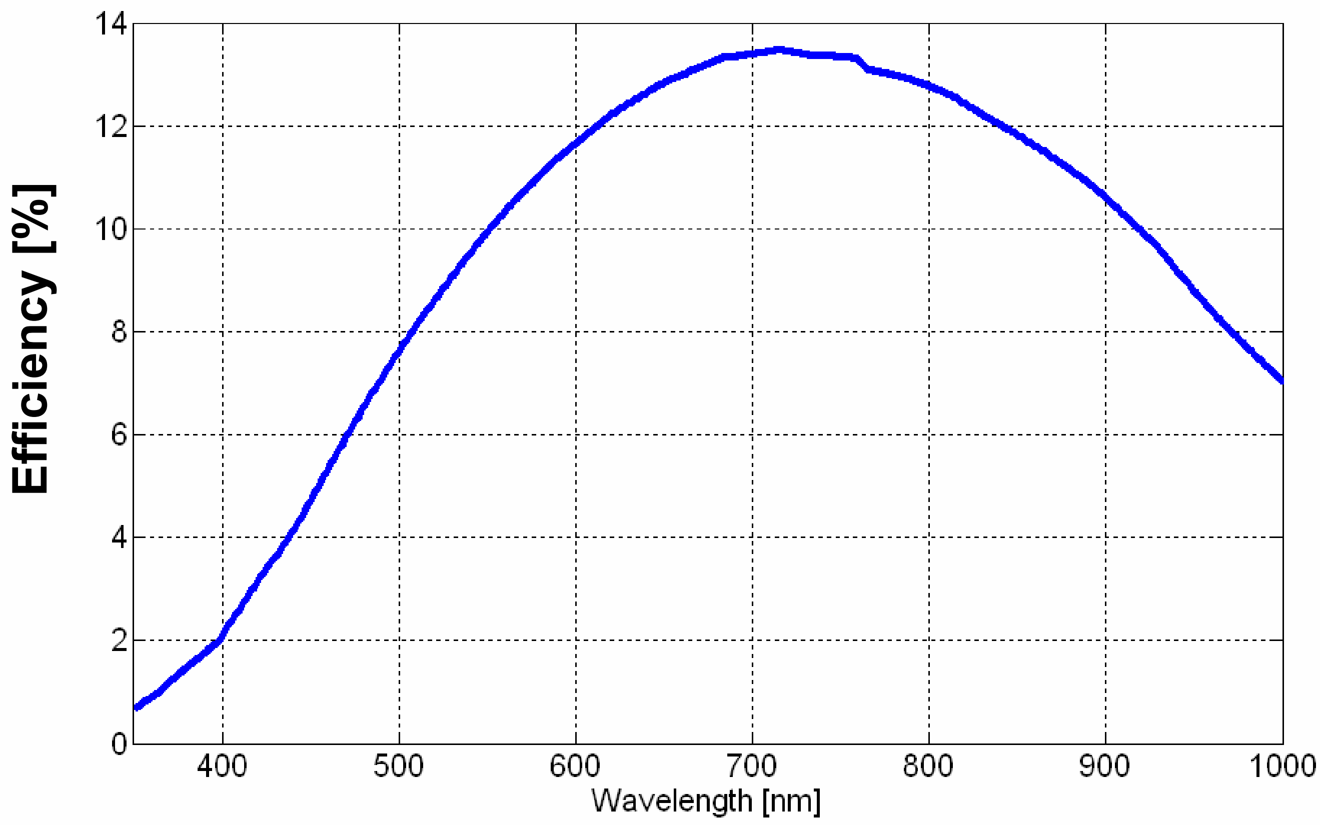


Fig.S7a: **Transmittance as a function of wavelength for pure water.** [PSOptimalityWaterEffectBatch1]

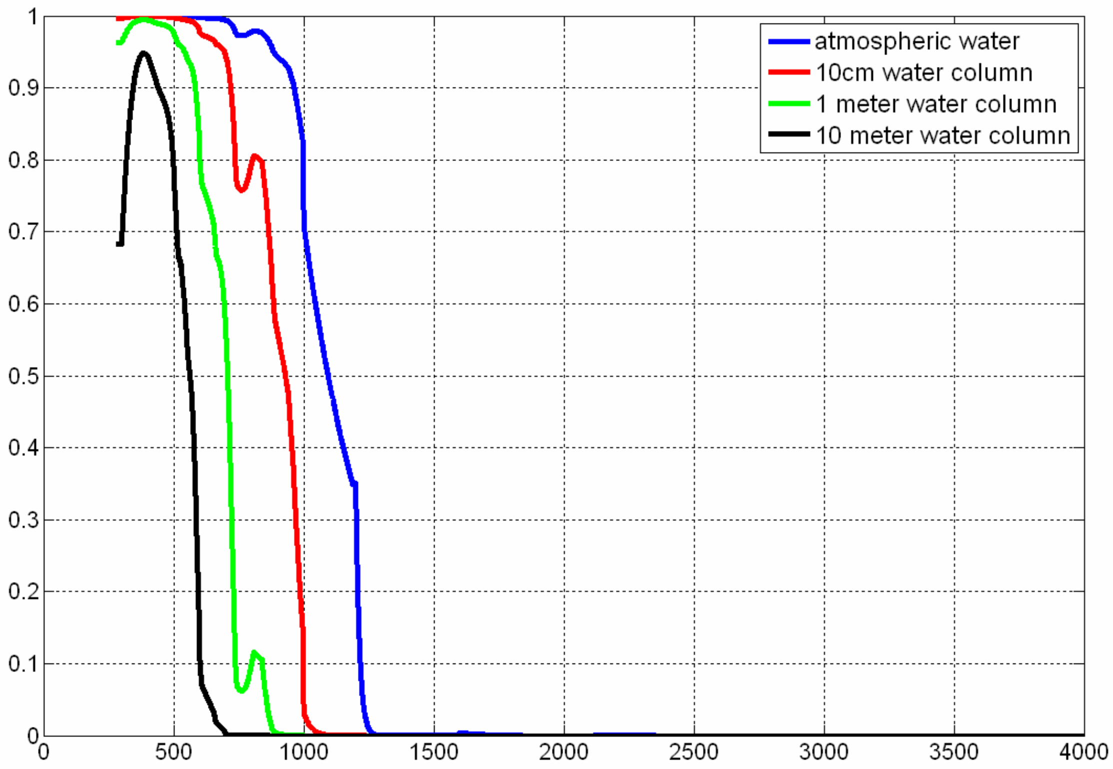


Fig.S7b: **Effect of water absorption on solar spectrum.**
[PSOptimalityWaterEffectBatch1]

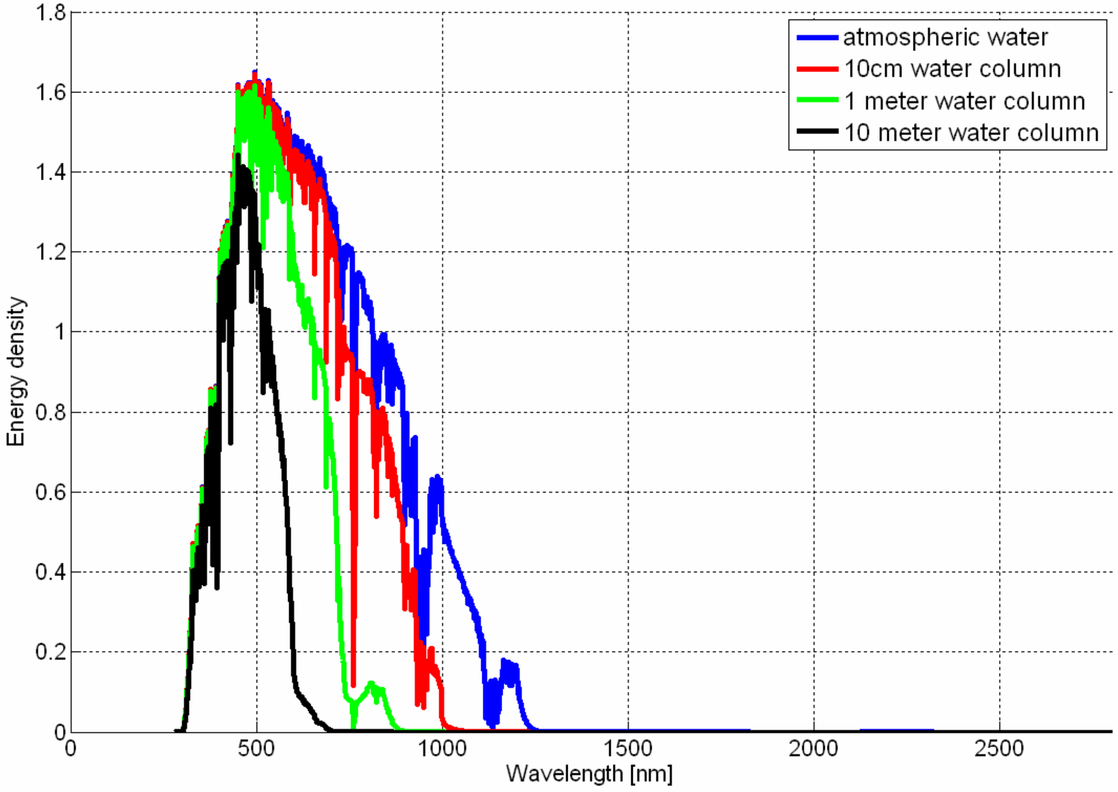


Fig.S7c: **Effect of water column on harvesting efficiency.**
[PSOptimalityWaterEffectBatch2]

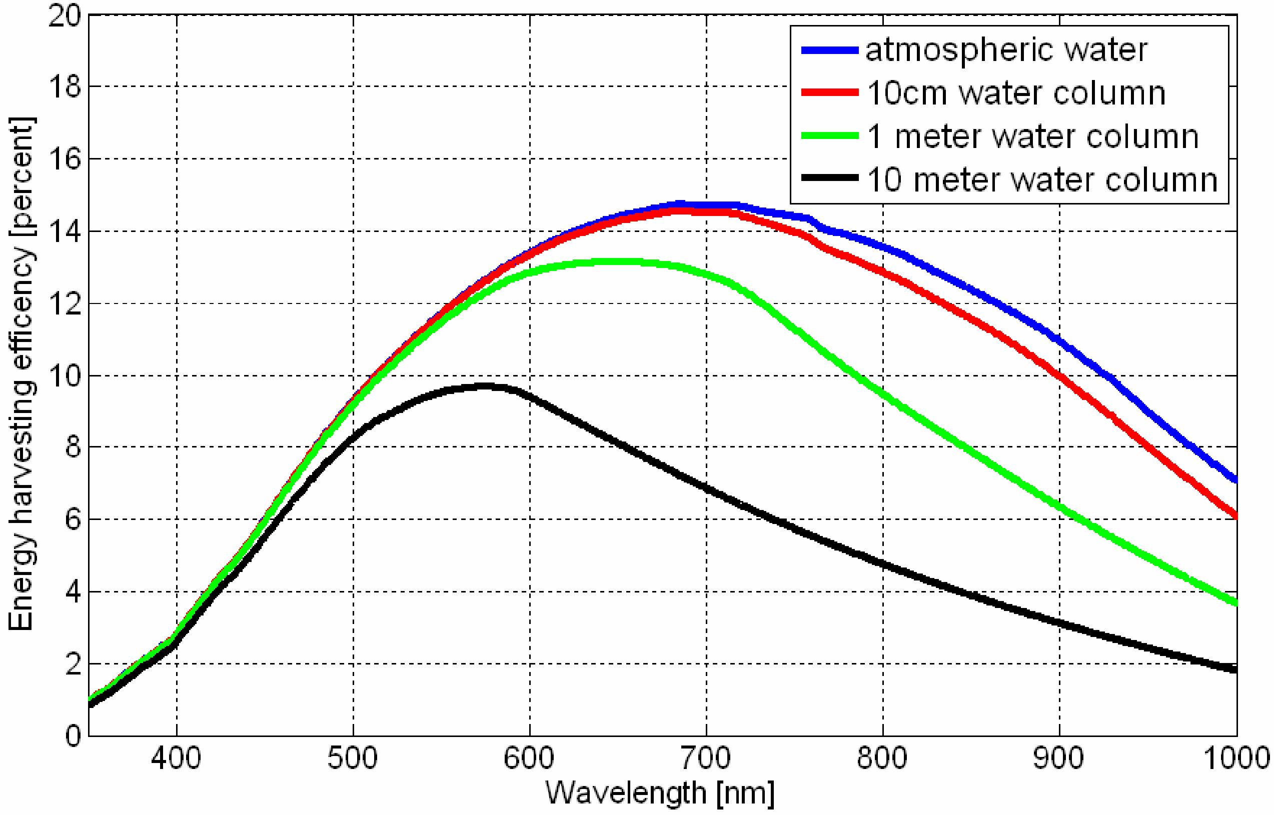
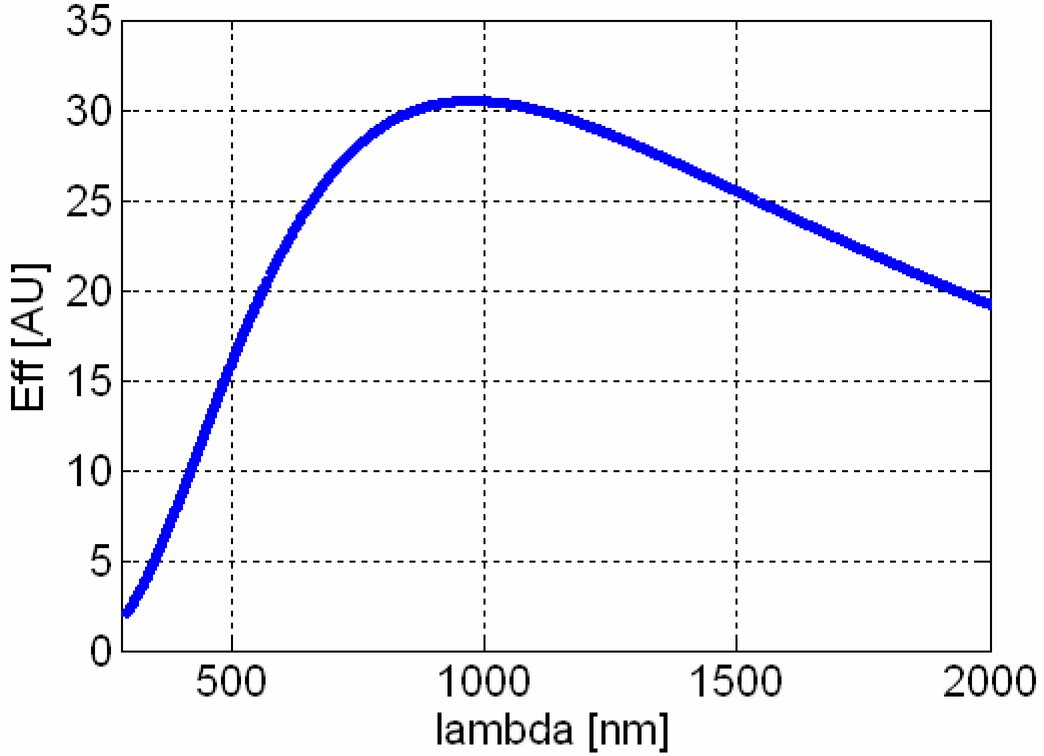


Fig.S8: **SQ or detailed balance limit on efficiency**
[PSOptimalitySQ4.m]



Calculation code using Matlab

```
load sunSpectrum1

lambda=data(:,1);
I_lambda=data(:,2);

numberPhotons=I_lambda.*lambda;

thermodynamicCost=1.2;

% loop through the range of bandgap wavelengths
for lambdaIndex=1:length(lambda),

    % calculate how many photons are absorbed
    photonsHarvested=sum(numberPhotons(1:lambdaIndex));

    % calculate energy per photon in eV
    energyPerPhoton=1280/lambda(lambdaIndex);

    % total energy harvested after deducting the thermodynamic cost
    energyHarvested(lambdaIndex)=photonsHarvested*(energyPerPhoton-thermodynamicCost);

end;

% total energy in the sun spectrum input
totalEnergy=1280*sum(I_lambda);

% Overall efficiency as a function of band gap wavelength
efficiencyVect=100*energyHarvested/totalEnergy;
```

Is there a downstream process that can be made better?

- Low efficiency under full solar flux because too many pigments per reaction center
- More photons absorbed than excited electrons can be processed
- Extra excitation energy is quenched by several mechanisms.
- Decreases overall efficiency at the whole culture level
- Not the selective force in natural settings where water column attenuates light and other organisms compete.

Experimental optimization of yield in the green algae Chlamydomonas

- Melis lab in Berkeley is experimenting with decreasing the antenna size by insertional mutagenesis.
- Efficiency was increased about 5 fold !

Reverse engineering photosynthesis regulation – main uncertainties

- For promoter library we will not be able to see regulation at the post-transcriptional level. Homologous recombination to achieve protein fusions can be performed in PCC6883.
- All strains sequenced, varying levels of annotation.
- Ability to detect reporters over high background of pigments
- Extent of regulation performed post transcriptionally that will be missed in a promoter library
- Functionality of fusion proteins in a fusion library

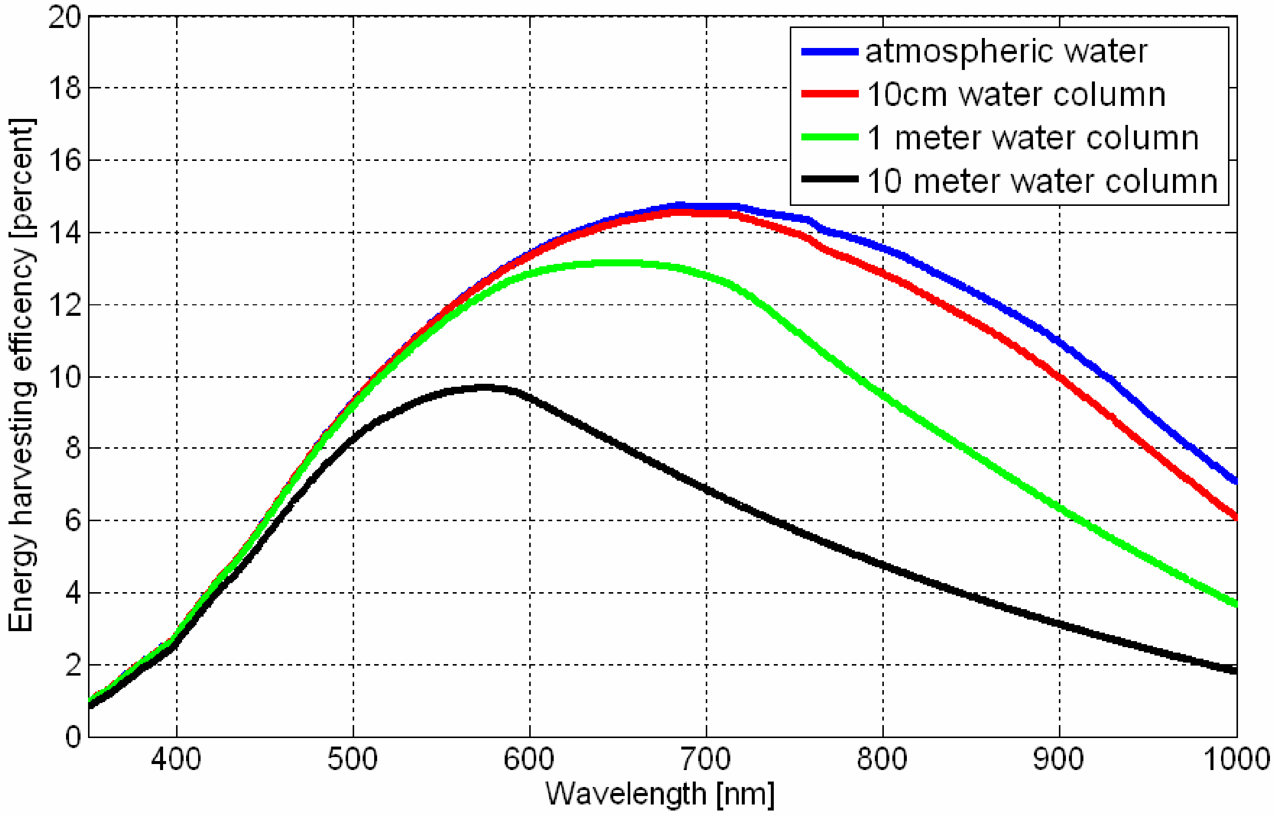
Purple, green-sulfur and helio bacteria use different wavelengths

- 790nm, 840nm and 870nm
- Account for less than 20% of world primary productivity
- Knowledge is more limited in estimating the thermo-kinetic cost
- From what I could gather not at the predicted maximum
- Possible explanations:
  - This analysis is not valid
  - Our knowledge is partial
  - There are other constraints

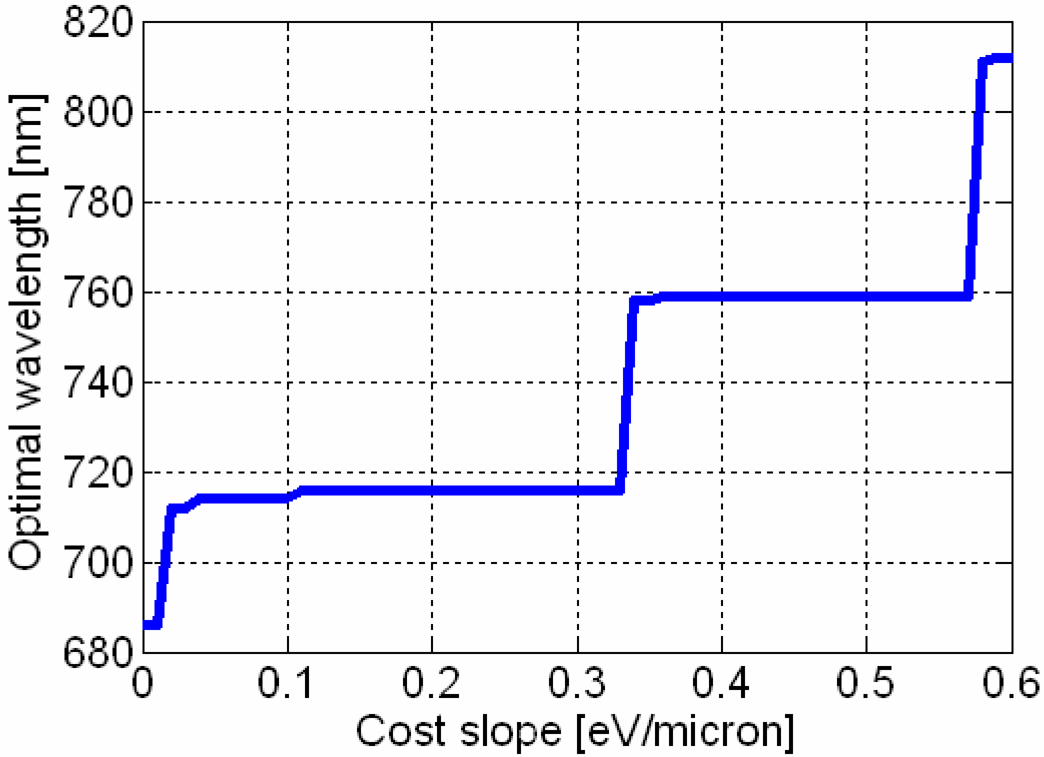
Does energy from photosynthesis ever limits growth?

- Often there is an over abundance of solar energy flux (photo-inhibition)
- Can become limiting from effects of season, time of day, competition, shading etc.
- Arantz, Delucia & Jordan (Ecology 2000, JEB 2000) find that a mutant (atrazine resistance in *Amaranthus hybridus*) that lowers the photosynthetic rate by 20-30% leads to a reduced fitness by about 40%.

Effect of water column on harvesting efficiency



Effect of thermodynamic cost dependence on wavelength on optimal wavelength of the reaction center.



If you think environmental questions are the biggest challenge for 21st century science

What biological system would you most be interested in understanding?