Thermal Radiation Modeling Workshop For SPIE Optics+Photonics 2017

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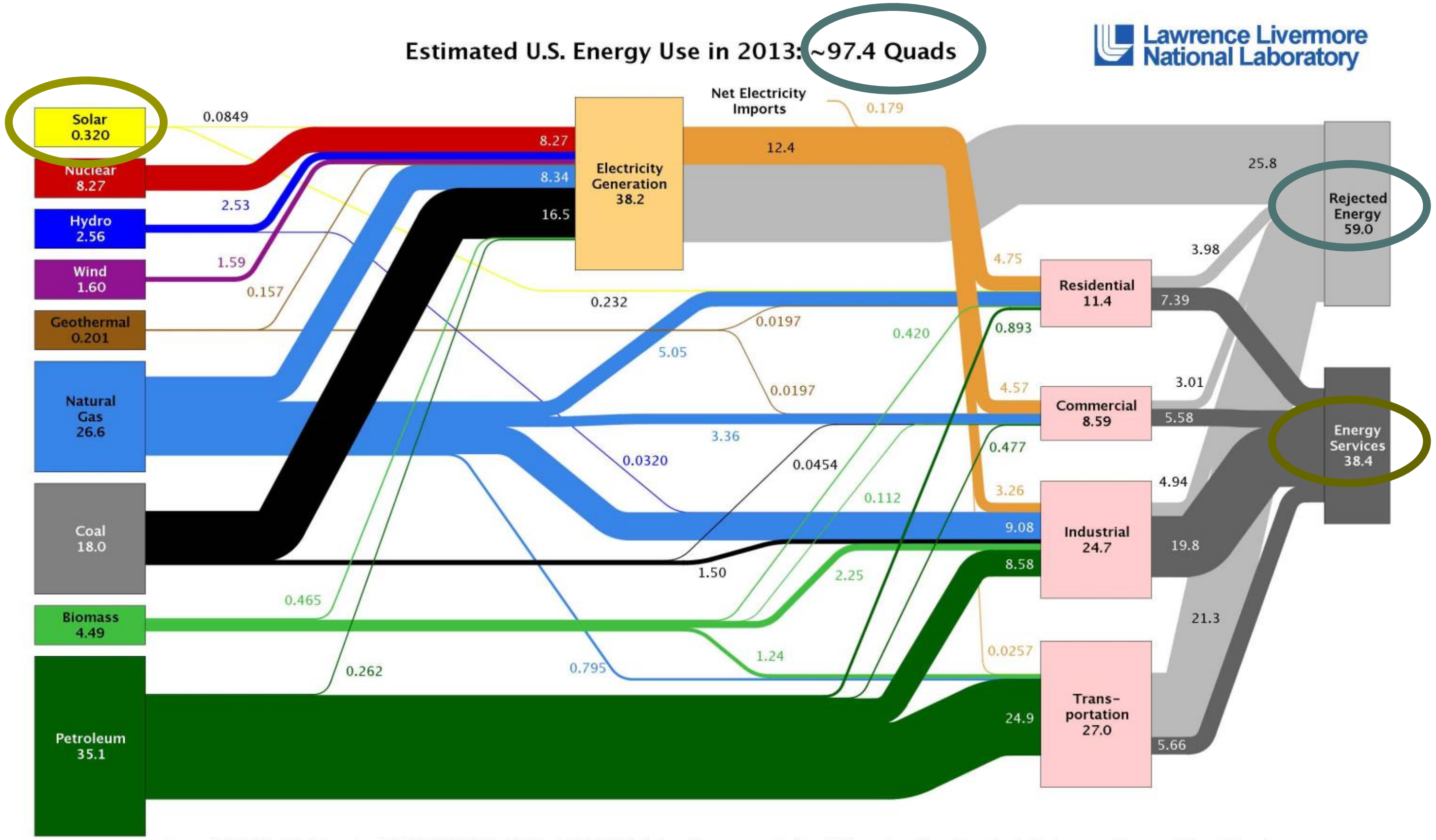
Brief History of Thermal Energy Harvesting

Year	Discovery	Significance	Innovators
1712	Atmospheric Engine	Pumping water out of mines	Thomas Newcomen
1776	Steam Engine	Mechanical workhorse of industrial revolution	James Watt
1870	Kirchoff's law of thermal radiation	Establishing centrality of blackbody in thermal radiation	Gustav Kirchoff
1879	Stefan-Boltzmann law	Calculating total radiated power	Josef Stefan
1900	Planck's law of blackbody radiation	Calculating radiation power spectrum	Max Planck
1956	Thermophotovoltaics	Converting thermal radiation into electricity	Henry Kolm
1960	Laser	Provides intense, monochromatic optical power	Schawlow & Townes
1962	Solar Cell Efficiency Limits	Provided a target for PV and TPV research	Shockley & Queisser
1979	Gallium antimonide cell	Provides suitable bandgap for TPV	Lew Fraas
2014	Photonic radiative cooling	Provides nearly ideal radiative cooling	Shanhui Fan

Key Concepts from Prior Research

- Carnot efficiency of heat engines
- Planck blackbody limit: centrality of blackbody in thermal radiation
- Shockley-Queisser limit of photovoltaics
- Additional losses at every step in practice

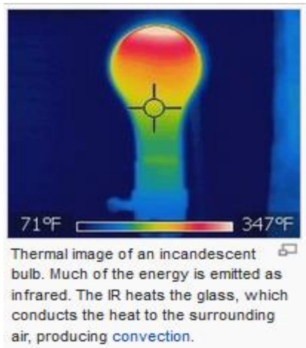
Energy Landscape Today



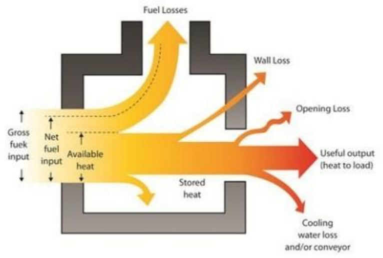
Source: LLNL 2014. Data is based on DOE/EIA-0035(2014-03), March, 2014. If this information or a reproduction of it is used, credit must be given to the Lawrence Livermore National Laboratory and the Department of Energy, under whose auspices the work was performed. Distributed electricity represents only retail electricity sales and does not include self-generation. EIA reports consumption of renewable resources (i.e., hydro, wind, geothermal and solar) for electricity in BTU-equivalent values by assuming a typical fossil fuel plant "heat rate." The efficiency of electricity production is calculated as the total retail electricity delivered divided by the primary energy input into electricity generation. End use efficiency is estimated as 65% for the residential and commercial sectors 80% for the industrial sector, and 21% for the transportation sector. Totals may not equal sum of components due to independent rounding. LLNL-MI-410527

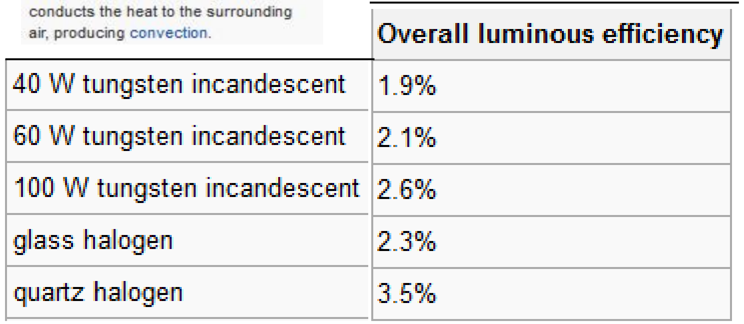
61% of raw energy wasted in 2013!

Too much parasitic loss in commonly used devices, like ovens and light bulbs



Thermal image of an incandescent bulb. Much of the energy is emitted as infrared. The IR heats the glass, which conducts the heat to the surrounding air, producing convection.





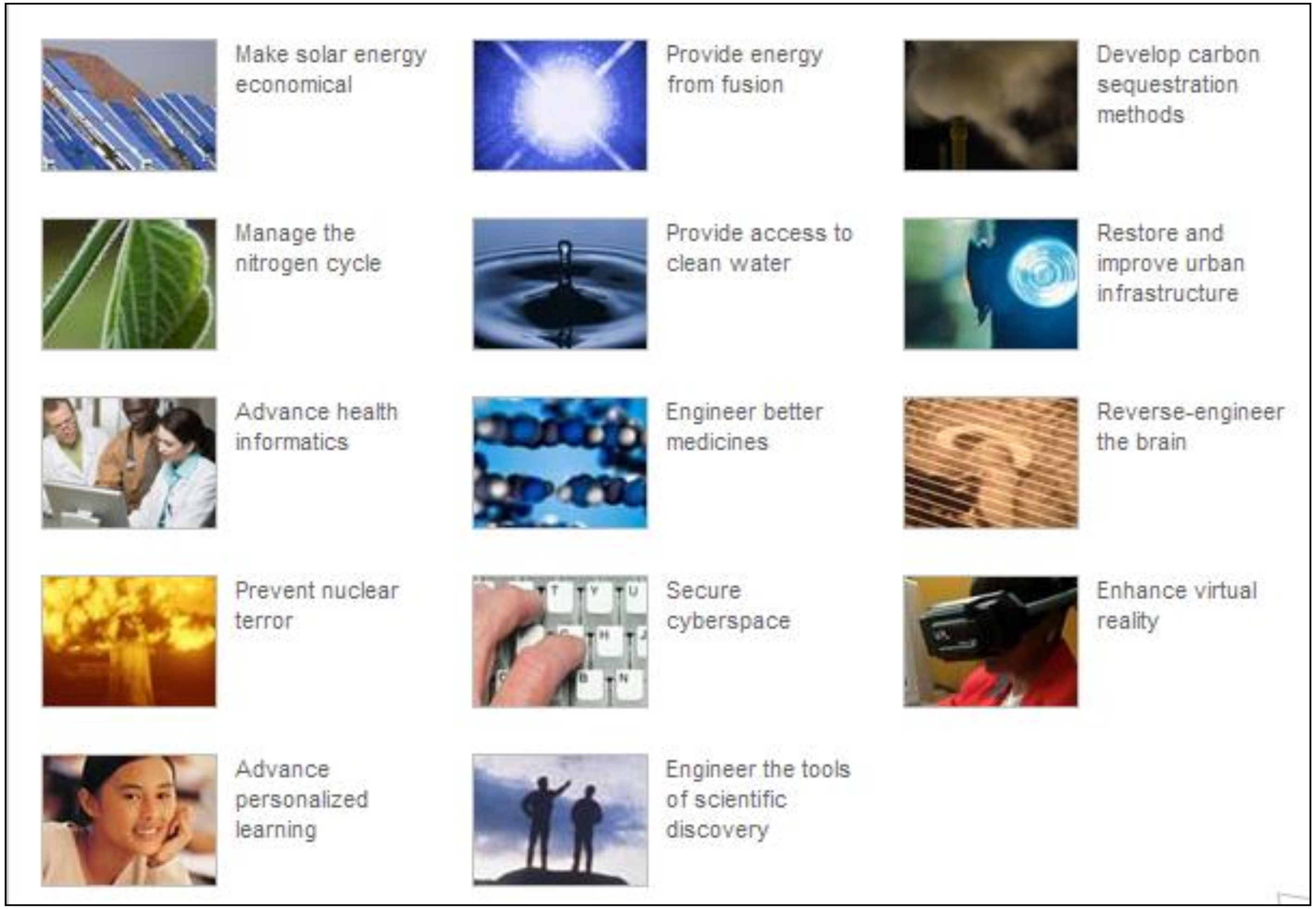
	Overall luminous efficiency
40 W tungsten incandescent	1.9%
60 W tungsten incandescent	2.1%
100 W tungsten incandescent	2.6%
glass halogen	2.3%
quartz halogen	3.5%

The chart above lists values of overall luminous efficacy and efficiency for several types of general service, 120-volt, 1000-hour lifespan incandescent bulb

NATIONAL ACADEMY OF ENGINEERING

NAE GRAND CHALLENGES FOR ENGINEERING

Challenges News Community



- Make solar energy economical
- Provide energy from fusion
- Develop carbon sequestration methods
- Manage the nitrogen cycle
- Provide access to clean water
- Restore and improve urban infrastructure
- Advance health informatics
- Engineer better medicines
- Reverse-engineer the brain
- Prevent nuclear terror
- Secure cyberspace
- Enhance virtual reality
- Advance personalized learning
- Engineer the tools of scientific discovery

14 Grand Challenges for Engineering in the 21st Century

MAKE SOLAR ENERGY ECONOMICAL

U.S. Department of Energy Solar Energy Technologies Program

Comments on "Make Solar Energy Economical"

SHAPE THE FUTURE

NAE Grand Challenges Scholars Program

Vest Scholars Program

Make Solar Energy Economical

Make Solar Energy Economical

- Key Challenges:
  - Novel earth-abundant materials
  - Reliable, low-cost packaging techniques
  - Energy storage (daily and seasonal)
- How simulations can help:
  - Provide predictions of performance of realistic, novel PV materials (e.g., using DFT)
  - Predict and optimize lifetime energy production (e.g., using ADEPT)
  - Design electrolyzers and fuel cells (e.g., using FEM multi-physics)

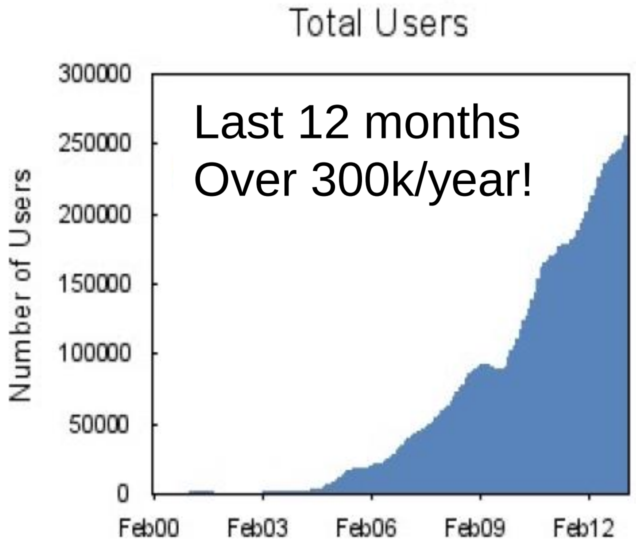
Lewis, N.S. 2007. Toward Cost-Effective Solar Energy Use. Science 315(5813): 798-801. DOI: 10.1126/science.1137014

WHAT IS NANOHUB AND S4?

- An open-access science gateway for cloud-based simulation tools and resources in nanoscale science and technology.
- Stanford Stratified Structure Solver (S4) is a frequency domain code to solve layered periodic structures.
- An input control file scripted in LUA outputs Absorption Spectrum using S-matrix Method

enabled by the HUBzero platform for simulation, learning, and collaboration

a major resource for computational nanotechnology



Last 12 months
Over 300k/year!

SETUP FOR HANDS-ON WORK

- Wireless ESSID: UNITE-9980; password: 78841109
- Nanohub login:
  - https://nanohub.org/
  - Create account via 'Signup' link in upper right
  - Login with institutional login, Facebook, or LinkedIn
- Bug reporting site
- https://nanohub.org/
- (upper right) **help** link
- Get the hands-on files

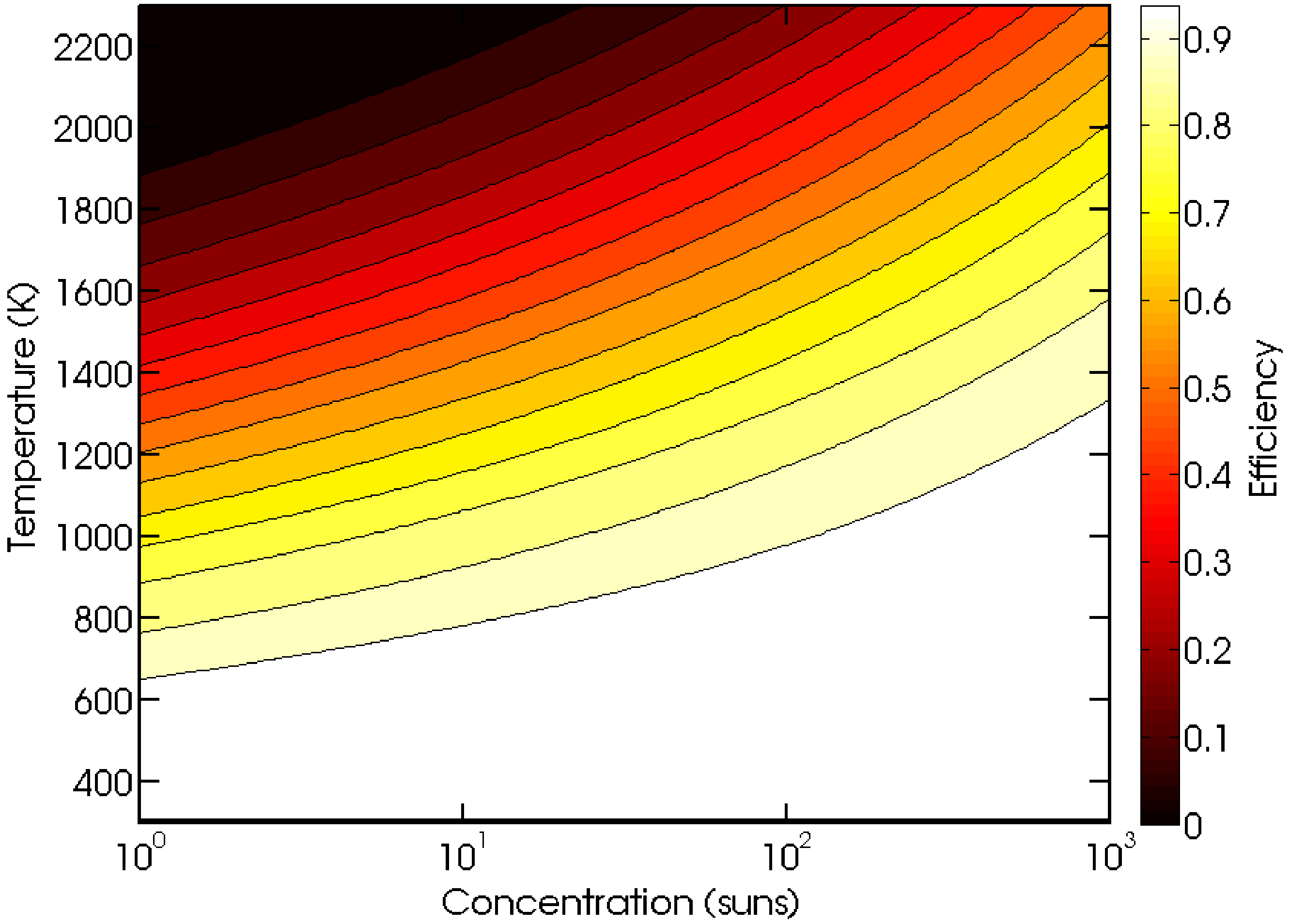
– https://nanohub.org/groups/thermalradiation

Step 1: Reach Maximum Temperature from Solar Heat

Key tool(s):

- S4sim

Selective Absorber: Maximum Thermal Transfer Efficiency



P. Bermel *et al.*, *Ann. Rev. Heat Transfer* (2012).

Thermal Transfer Efficiency

$$\eta_t = B\overline{\alpha} - \frac{\overline{\epsilon}\sigma T^4}{CI}$$

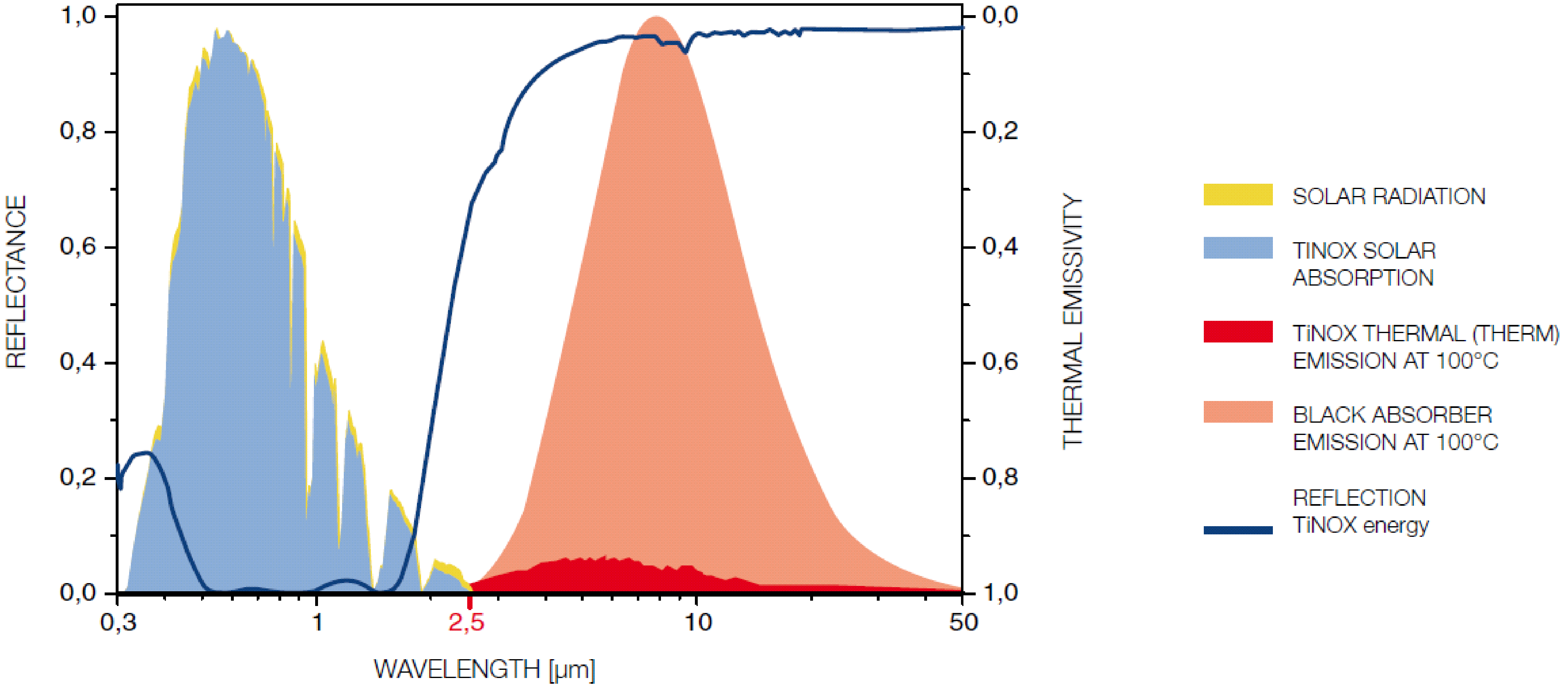
Spectrally-averaged absorptivity

$$\overline{\alpha} = \frac{1}{I}\int_0^\infty d\lambda \int_0^{\theta_c} d\theta \left[\epsilon(\lambda,\theta)\sin 2\theta \frac{dI}{d\lambda}\right]$$

Spectrally-averaged emissivity

$$\overline{\epsilon} = \frac{1}{\sigma T^4}\int_0^\infty d\lambda \int_0^{\pi/2} d\theta \left\{\frac{2hc^2\epsilon(\lambda,\theta)\sin 2\theta}{\lambda^5\left[e^{hc/\lambda kT}-1\right]}\right\}$$

Best Commercial Selective Solar Absorbers: T=400 K (1 sun)

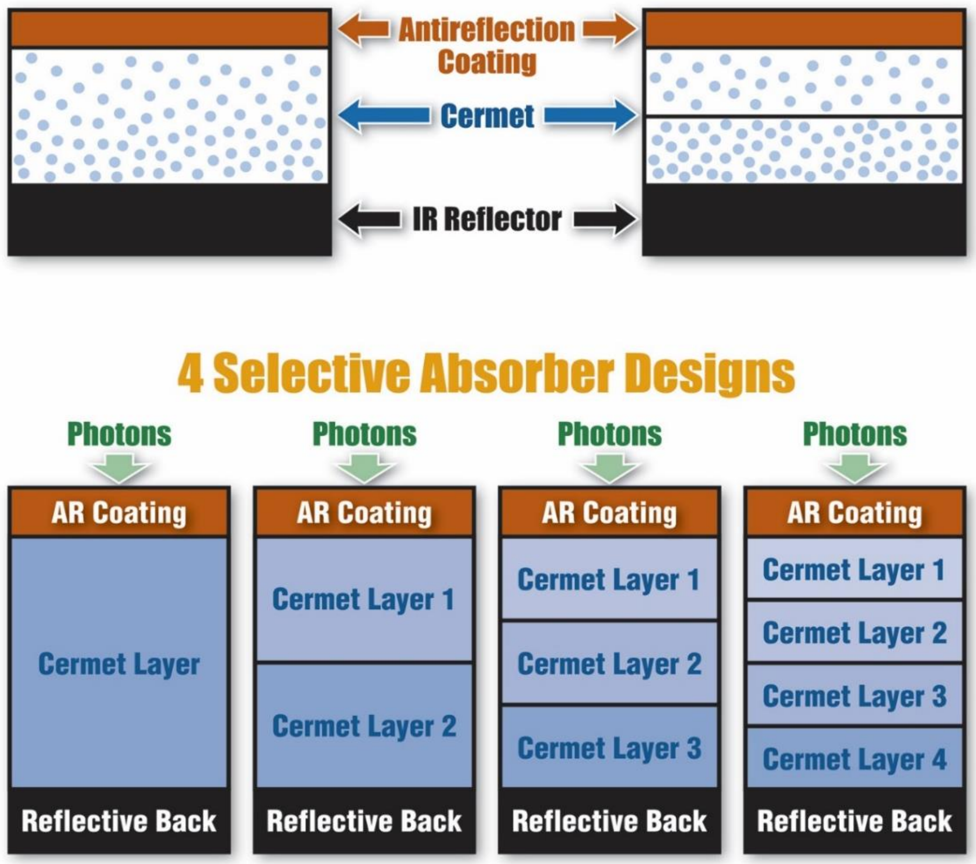


Almeco-TiNOX Solar

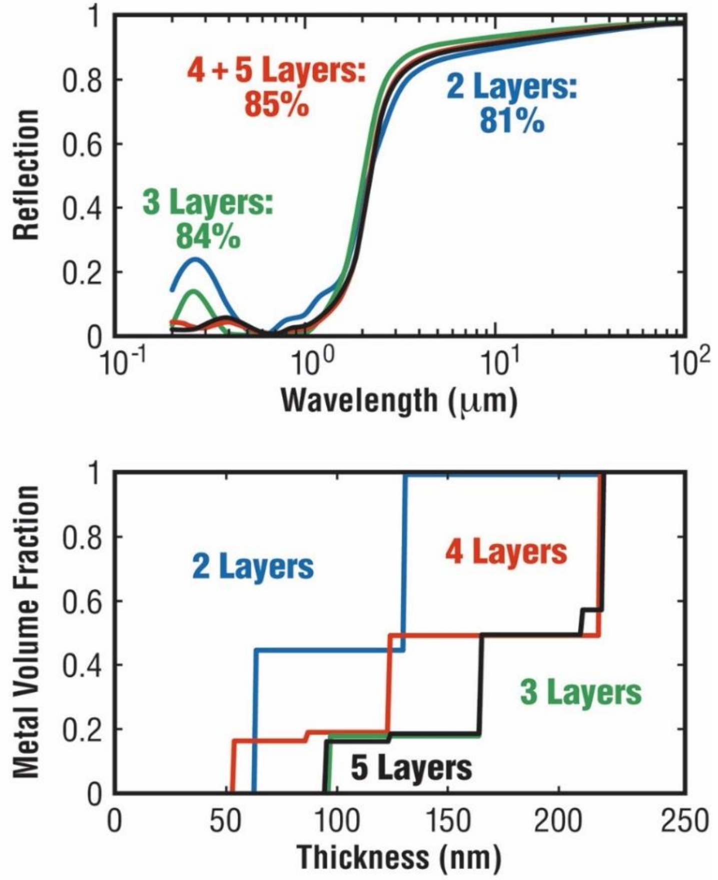
η_t = 90%; α = 95%; ε = 5%

http://www.almecogroup.com/en/pagina/16-solar

Selective Solar Absorbers at T=1000 K (100 suns)



5 Layer Optimization Yields: $\eta_t = 85\%$; $\alpha = 95\%$; $\varepsilon = 17\%$



D. Chester *et at.*, *Opt. Express* **19**, A245 (2011).

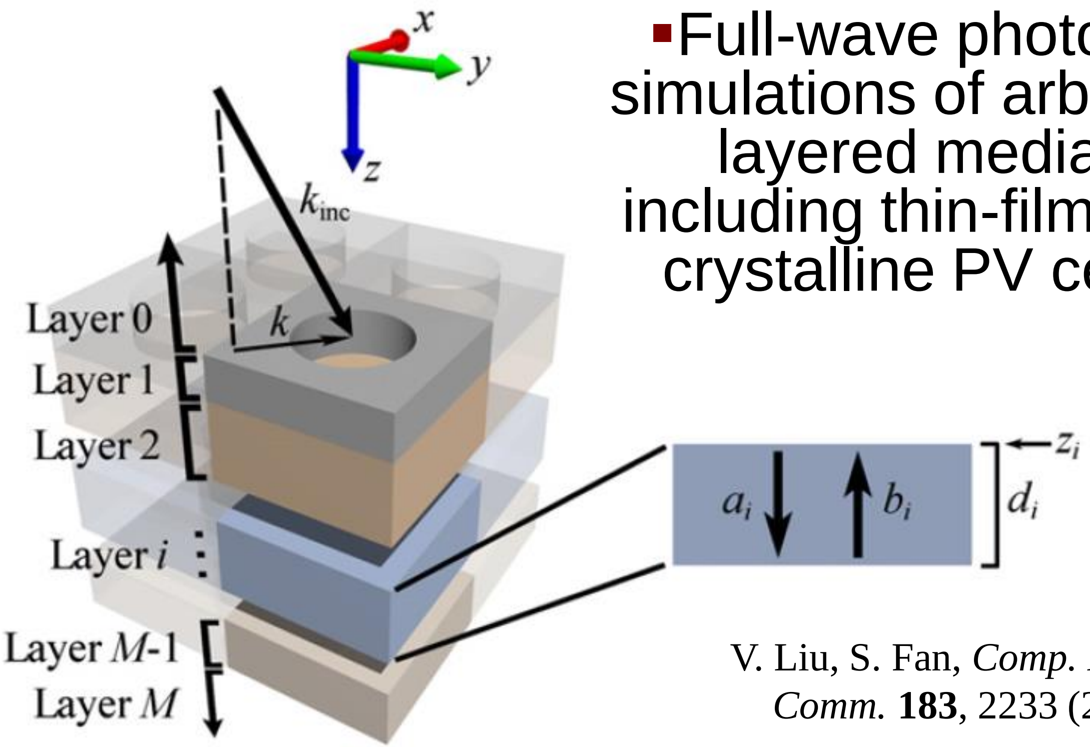
P. Bermel *et al.*, Energy Environ. Sci. (2016)

Selective Solar Absorbers

Schematic of the structure for selective absorber based on Si substrate with 215nm Si_3N_4 front anti-reflection coating (ARC) and 300nm Ag back reflection layer. Heights are not to scale.

H. Tian et al., *Appl. Phys. Lett.* (2017)

Photonic Simulations with S^4



- Full-wave photonic simulations of arbitrary layered media, including thin-film and crystalline PV cells

V. Liu, S. Fan, *Comp. Phys. Comm.* **183**, 2233 (2012)

https://nanohub.org/tools/s4sim/

S-Matrix Method: Advantages

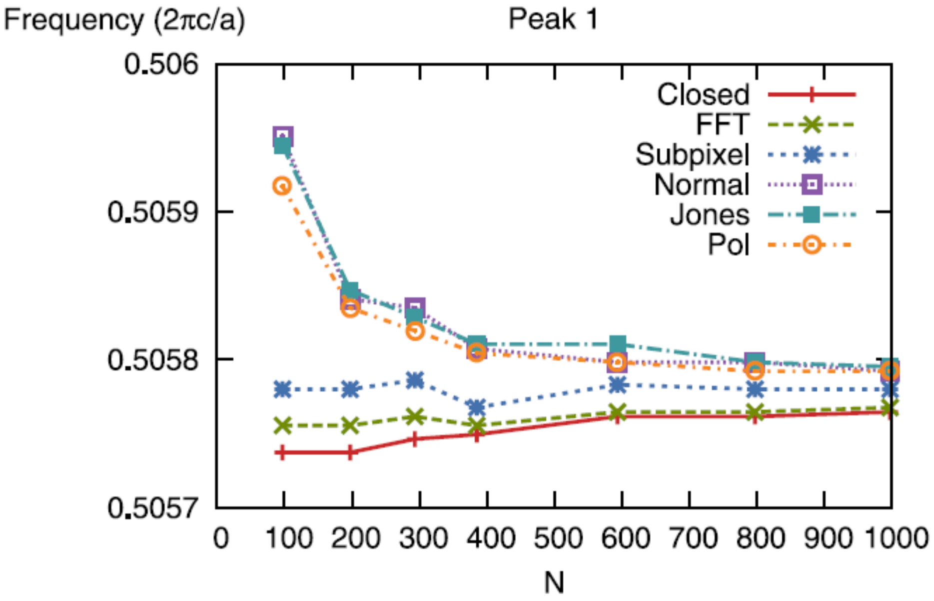
- No *ad hoc* assumptions regarding structures
- Applicable to wide variety of problems
- Suitable for eigenmodes or high-*Q* resonant modes at single frequency
- Can treat layers with large difference in length scales
- Computationally tractable enough on single core machines

S-Matrix Method: Disadvantages

- Accurate solutions obtained more slowly as the following increase:
    - Number of layers
    - Absolute magnitude of Fourier components (especially for metals)
    - Number of plane-wave components (~N^3)
- Relatively slow for broad-band problems (time-domain is a good alternative)

Photonic Simulations with S^4

Accuracy improves systematically with computing power



V. Liu, S. Fan, *Comp. Phys. Comm.* **183**, 2233 (2012)

S^4: Lua Control Files

- Obtain a new, blank simulation object with no solutions:

```
S = S4.NewSimulation()
```

- Define all materials:

```
S:AddMaterial('name', {eps_real, eps_imag})
```

- Add all layers:

```
S:AddLayer('name', thickness, 'material_name')
```

- Add patterning to layers:

```
S:SetLayerPatternCircle('layer_name', 'inside_material', {center_x, center_y},
radius)
```

S^4: FMM Formulations

- Specify the excitation mechanism:

```
S:SetExcitationPlanewave(
        {angle_phi, angle_theta}, -- phi in [0,180), theta in [0,360)
        {s_pol_amp, s_pol_phase}, -- phase in degrees
        {p_pol_amp, p_pol_phase})
```

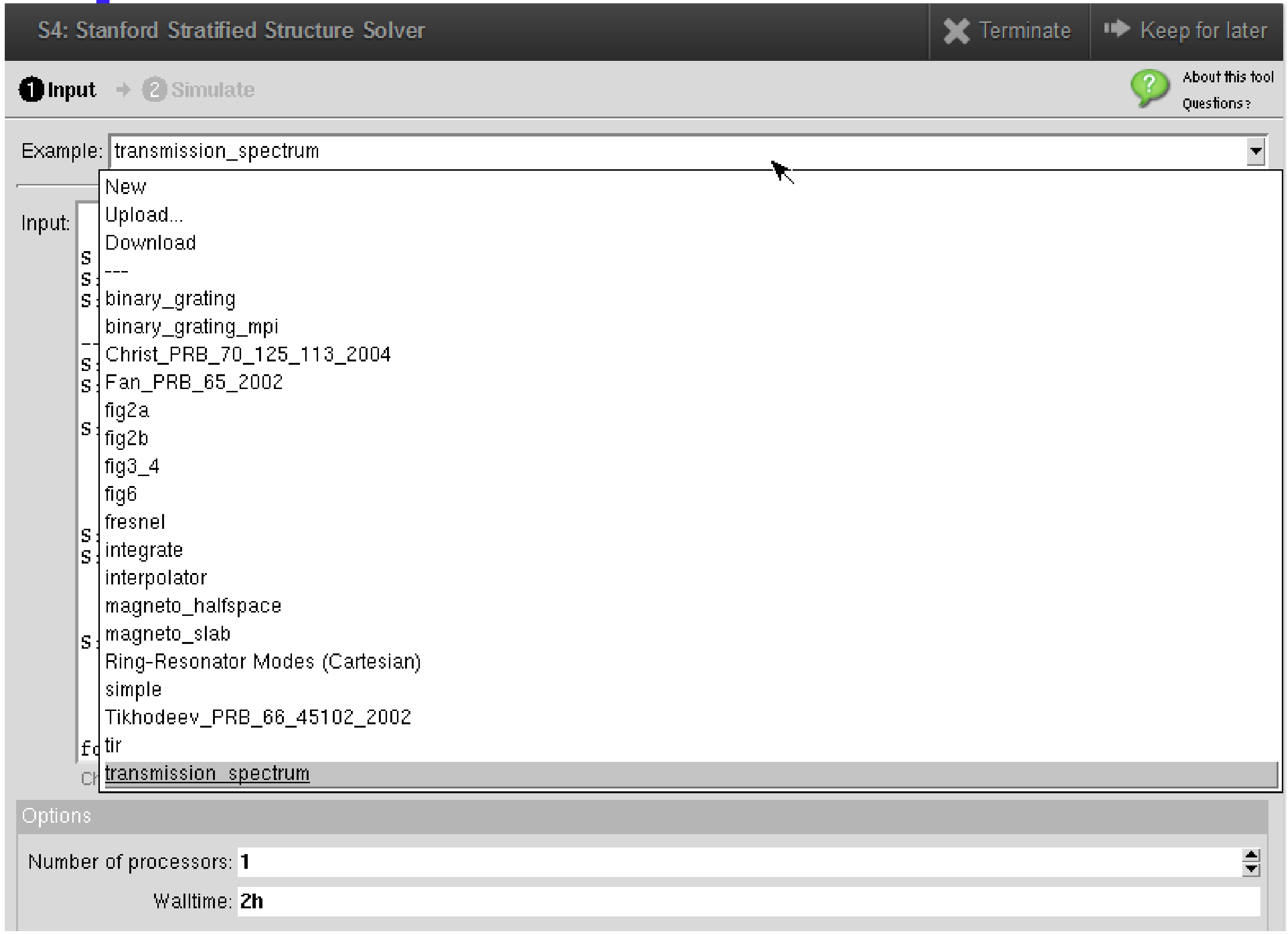
- Specify the operating frequency:

```
S:SetFrequency(0.4)
```

- Obtain desired output:

```
forward_power, backward_power = S:GetPoyntingFlux('layer_name', z_offset)
print(forward_power, backward_power)
```

S^4: Input

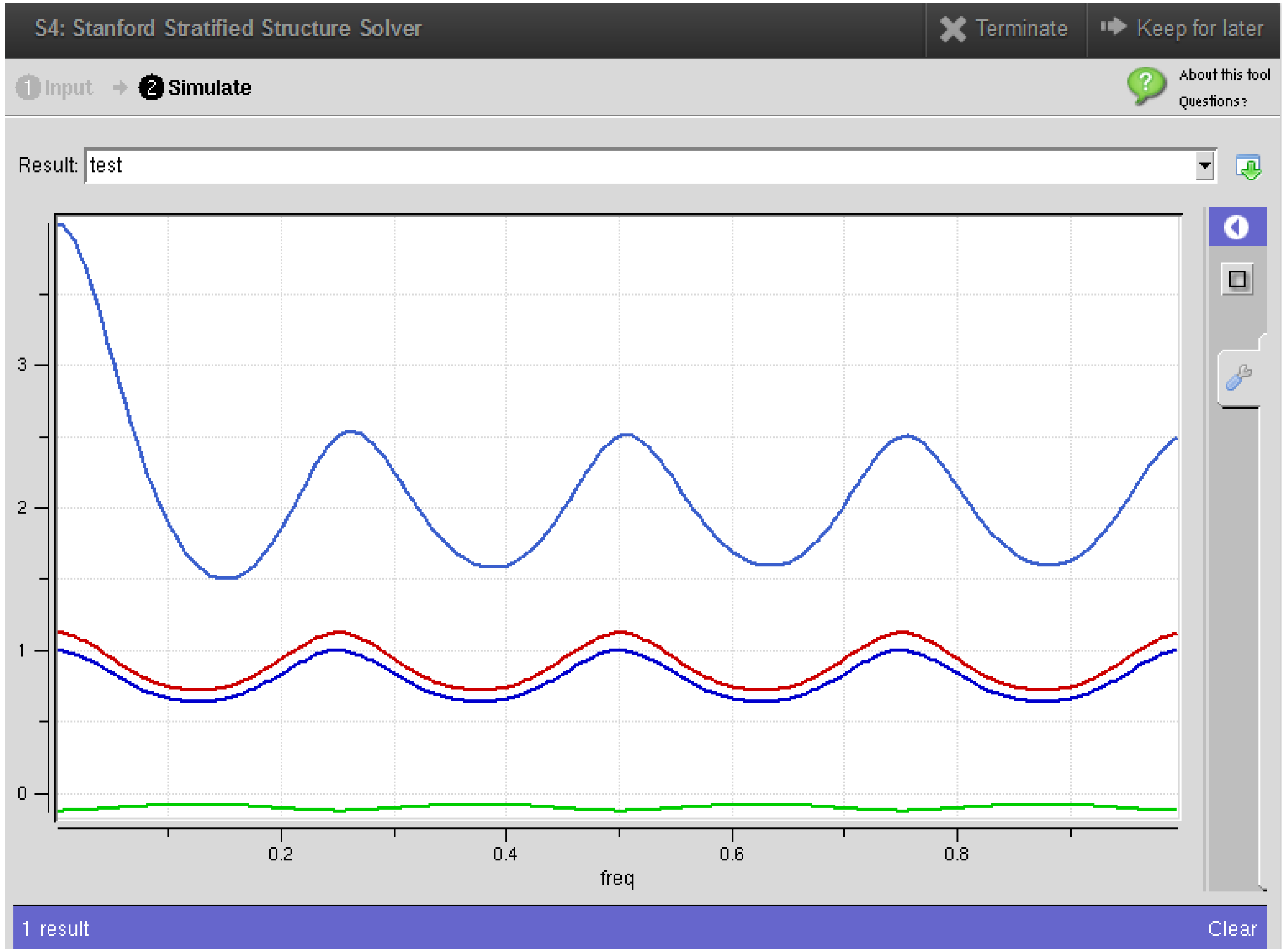


Number of processors: 1

Walltime: 2h

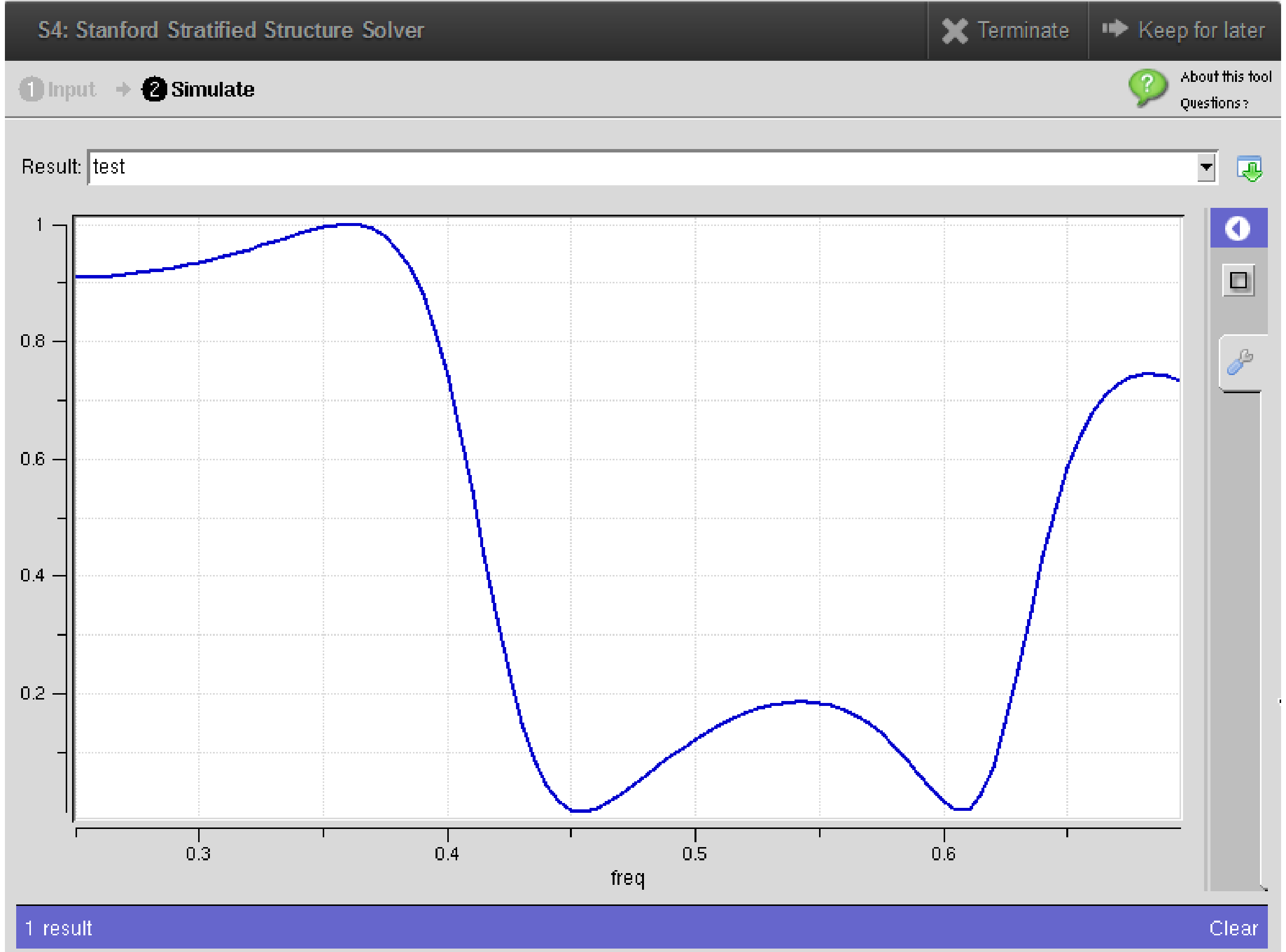
Can choose several examples drawn from the literature

S^4: Output



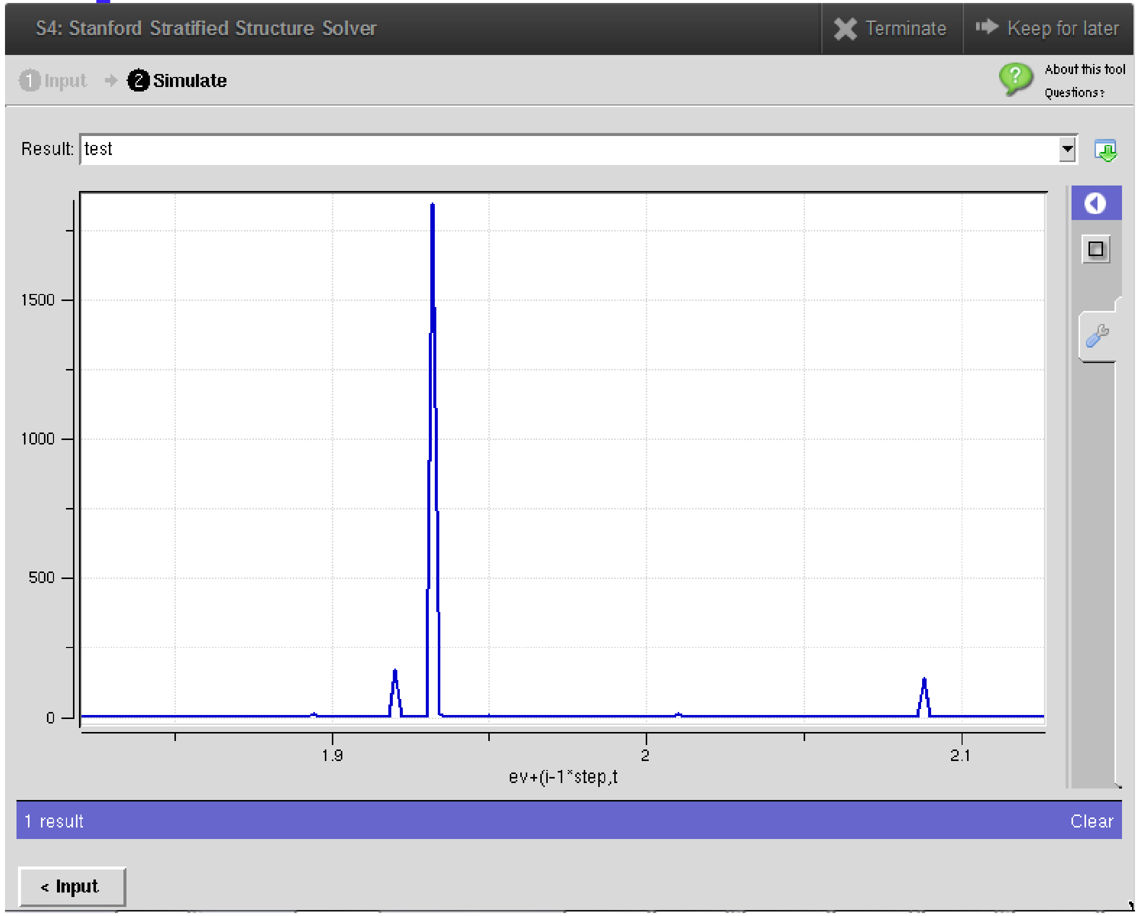
Transmission through multilayer stack matches analytical expression

S^4: Output



Transmission through 1D square grating of silicon and air

S^4: Output

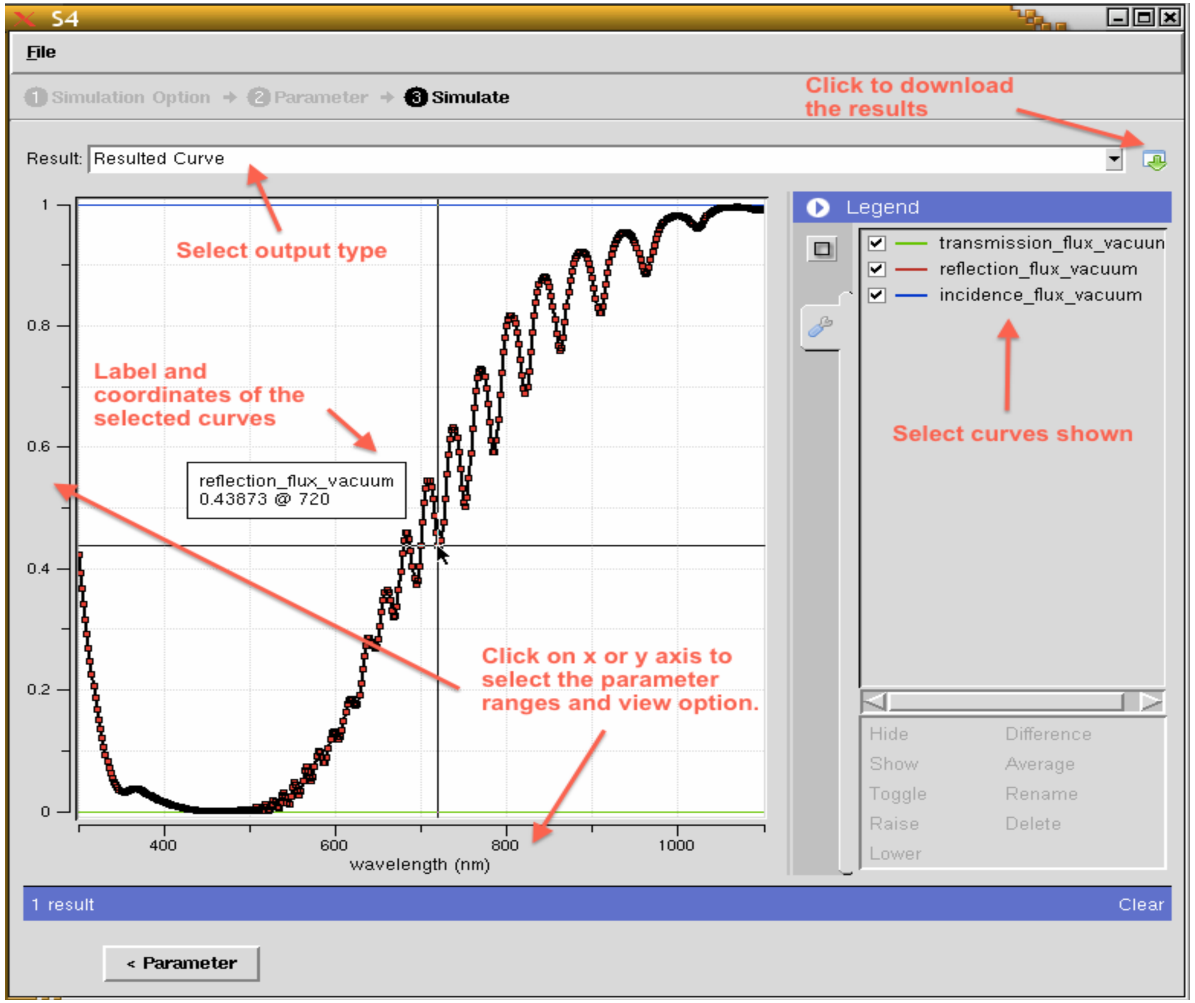


Result: test

1 result

- Transmission from Fig. 4 of Tikhodeev *et al*., *Phys. Rev. B* **66**, 045102 (2002).

S4sim: Output Window



Result: Resulted Curve

reflection_flux_vacuum
0.43873 @ 720

☑ transmission_flux_vacuun
☑ reflection_flux_vacuum
☑ incidence_flux_vacuum

Click to download the results

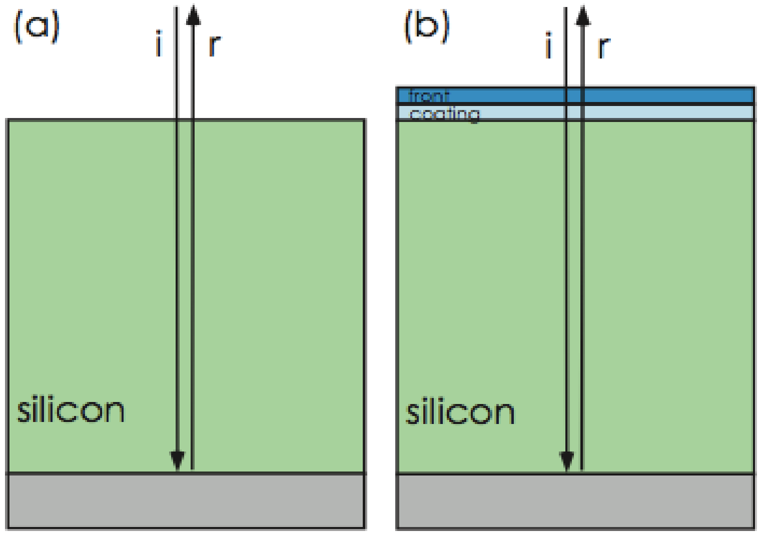
Select output type

Label and coordinates of the selected curves

Select curves shown

Click on x or y axis to select the parameter ranges and view option.

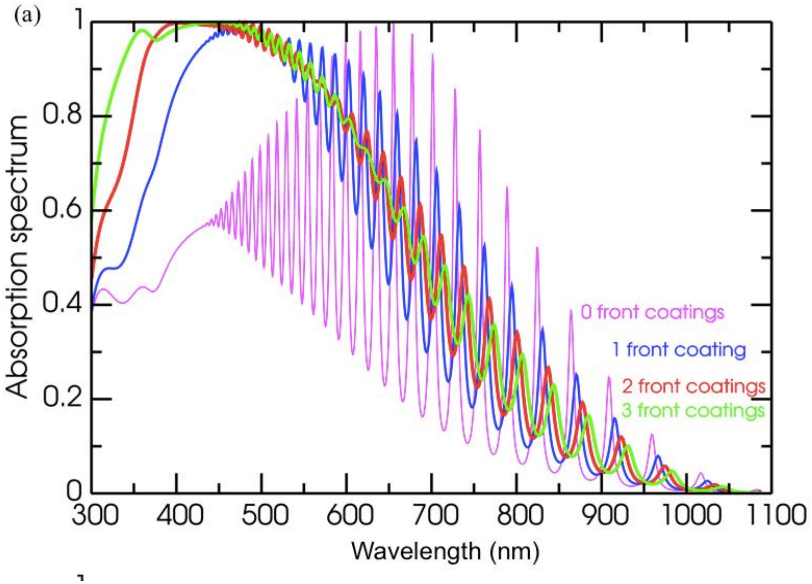
S4sim Example: PV Front Coating



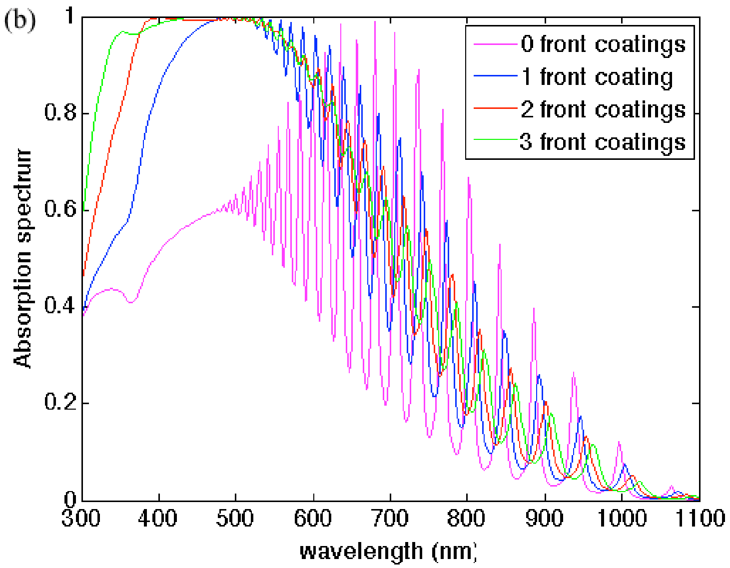
Number of front coating layers	1		2		3	
Relative permittivity	Real	Imag	Real	Imag	Real	Imag
Layer 1	4.32	0	2.37	0	1.80	0
Layer 2			9.12	0	5.71	0
Layer 3					14.36	0

Number of front coating layers	1	2	3
Thickness (nm)			
Layer 1	60	82.3	91.0
Layer 2		38.9	53.1
Layer 3			29.9

S4sim Example: PV Front Coating



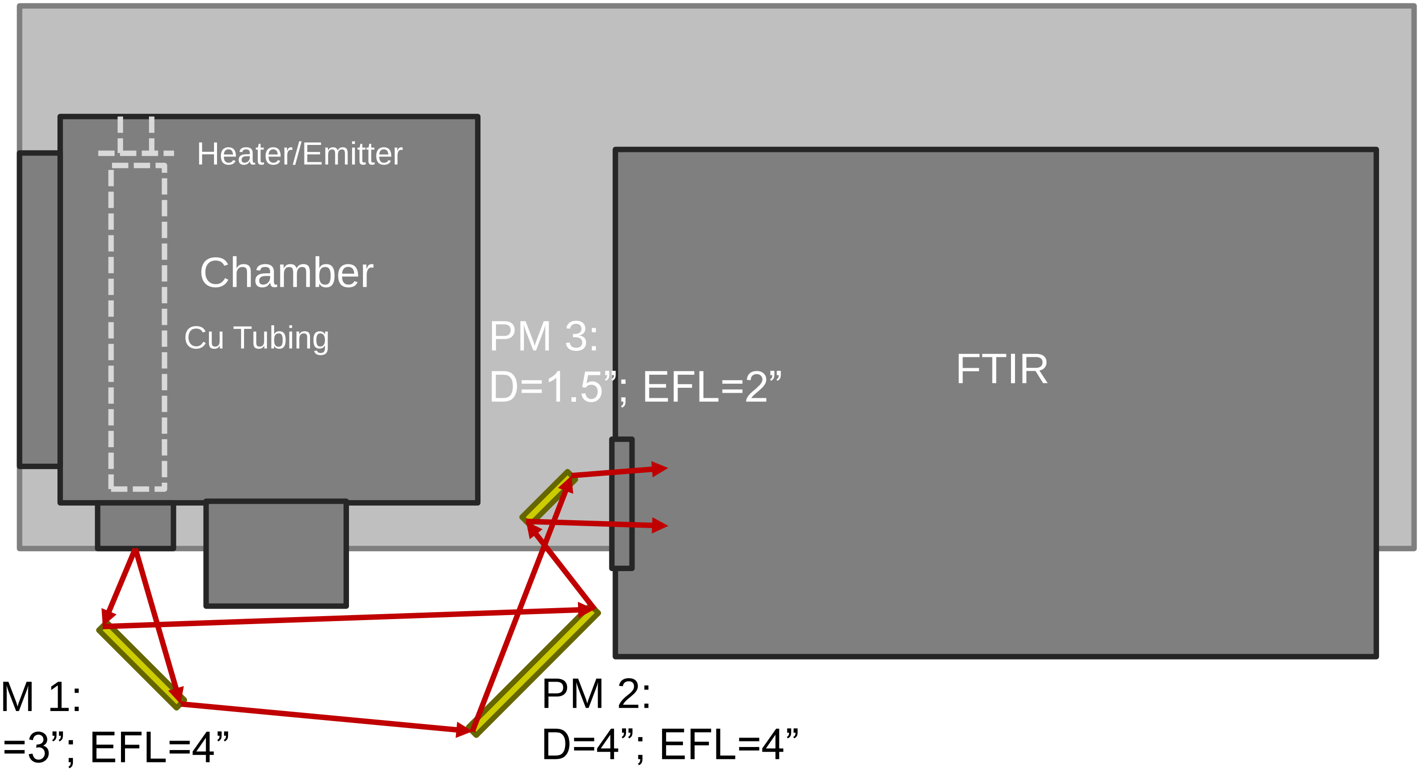
Results from M. Ghebrebrhan, P. Bermel, Y. Avniel, J. Joannopoulos, and S. Johnson, Optics Express 17, 7505-7518 (2009).



Results generated by S4sim

Direct Thermal Emission Measurement System

H. Tian et al., *Appl. Phys. Lett.* (2017)

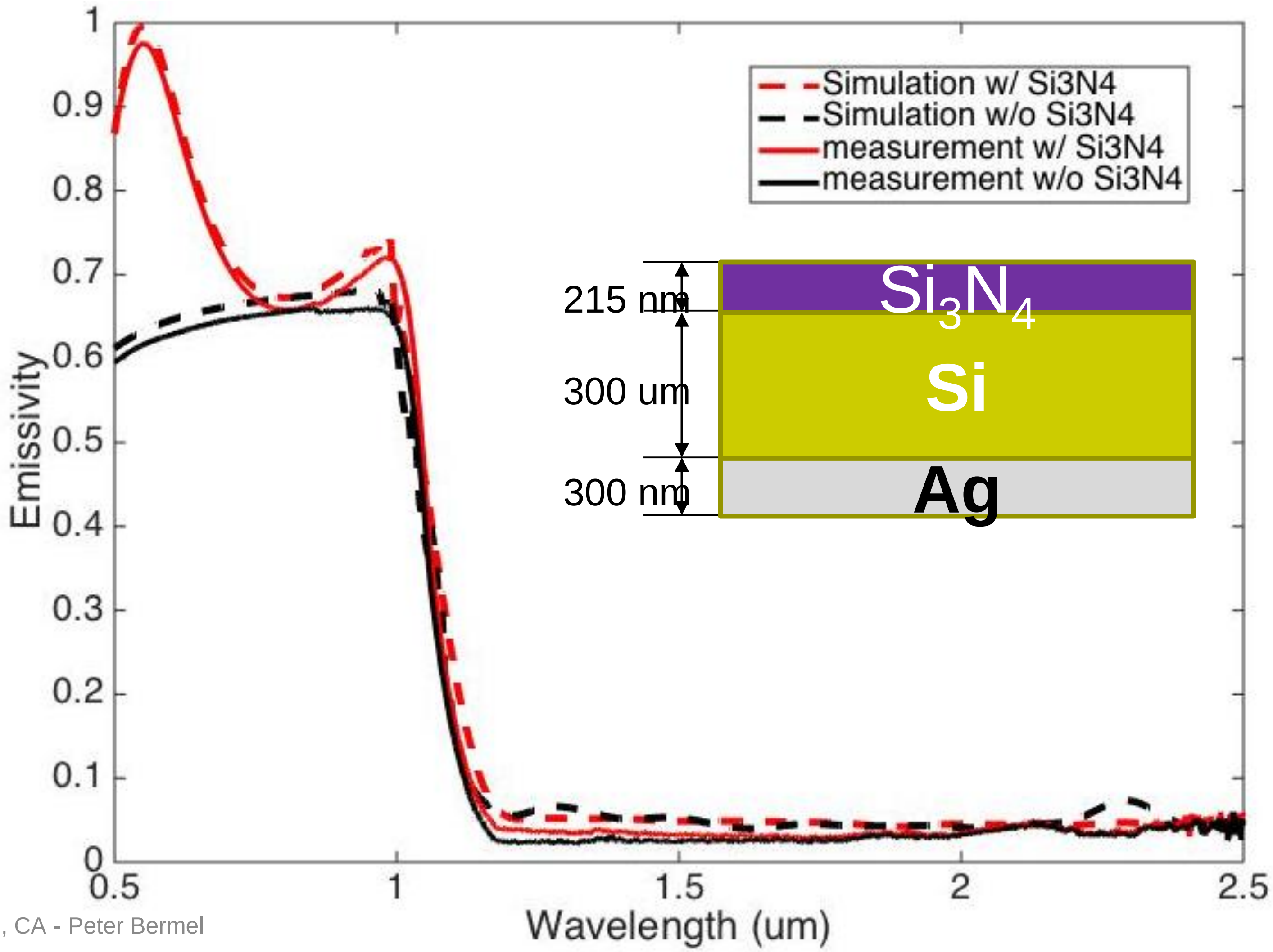


The sample is heated by the heater, and the emitted light is collected and guided by the Cu tube, transmitted through a CaF_2 window, reflected by three off-axis parabolic mirrors (PM 1, 2, and 3, Edmund Optics) to a Fourier Transform InfraRed (FTIR) spectrometer with a mercury cadmium telluride detector and KBr beam splitter (Thermo Fisher Nicolet 670).

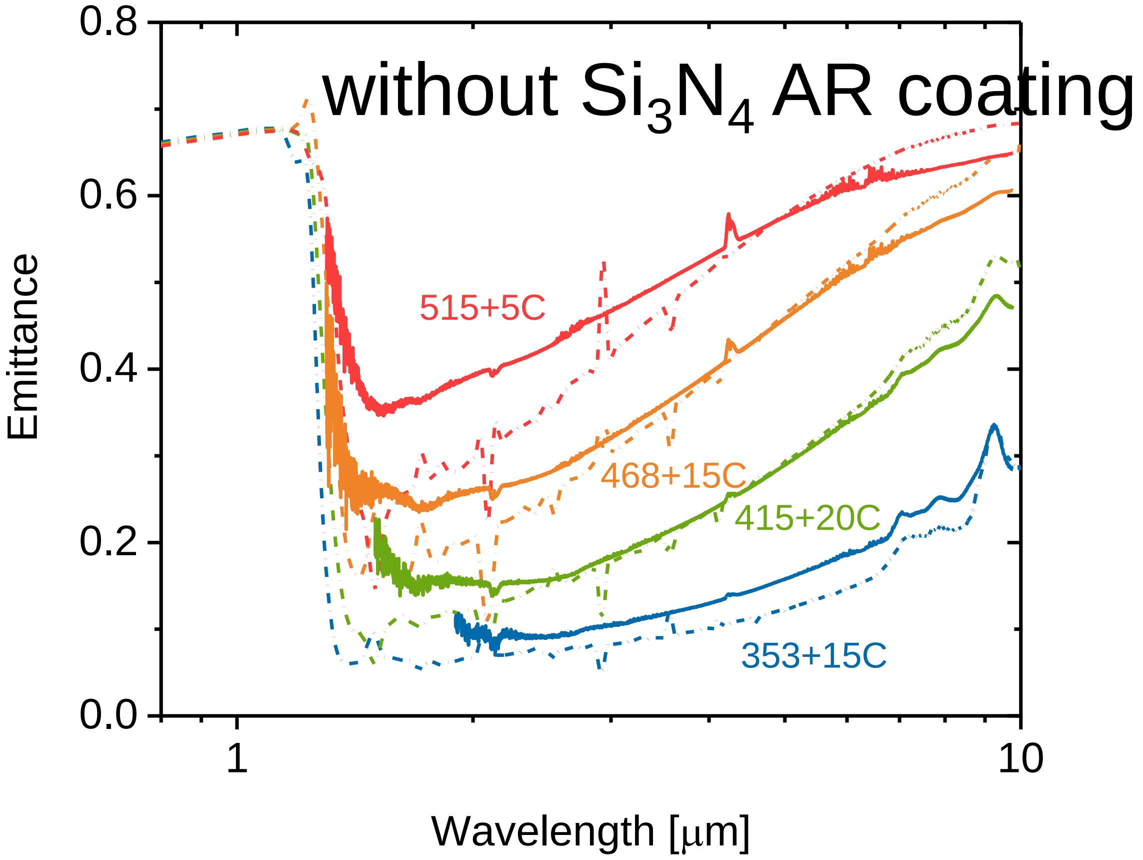
300 μm Si Experiment & Simulation at Room Temperature

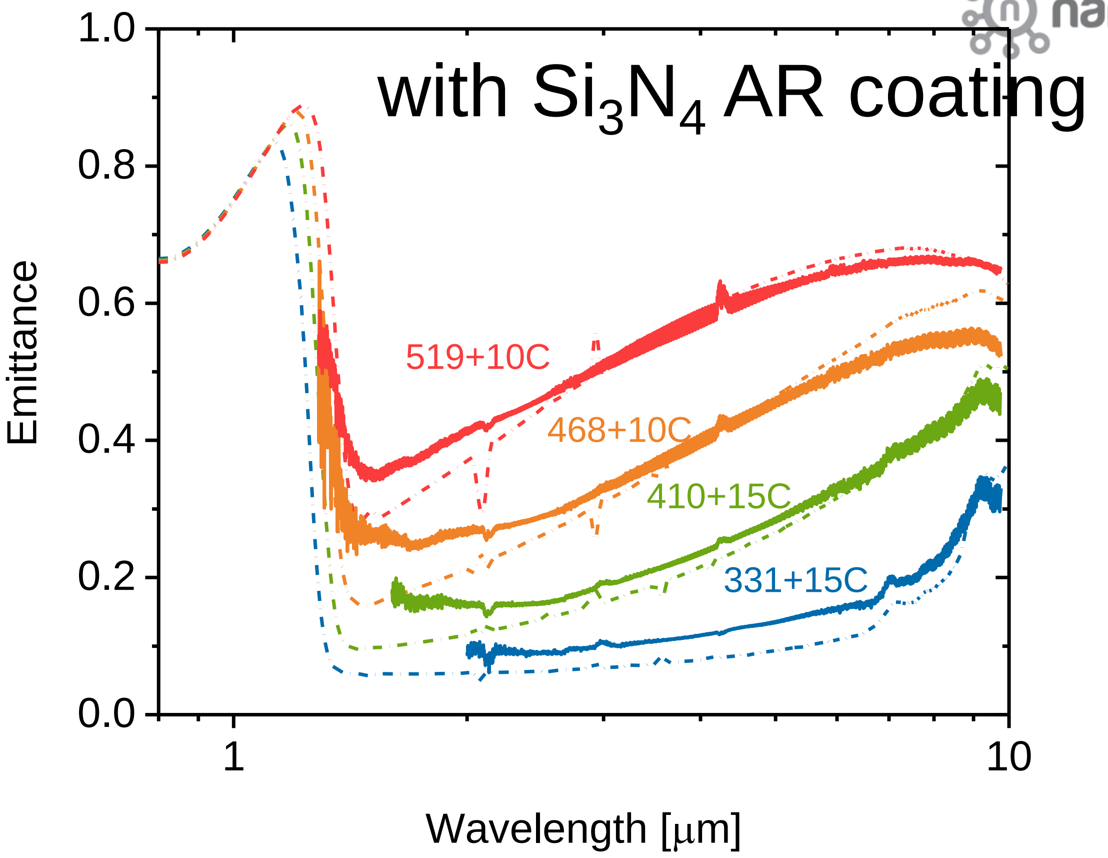
Measurement (solid lines) and simulation (dashed lines) of the emissivity of selective absorbers with (red lines) and without (black lines) front coating at room temperature. Measurements performed by a Lambda 950 spectrophotometer with an integrating sphere (Labsphere). The thicknesses of Si_3N_4, Si and Ag are 215nm, 300 μm and 300nm respectively.

H. Tian et al., *Appl. Phys. Lett.* (2017)



300 μm Si Experiment & Simulation at High Temperatures





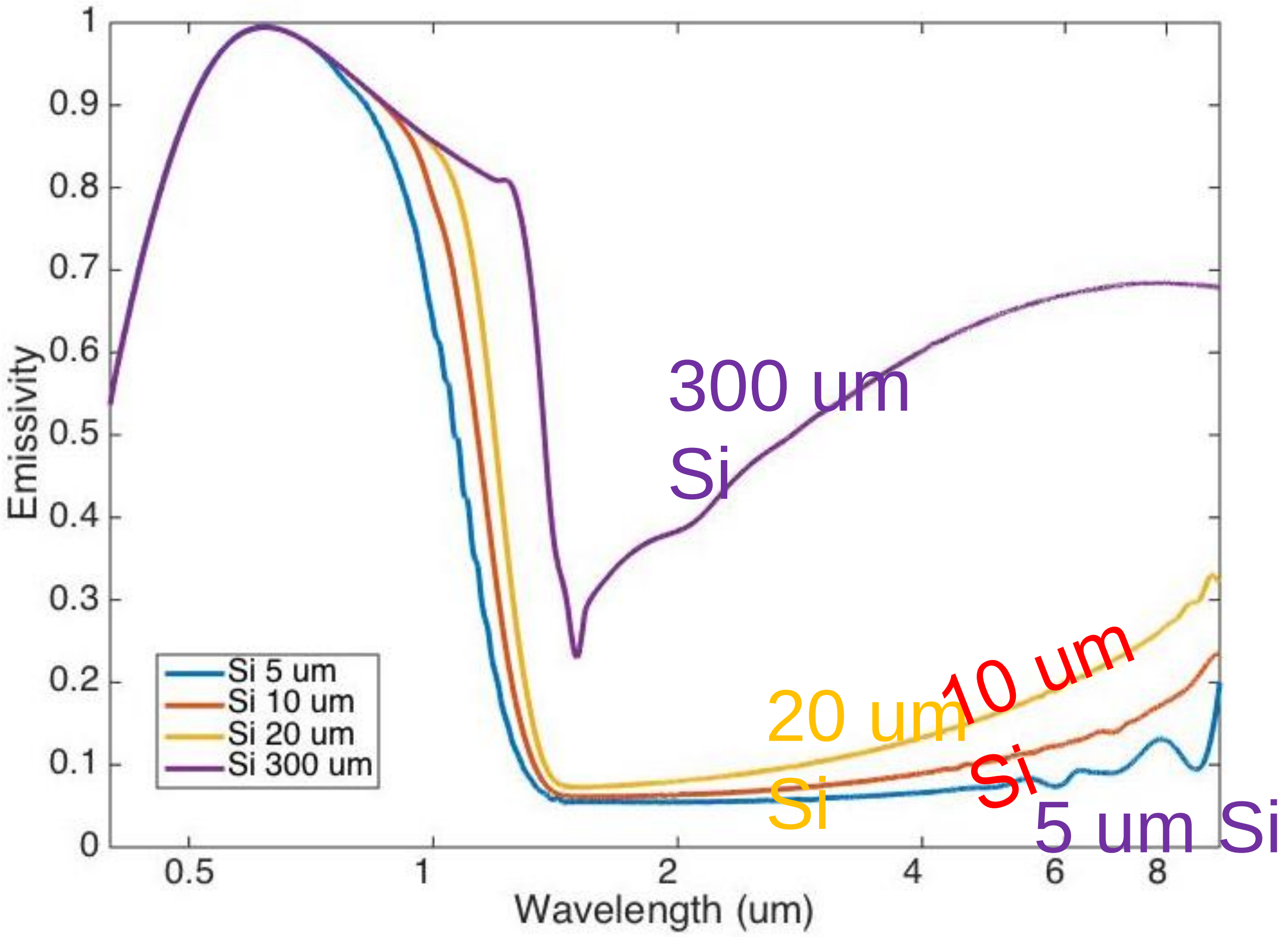
High spectral selectivity is observed at 468 °C in both samples, with a cutoff wavelength of approximately 1.3 μm. Higher short-wavelength emittance is both predicted and observed for the structure with a Si_3N_4 AR coating

H. Tian et al., *Appl. Phys. Lett.* (2017)

Thin Si film optimization targeted @ 550 °C

Emissivity for selective absorbers with different Si thicknesses. Optimal Si_3N_4 thickness is used for each curve which is 80 nm. The temperature is set at 550℃ and the F-P interference around the Mid-IR is smoothed out for more clear comparison. Less MWIR absorption is experienced for thinner layers of silicon because all samples are in the intrinsic regime, and free carrier absorption dominates.

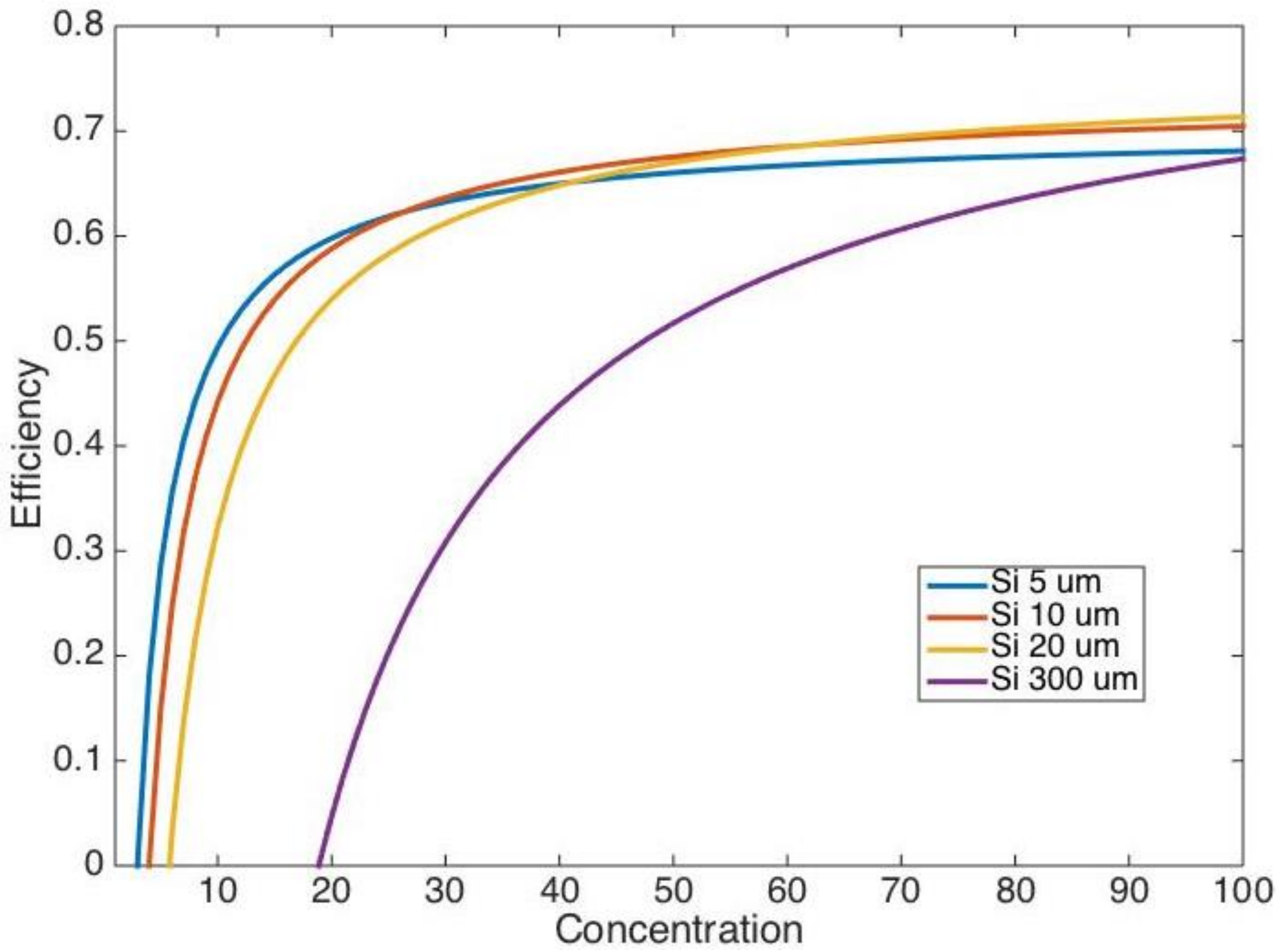
H. Tian et al., *Appl. Phys. Lett.* (2017)



Optimization Summary for 550 °C

Dependence of solar thermal transfer efficiency η_t for different Si thicknesses on the concentration. The Si_3N_4 thickness is fixed at 80nm, and the temperature is 550C. Thinner layers of silicon experience less reradiation; however layers which are too thin have less absorption, which puts an upper bound on η_t.

H. Tian et al., *Appl. Phys. Lett.* (2017)



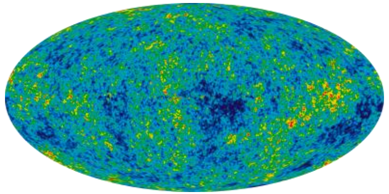
Step 2: Reach Below Ambient Temperatures under Sunlight

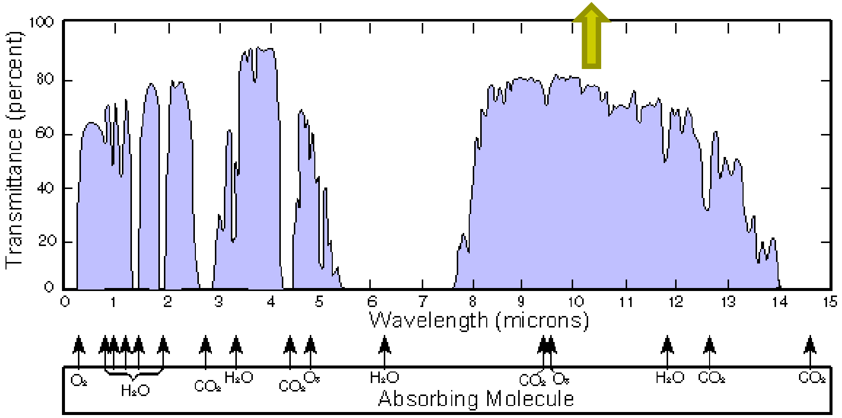
Key tools:

- RadCool

Radiative Cooling for Passive Thermal Management

3 K microwave background



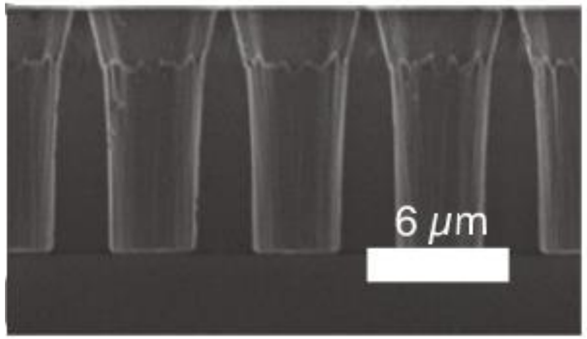


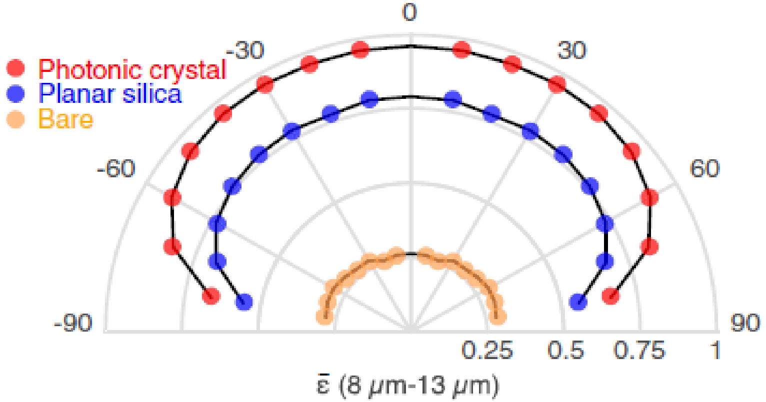
The sky transparency window allows radiative cooling outdoors

Questions:

1. Any alternative coolers to PhCs?
2. What is the temperature reduction and performance improvement by applying radiative cooling to hybrid or STPV systems?

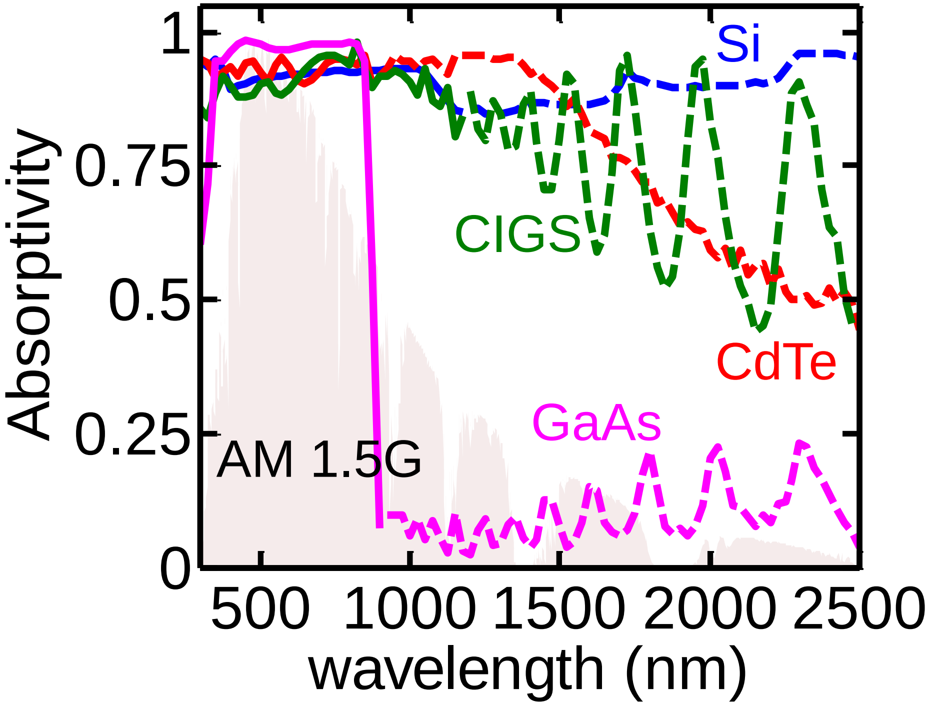
Photonic Crystal

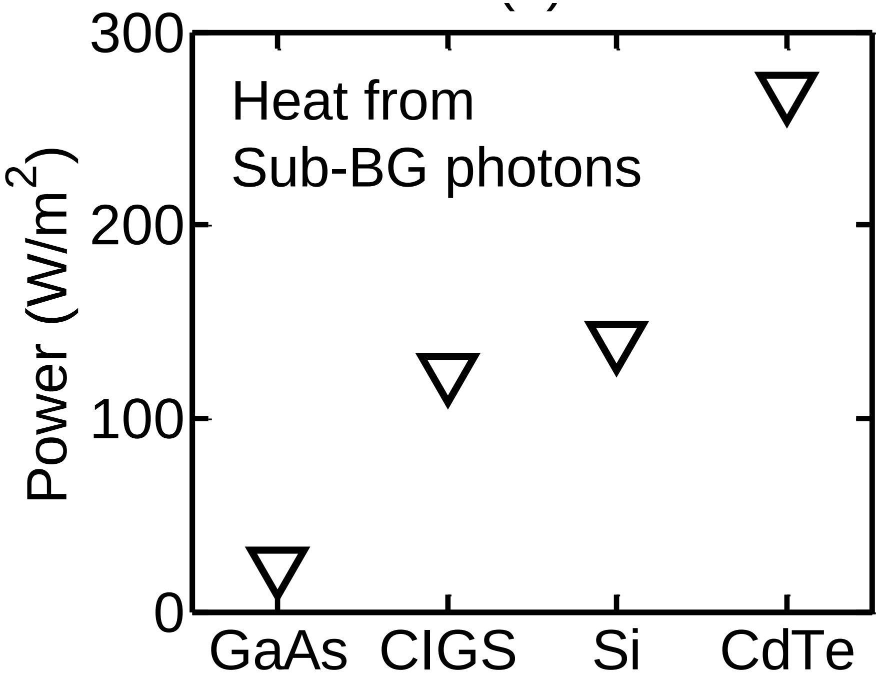




Zhu, Linxiao *et.al Proceedings of the National Academy of Sciences* 112.40 (2015): 12282-12287.

Most PV cells experience heating from sub-bandgap absorption

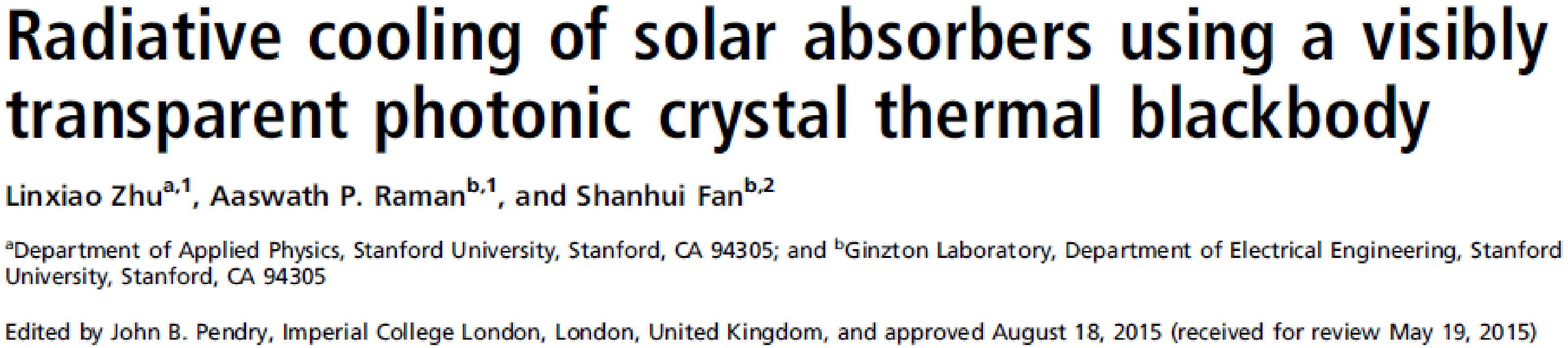




In c-Si cells, degradation processes with activation energy of 0.85 eV are accelerated almost a factor of 2 for every 10 K temperature difference

X. Sun *et al*., *IEEE J. Photovolt.* (submitted, July 2016)

Radiative cooling on PV devices

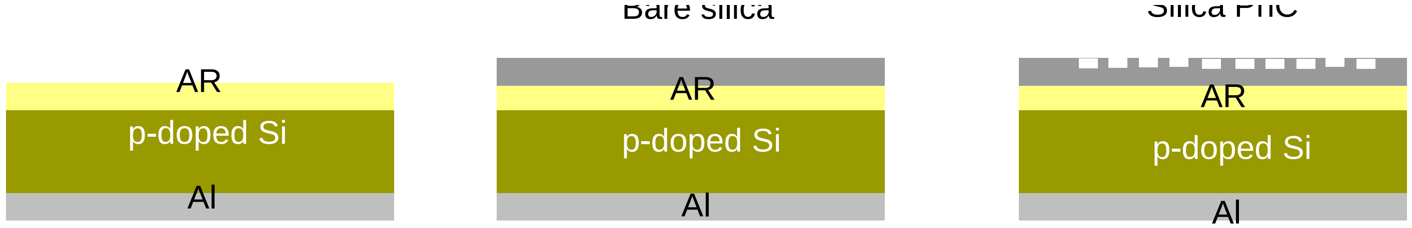


Radiative cooling of solar absorbers using a visibly transparent photonic crystal thermal blackbody

Linxiao Zhu[a,1], Aaswath P. Raman[b,1], and Shanhui Fan[b,2]

[a]Department of Applied Physics, Stanford University, Stanford, CA 94305; and [b]Ginzton Laboratory, Department of Electrical Engineering, Stanford University, Stanford, CA 94305

Edited by John B. Pendry, Imperial College London, London, United Kingdom, and approved August 18, 2015 (received for review May 19, 2015)



Bare absorber

Bare absorber +silica

Bare absorber +silica PhC

- Silica/silica PhC layer should at least preserve the solar absorption of the absorber
- Silica/silica PhC layer is expected to enhance the thermal emittance at the IR window

Radiative cooling on PV devices

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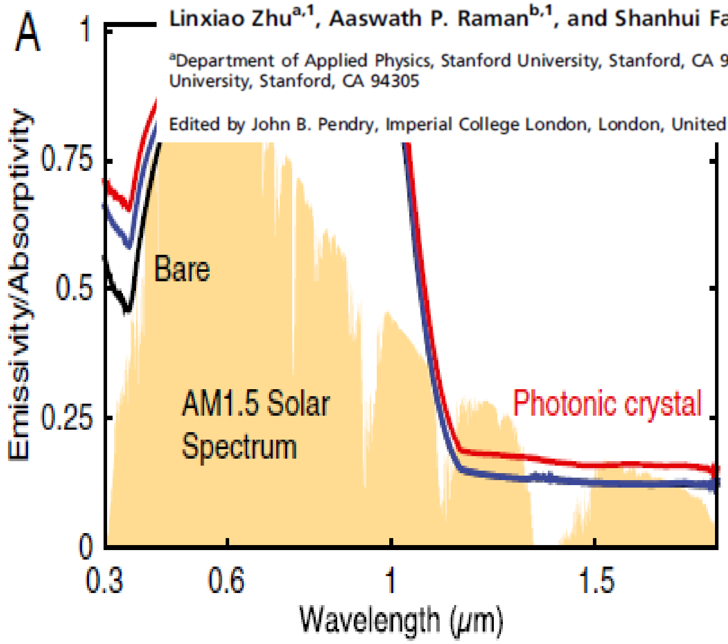
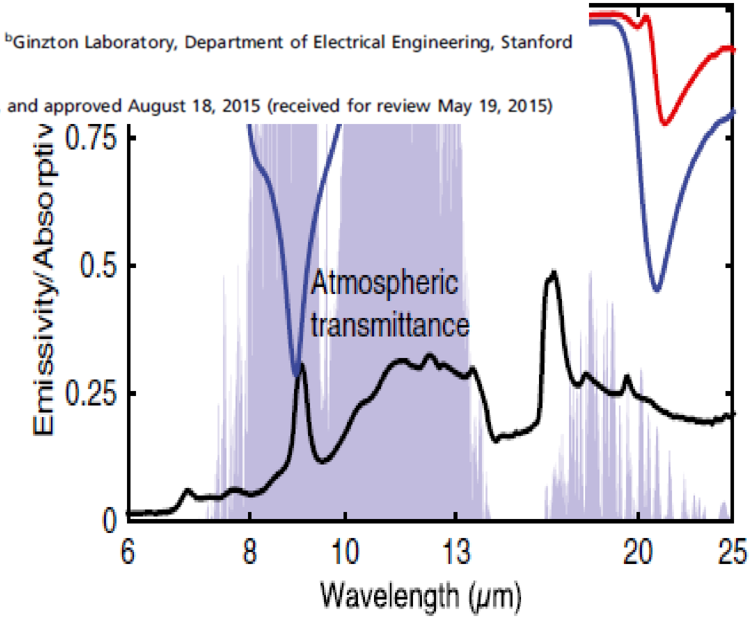


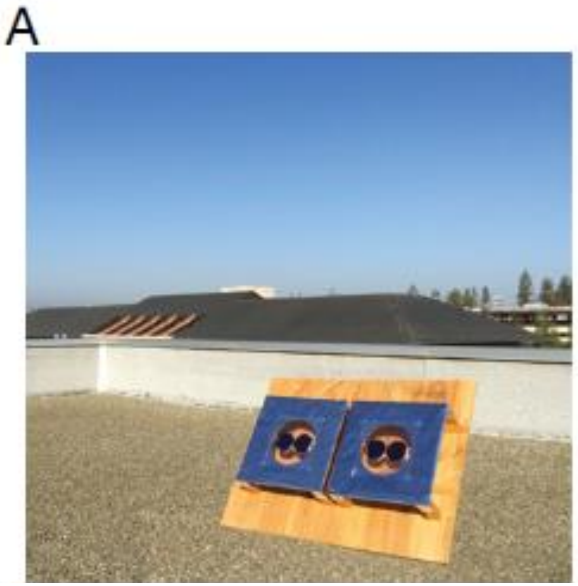
Solar absorption of the three structures

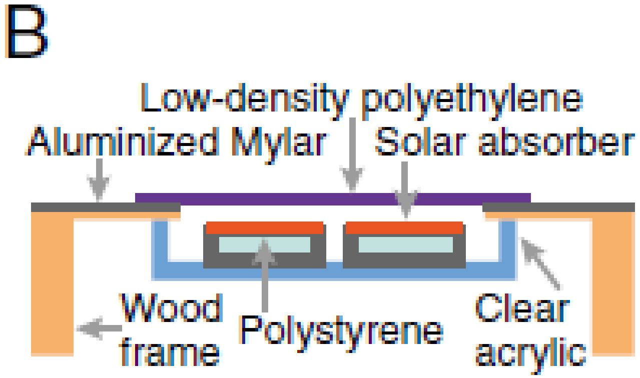


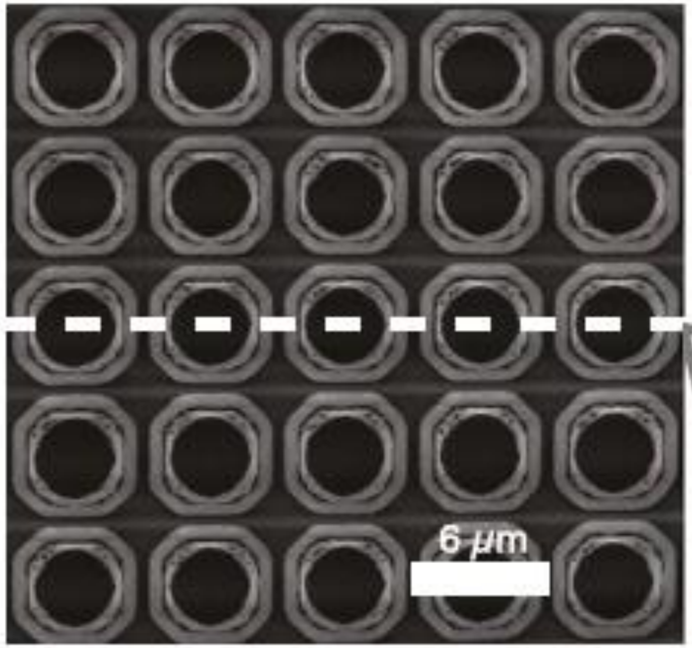
Emissivity spectra of the three structures at the IR window

Experimental setup

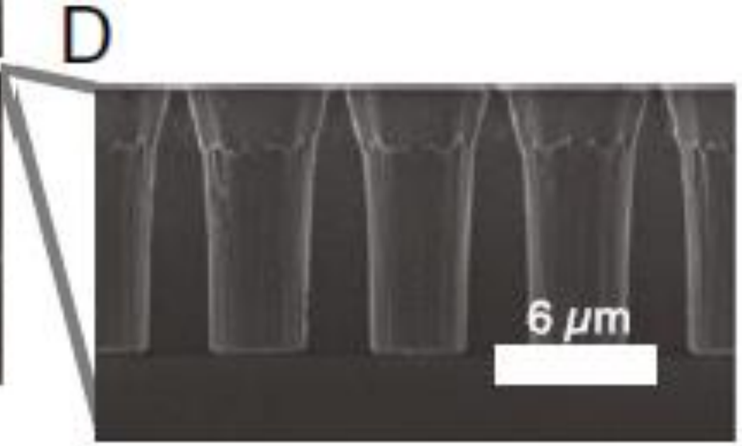
Zhu, Linxiao *et.al Proceedings of the National Academy of Sciences* 112.40 (2015): 12282-12287.





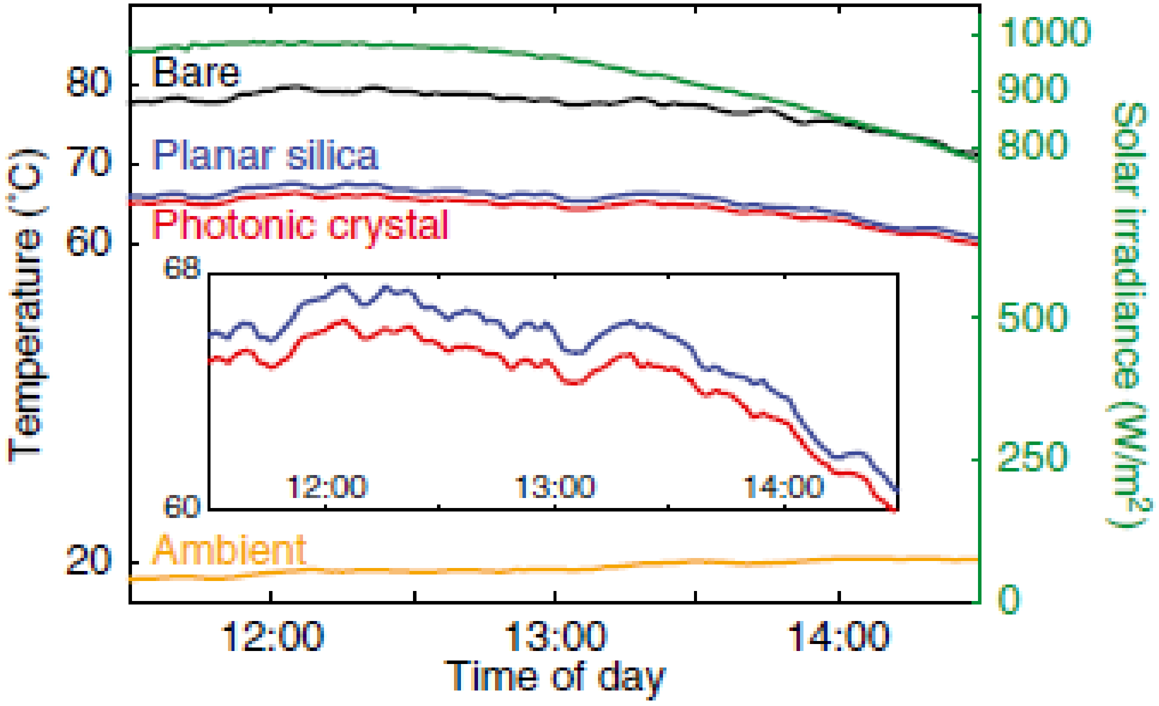


Periodicity: 6 μm;
Depth: 10 μm;

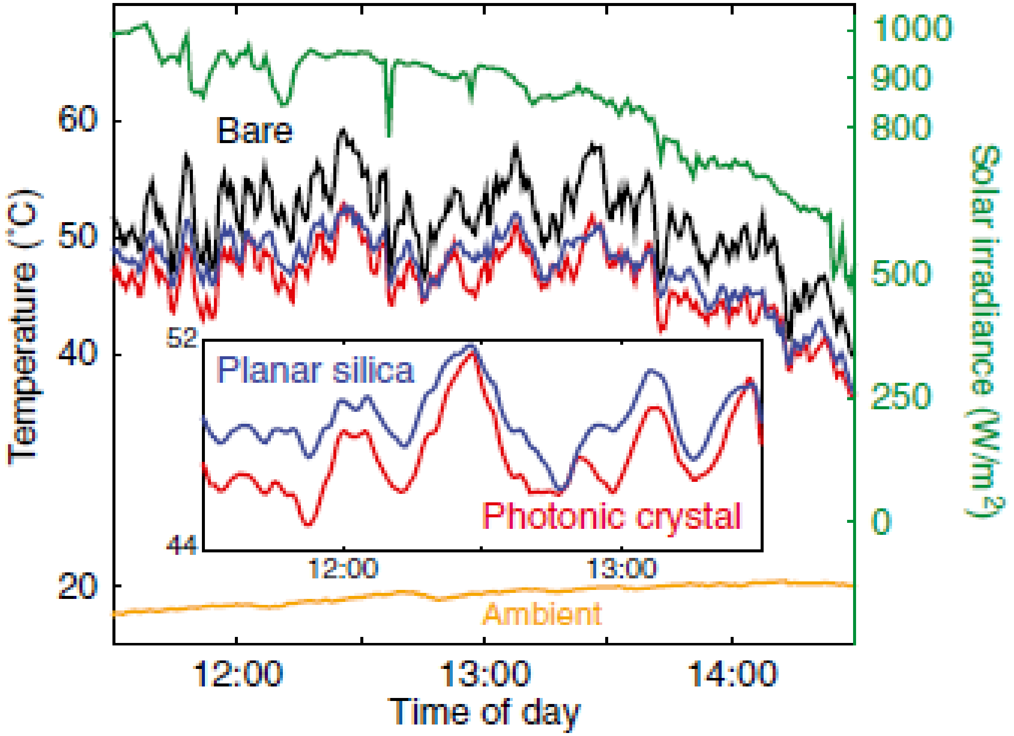


The container allows control over convection

Effects of radiative cooling



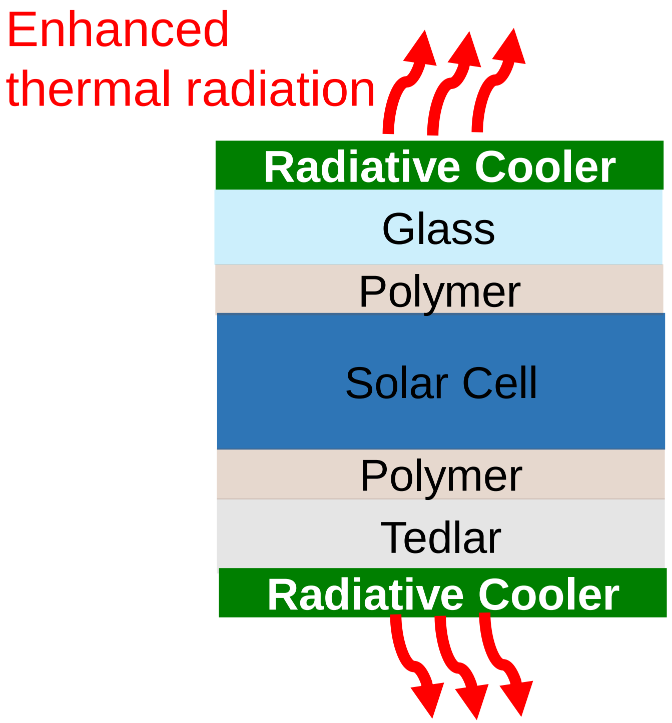
Without convection



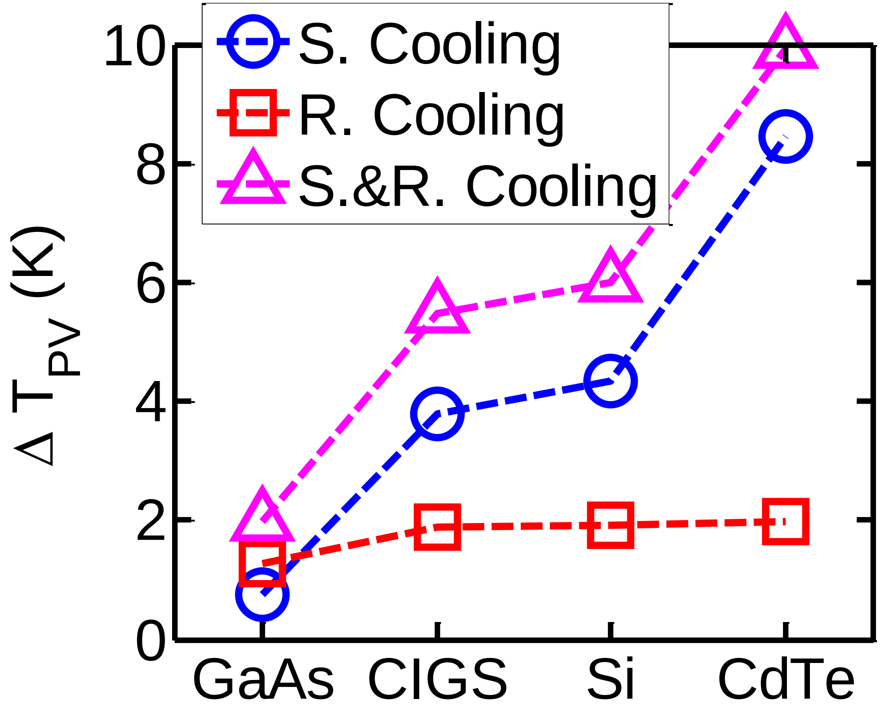
With convection

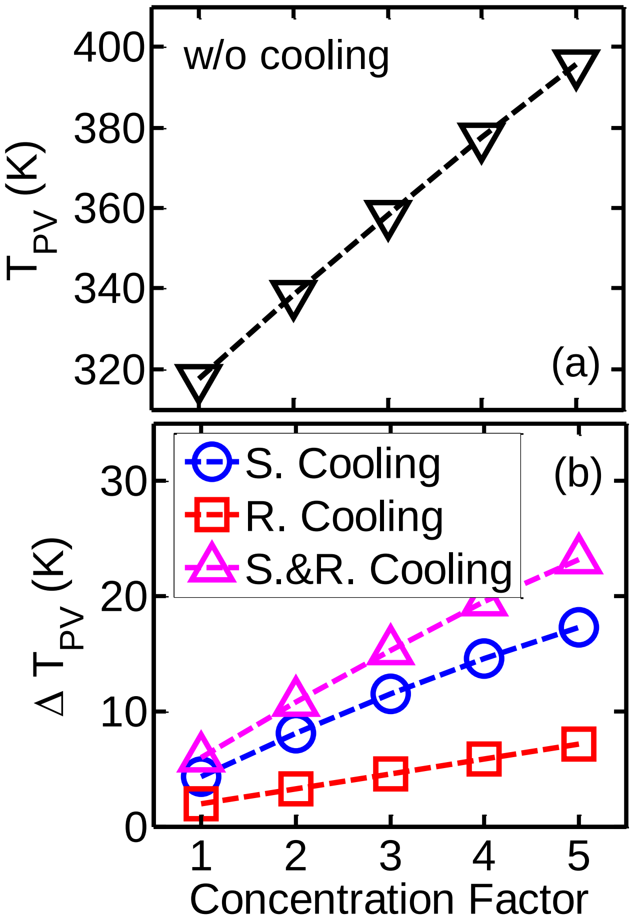
Zhu, Linxiao *et.al Proceedings of the National Academy of Sciences* 112.40 (2015): 12282-12287.

Benefits of radiative cooling extend across many PV technologies and installations


Enhanced thermal radiation

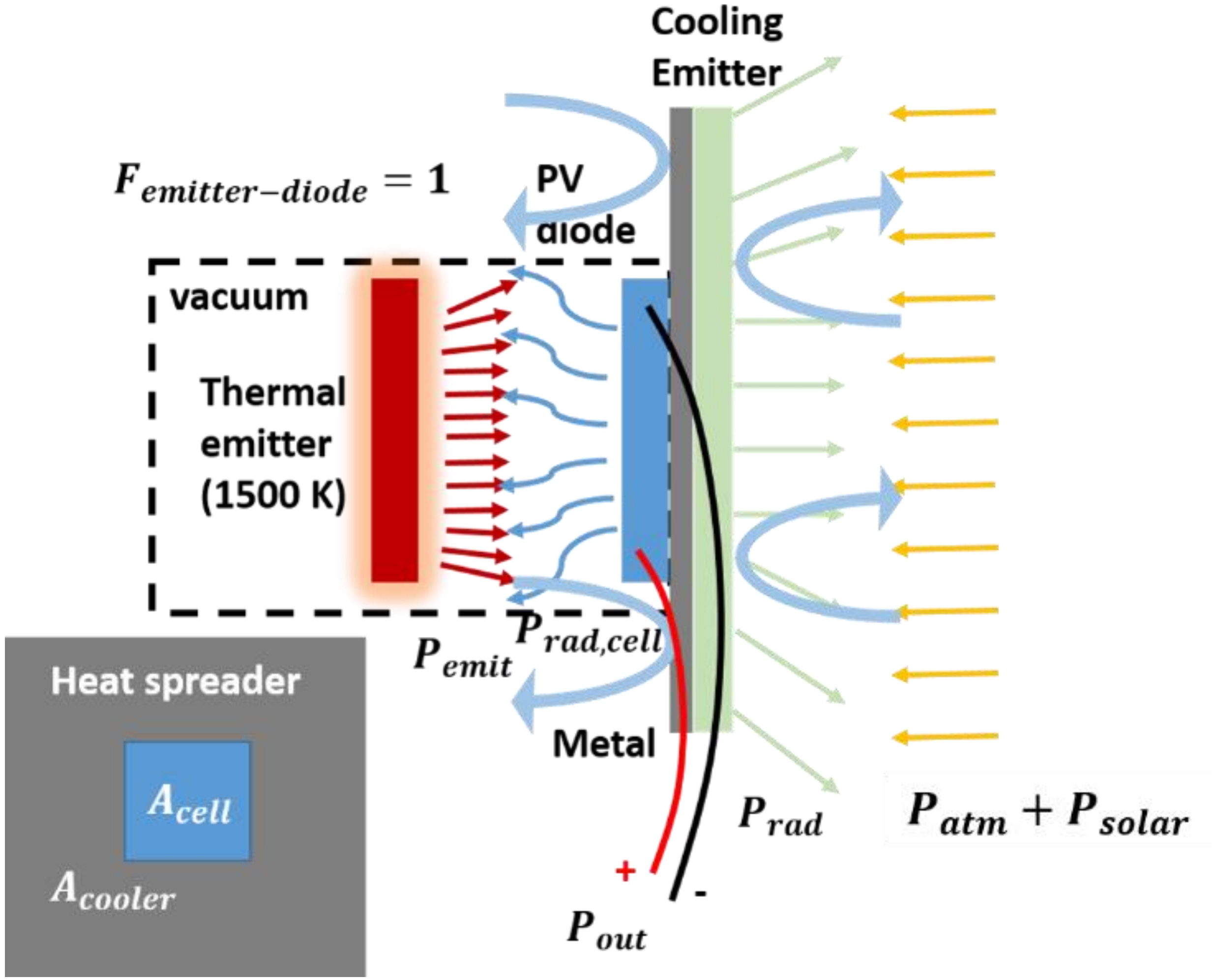
Radiative Cooler
Glass
Polymer
Solar Cell
Polymer
Tedlar
Radiative Cooler





X. Sun *et al.*, *IEEE J. Photovolt.* (submitted, July 2016)

Self-Consistent Modeling of Radiative Cooling for Passive Thermal Management



P_{emit}: emission power from thermal emitter at T_E

$P_{rad,cell}$: radiative recombination of the PV diode at T_C

P_{out}: electrical output power from PV diode (**SQ Limit**)

P_{rad}: radiation power from the cooling emitter at T_C

P_{atm}: radiation power from atmosphere (300 K)

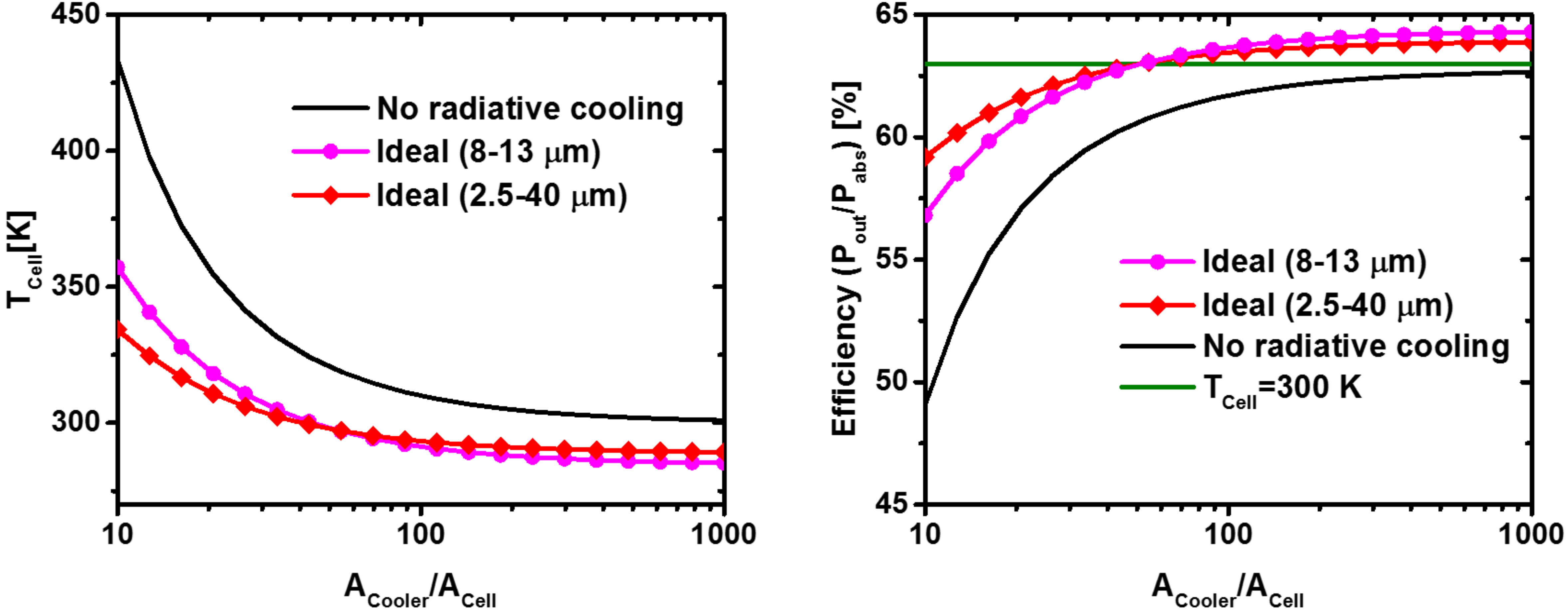
P_{conv}: convection power at the exposed surface

$R = A_{cooler}/A_{cell}$ (Area ratio)

$$P_{emit}(T_E, E > E_g) + R \cdot P_{atm} = P_{out}(T_C) + P_{rad,cell}(T_C) + R \cdot P_{rad}(T_C) + (2R - 1) \cdot P_{conv}$$

Z. Zhou *et al.*, *SPIE Conf. Proc.* (2016).

Radiative Cooling Reduces Temperature and Improves Performance Substantially



Z. Zhou *et al*., *SPIE Conf. Proc.* (submitted).

Methods

- Radiative cooling – a passive technique that dissipates heat into remote space via thermal radiation
- Develop a simulation tool, RadCool, to model radiative cooling

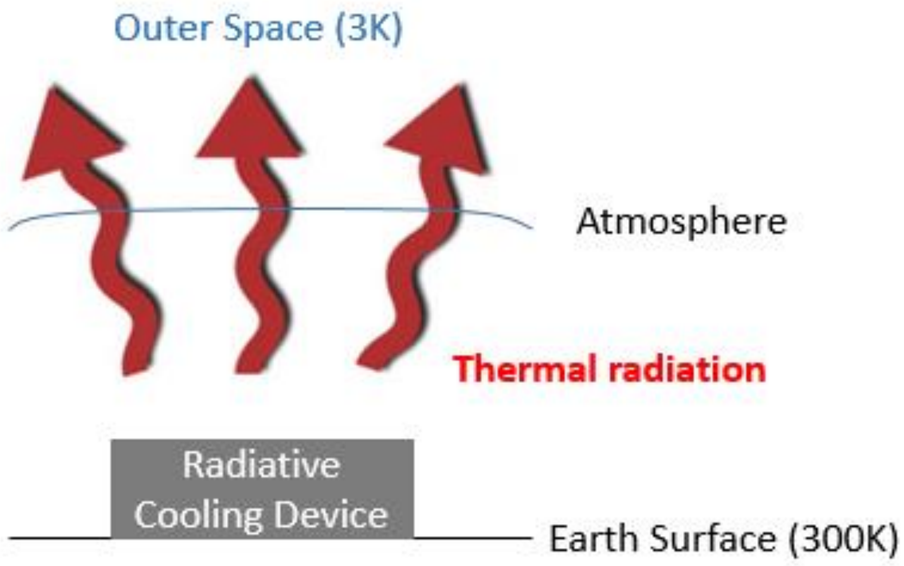


Figure 3. Radiative cooling concept

System overview

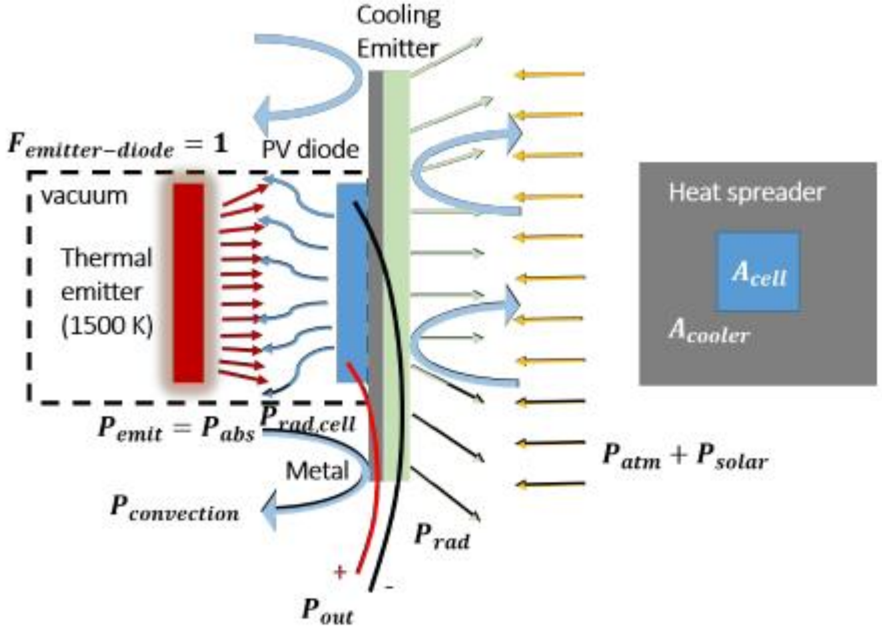
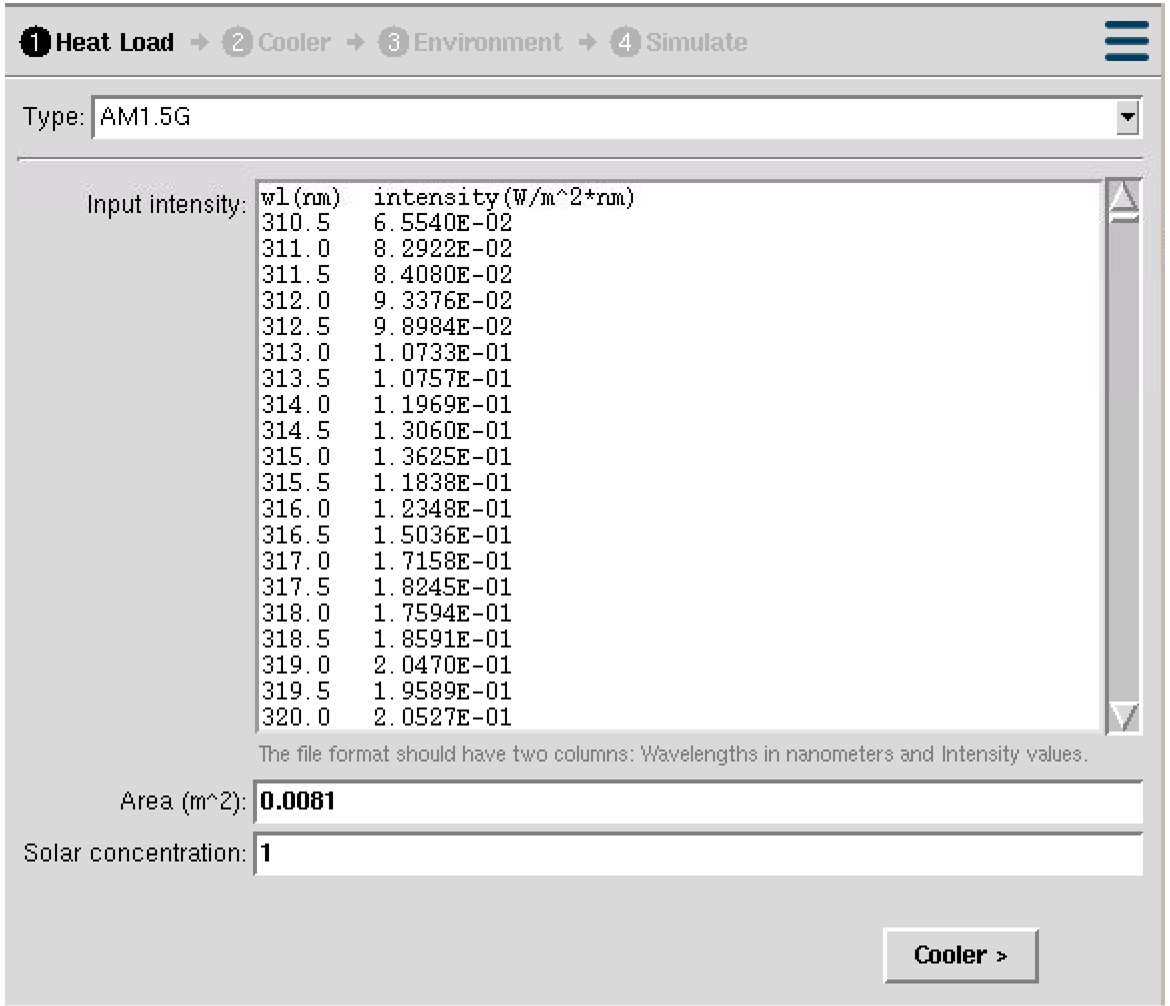


Figure 4. Schematic of the TPV system with a radiative coo

Equilibrium heat transfer analysis: $P_{abs} + P_{atm} + P_{sun} = P_{rad} + P_{rad,cell} + P_{out} + P_{cov}$

[3] Z. Zhou, X. Sun and P. Bermel, "Radiative cooling for thermophotovoltaic systems," Proc. of SPIE, vol. 9973, 2016.

Simulation tool - input



Type: AM1.5G

Input intensity:

```
wl(nm)   intensity(W/m^2*nm)
310.5    6.5540E-02
311.0    8.2922E-02
311.5    8.4080E-02
312.0    9.3376E-02
312.5    9.8984E-02
313.0    1.0733E-01
313.5    1.0757E-01
314.0    1.1969E-01
314.5    1.3060E-01
315.0    1.3625E-01
315.5    1.1838E-01
316.0    1.2348E-01
316.5    1.5036E-01
317.0    1.7158E-01
317.5    1.8245E-01
318.0    1.7594E-01
318.5    1.8591E-01
319.0    2.0470E-01
319.5    1.9589E-01
320.0    2.0527E-01
```

The file format should have two columns: Wavelengths in nanometers and Intensity values.

Area (m^2): 0.0081

Solar concentration: 1

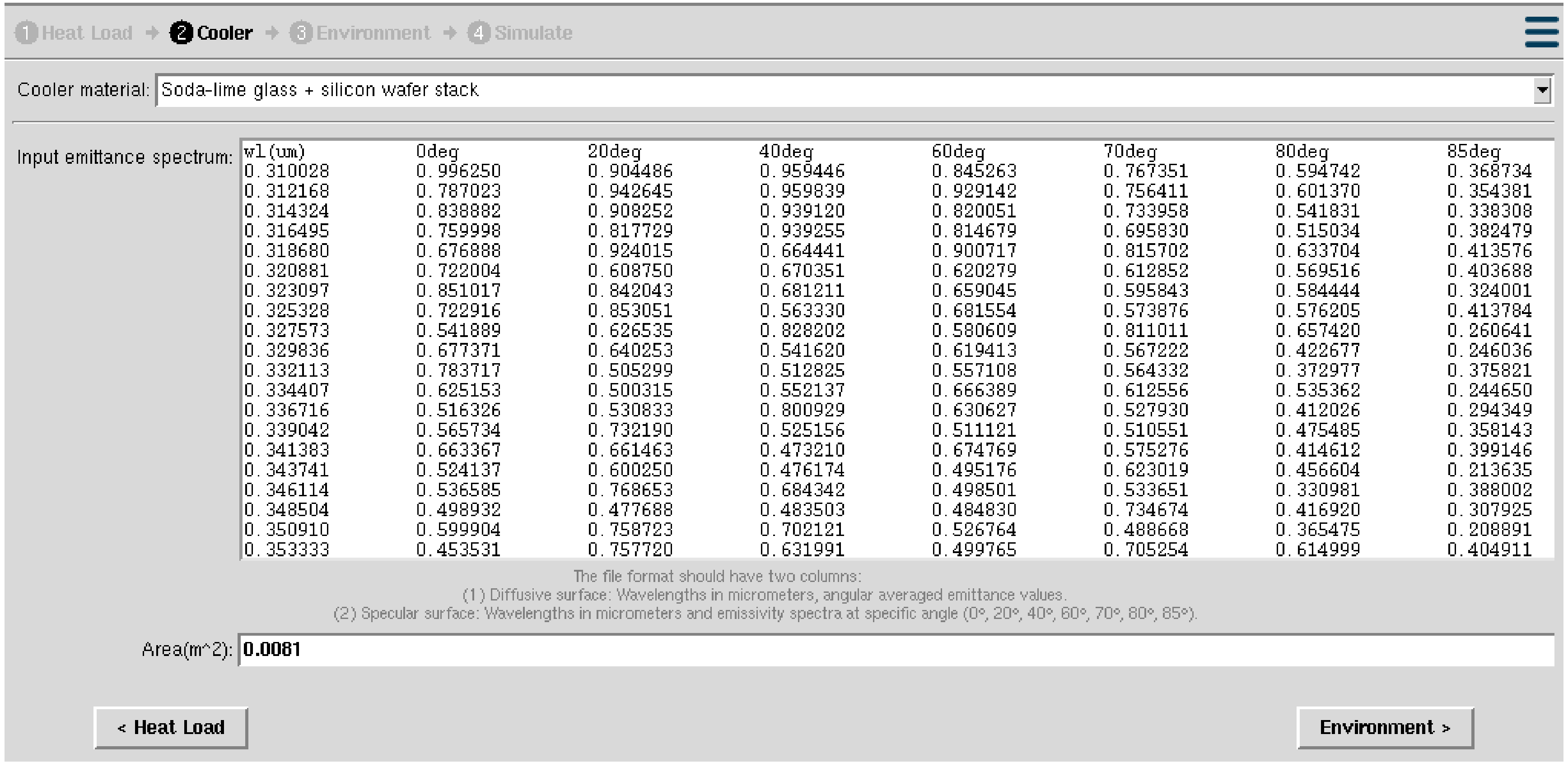
Heat load phase

- Solar absorption power

$$P_{sun} = conc.* A * \int_{0}^{\infty} d\lambda \varepsilon(\lambda) I_{AM1.5}(\lambda)$$

*Assuming incidence angle is 0

Simulation tool - input



Cooler material: Soda-lime glass + silicon wafer stack

Input emittance spectrum:

wl(um)	0deg	20deg	40deg	60deg	70deg	80deg	85deg
0.310028	0.996250	0.904486	0.959446	0.845263	0.767351	0.594742	0.368734
0.312168	0.787023	0.942645	0.959839	0.929142	0.756411	0.601370	0.354381
0.314324	0.838882	0.908252	0.939120	0.820051	0.733958	0.541831	0.338308
0.316495	0.759998	0.817729	0.939255	0.814679	0.695830	0.515034	0.382479
0.318680	0.676888	0.924015	0.664441	0.900717	0.815702	0.633704	0.413576
0.320881	0.722004	0.608750	0.670351	0.620279	0.612852	0.569516	0.403688
0.323097	0.851017	0.842043	0.681211	0.659045	0.595843	0.584444	0.324001
0.325328	0.722916	0.853051	0.563330	0.681554	0.573876	0.576205	0.413784
0.327573	0.541889	0.626535	0.828202	0.580609	0.811011	0.657420	0.260641
0.329836	0.677371	0.640253	0.541620	0.619413	0.567222	0.422677	0.246036
0.332113	0.783717	0.505299	0.512825	0.557108	0.564332	0.372977	0.375821
0.334407	0.625153	0.500315	0.552137	0.666389	0.612556	0.535362	0.244650
0.336716	0.516326	0.530833	0.800929	0.630627	0.527930	0.412026	0.294349
0.339042	0.565734	0.732190	0.525156	0.511121	0.510551	0.475485	0.358143
0.341383	0.663367	0.661463	0.473210	0.674769	0.575276	0.414612	0.399146
0.343741	0.524137	0.600250	0.476174	0.495176	0.623019	0.456604	0.213635
0.346114	0.536585	0.768653	0.684342	0.498501	0.533651	0.330981	0.388002
0.348504	0.498932	0.477688	0.483503	0.484830	0.734674	0.416920	0.307925
0.350910	0.599904	0.758723	0.702121	0.526764	0.488668	0.365475	0.208891
0.353333	0.453531	0.757720	0.631991	0.499765	0.705254	0.614999	0.404911

The file format should have two columns:
(1) Diffusive surface: Wavelengths in micrometers, angular averaged emittance values.
(2) Specular surface: Wavelengths in micrometers and emissivity spectra at specific angle (0°, 20°, 40°, 60°, 70°, 80°, 85°).

Area(m^2): 0.0081

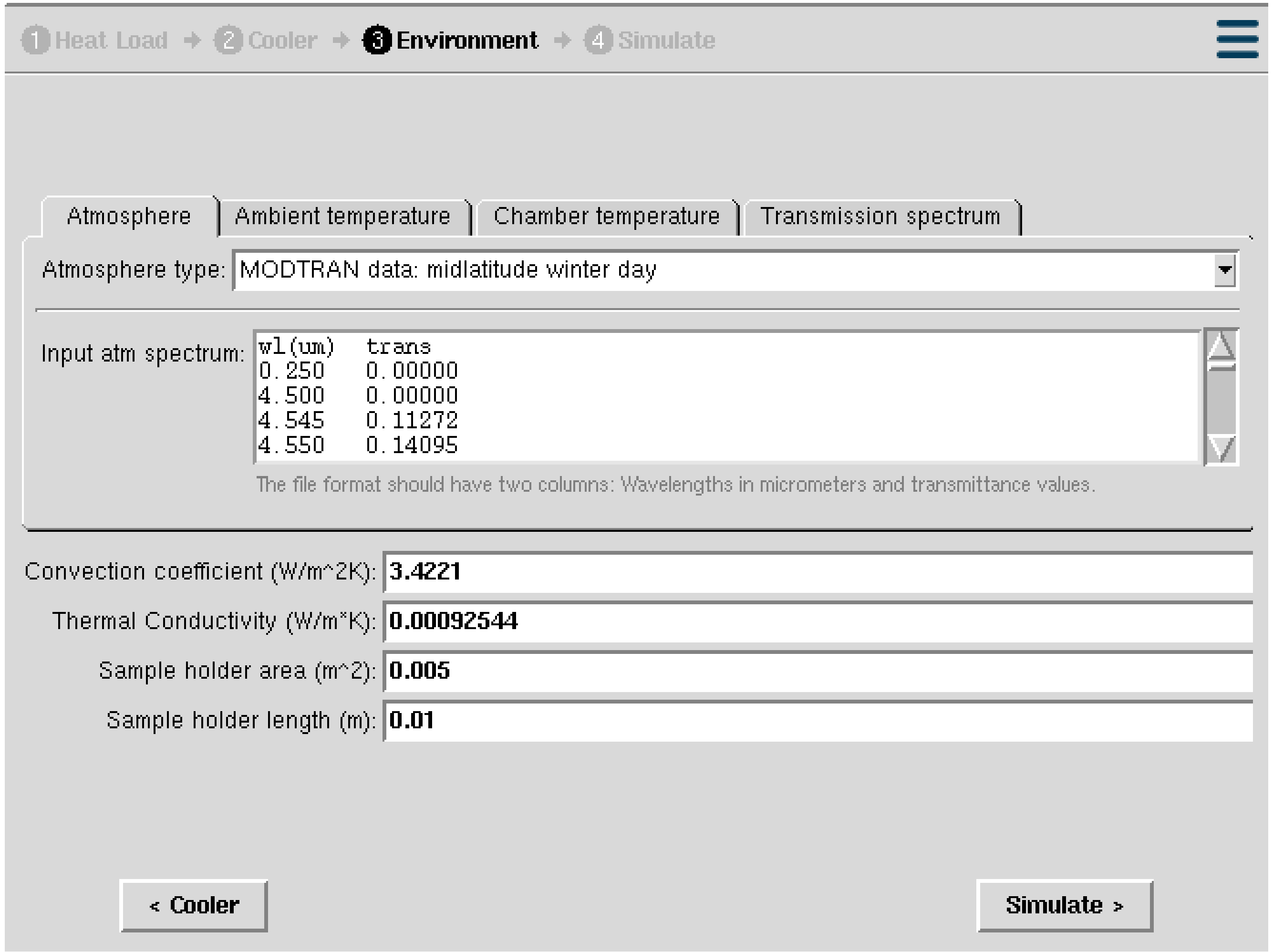
Cooler phase

- Thermal radiated power

$$P_{rad} = \int d\Omega cos\theta \int_0^{\infty} d\lambda I_{BB} \varepsilon$$

*I_{BB} is the spectral radiance of a blackbody at temperature T

simulation tool - input



Atmosphere type: MODTRAN data: midlatitude winter day

Input atm spectrum:

```
wl(um)   trans
0.250    0.00000
4.500    0.00000
4.545    0.11272
4.550    0.14095
```

The file format should have two columns: Wavelengths in micrometers and transmittance values.

Convection coefficient (W/m^2K): 3.4221

Thermal Conductivity (W/m*K): 0.00092544

Sample holder area (m^2): 0.005

Sample holder length (m): 0.01

Environment Phase

- Absorbed thermal radiation from the atmosphere

$$P_{atm} = \int d\Omega cos\theta \int_0^\infty d\lambda I_{BB} \varepsilon(\lambda,\Omega) \varepsilon_{atm}(\lambda,\Omega)$$

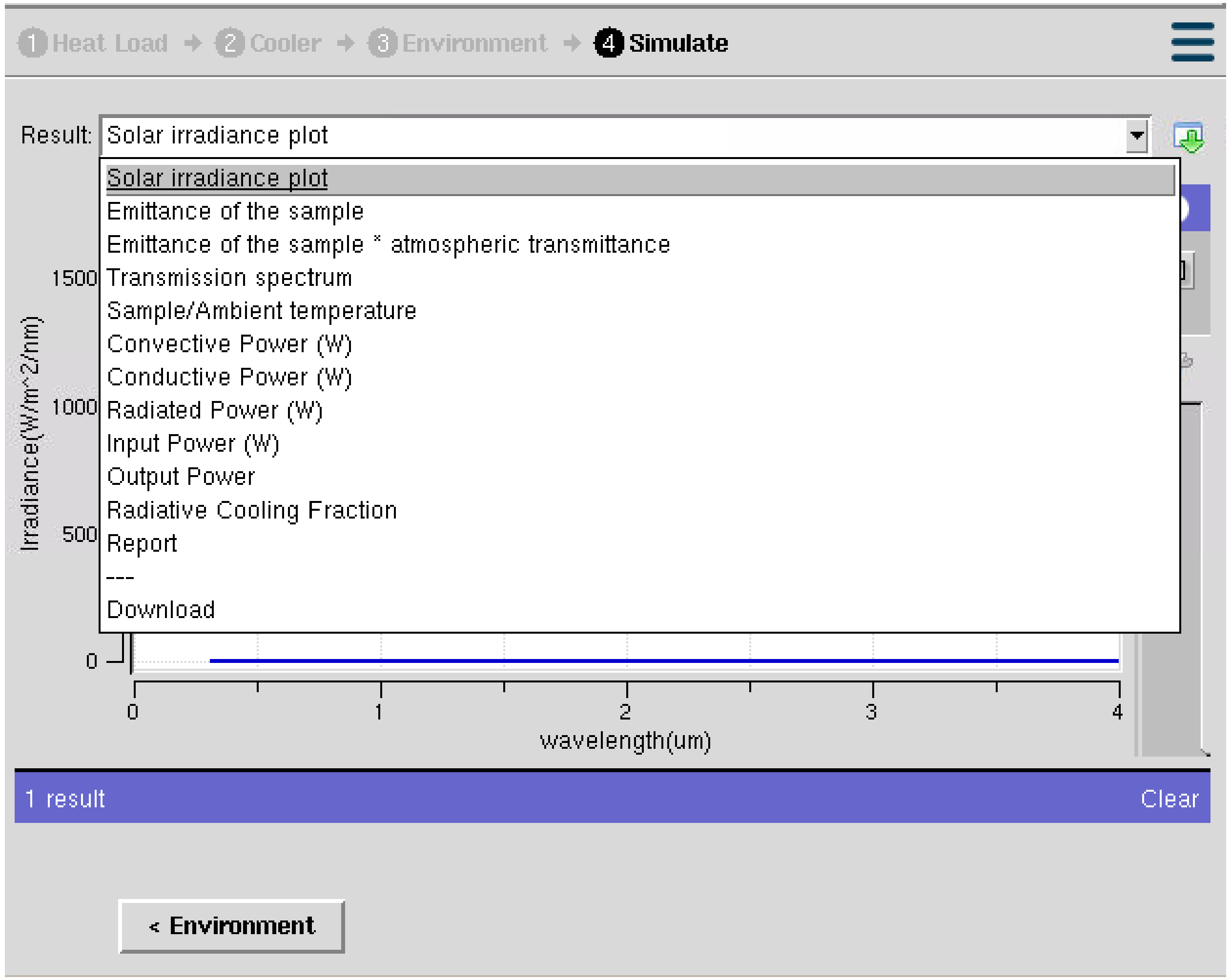
- Conductive Power

$$P_{cod} = K * (T - T_{chamb})$$

- Convective Power

$$P_{cov} = 2 \, * h_c * A \, * (T - T_{chamb})$$

Simulation tool - output

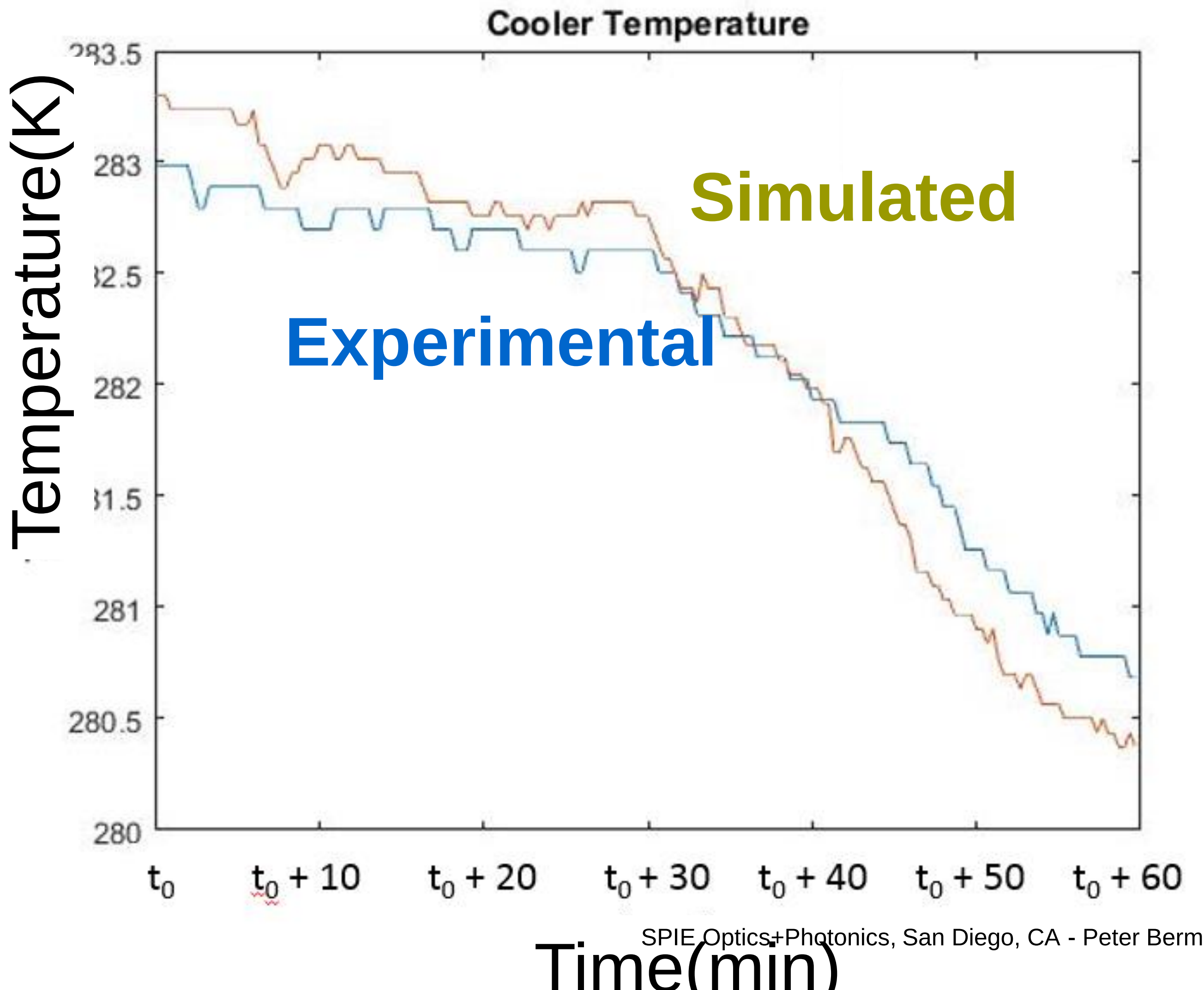


Result: Solar irradiance plot

The steady-state temperature T of the sample is determined by:

$$P_{rad}(T) - P_{atm}(T_{amb}) - P_{sun} + P_{cod+cov} = 0$$

Experimental verification



Experimental data

- Area ratio of the heat load and the cooler: 1
- Cooling material: silicon wafer with soda-lime glass
- Transmission spectrum: polyethylene film

Ambient temperature on the day of the experiment: ~290K

Conclusions/future work

- RadCool successfully models radiative cooling system in a graphical interface
- More experiments need to be done to confirm the generality of the system and modeling approach
- RadCool can be connected directly with the existing TPV model
- The radiative cooling technique is not limited to TPV systems
  - Potential applications include solar cell cooling, infrared detectors, and sensitive electronic devices that are used outdoors.

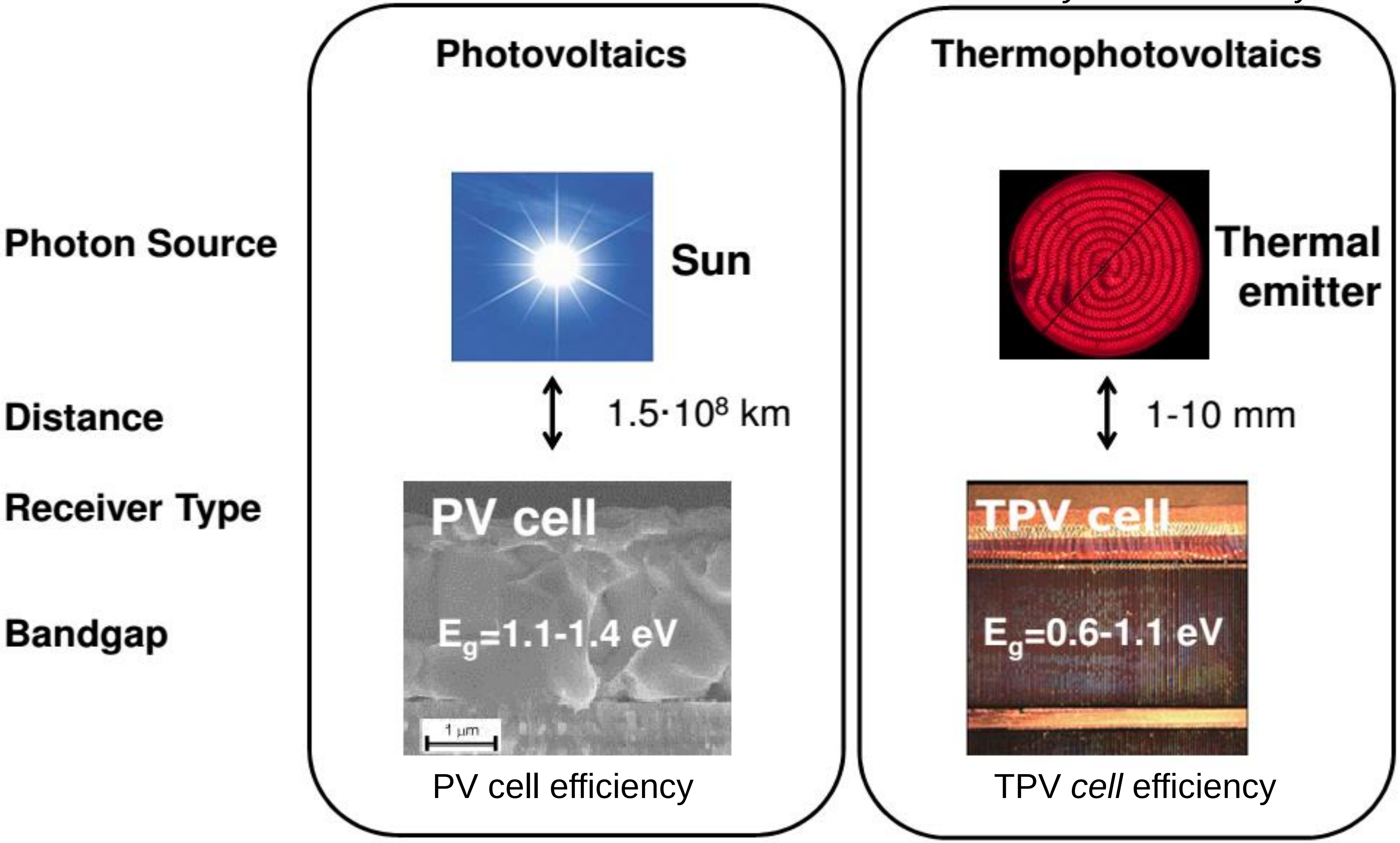
Step 3: Combine Hot and Cold Objects for Maximum Efficiencies

Key tools:

- TPXsim
- TPVexpt

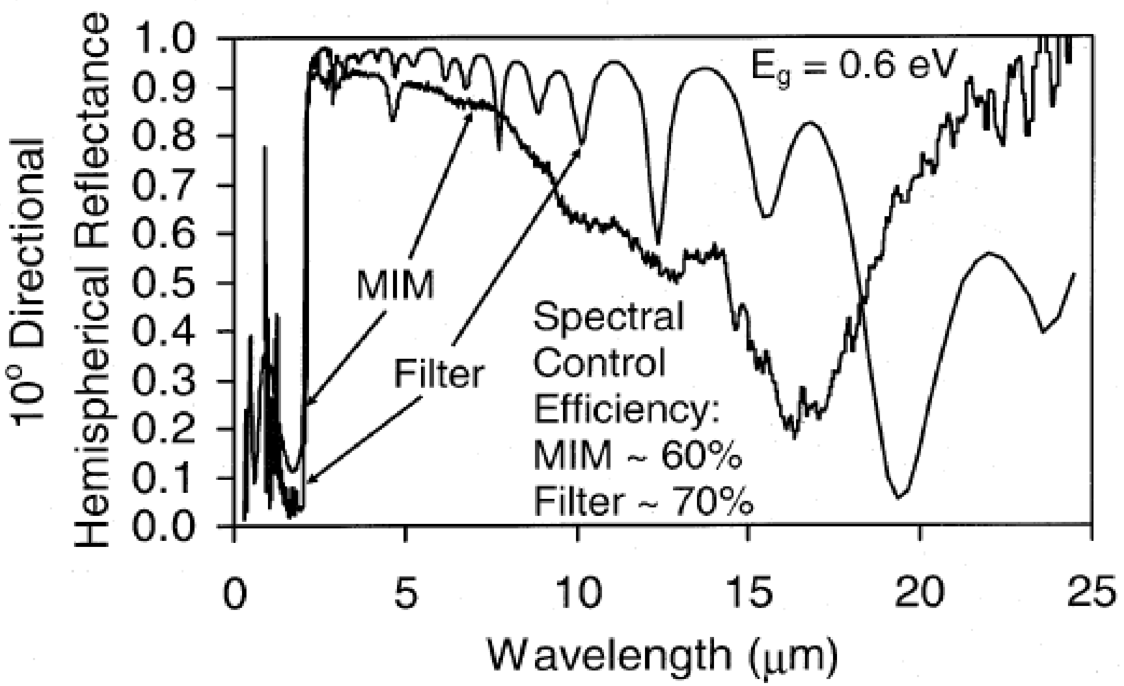
What Makes TPV Different from PV?

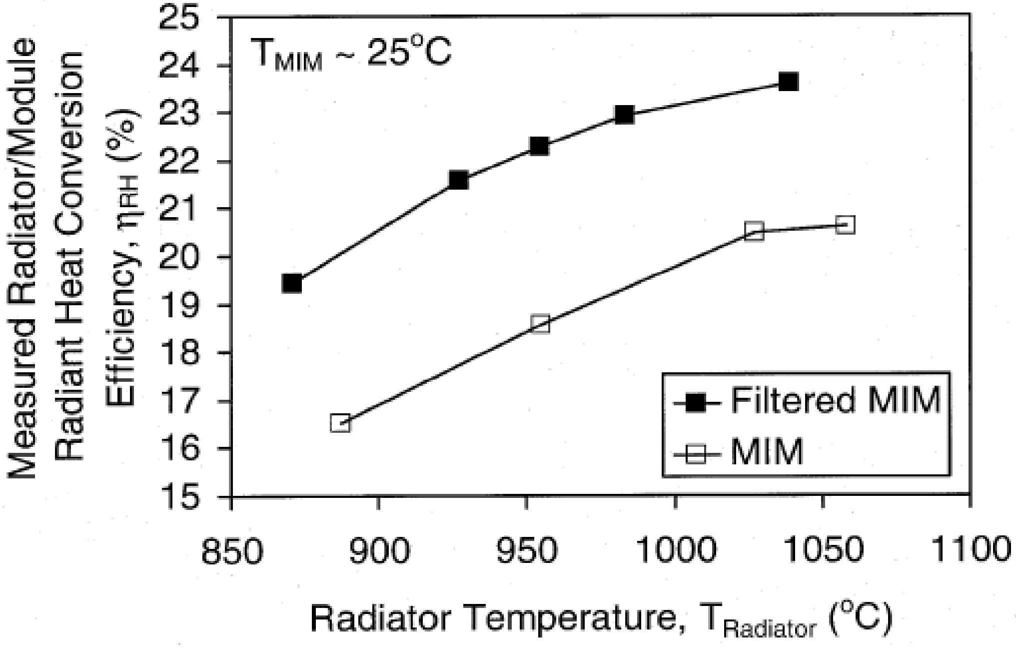
TPV *system* efficiency



	Photovoltaics	Thermophotovoltaics
Photon Source	**Sun**	**Thermal emitter**
Distance	$1.5 \cdot 10^8$ km	1-10 mm
Receiver Type	**PV cell**	**TPV cell**
Bandgap	E_g=1.1-1.4 eV	E_g=0.6-1.1 eV
	PV cell efficiency	TPV *cell* efficiency

23% Demonstrated TPV Electric Generation Efficiency with Spectral Control



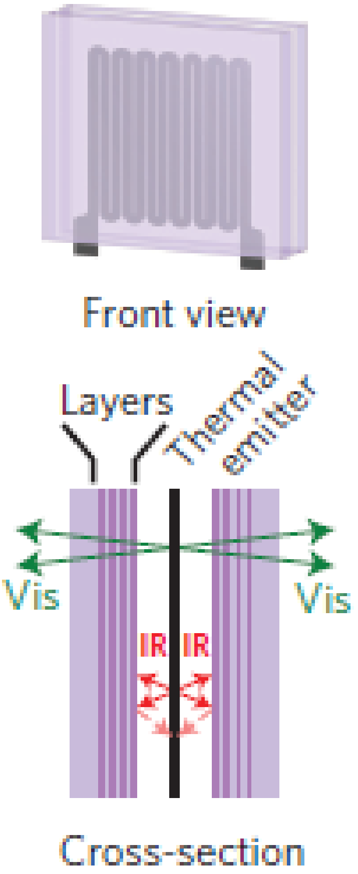


Reflection spectrum for optical filter and receiver

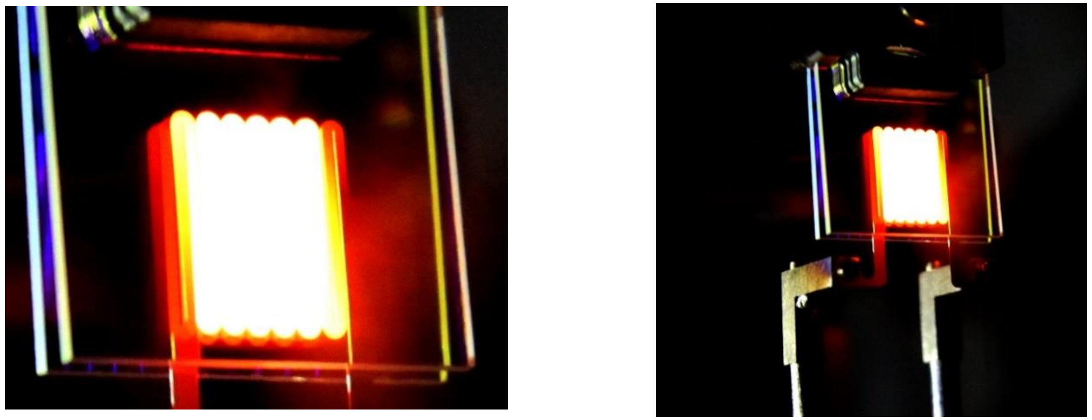
Efficiency in converting radiation to electricity

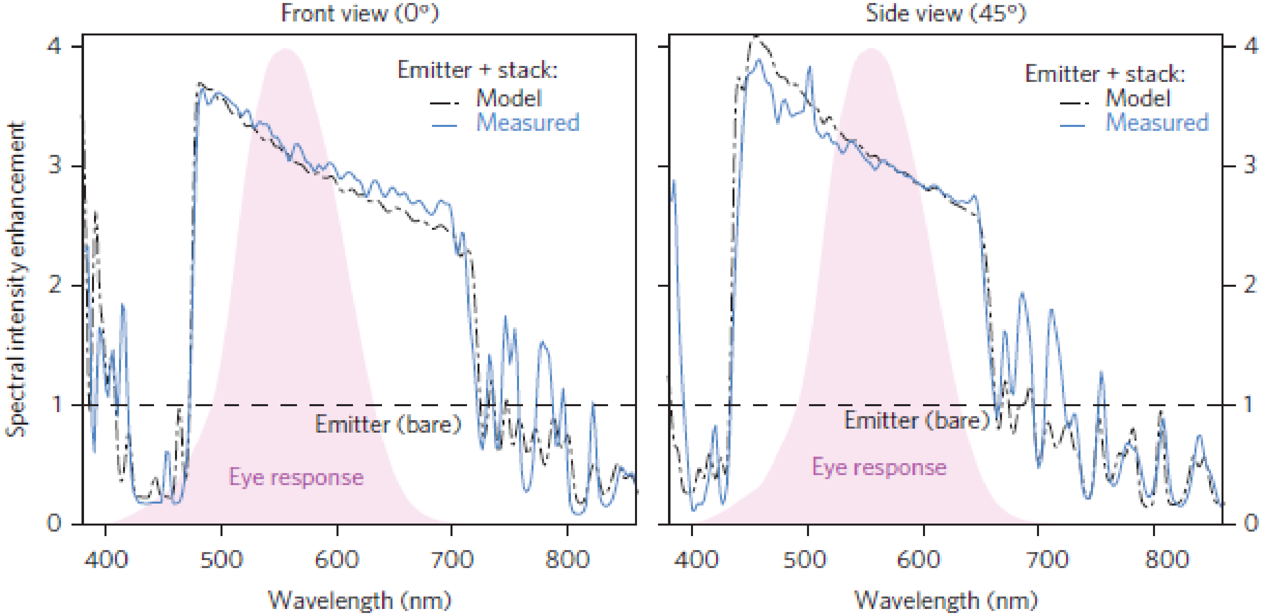
B. Wernsman *et al.*, *IEEE Trans. Electron Dev.* **51**, 512 (2004)

Photon Recycling Can Greatly Reshape High Temperature Thermal Emission

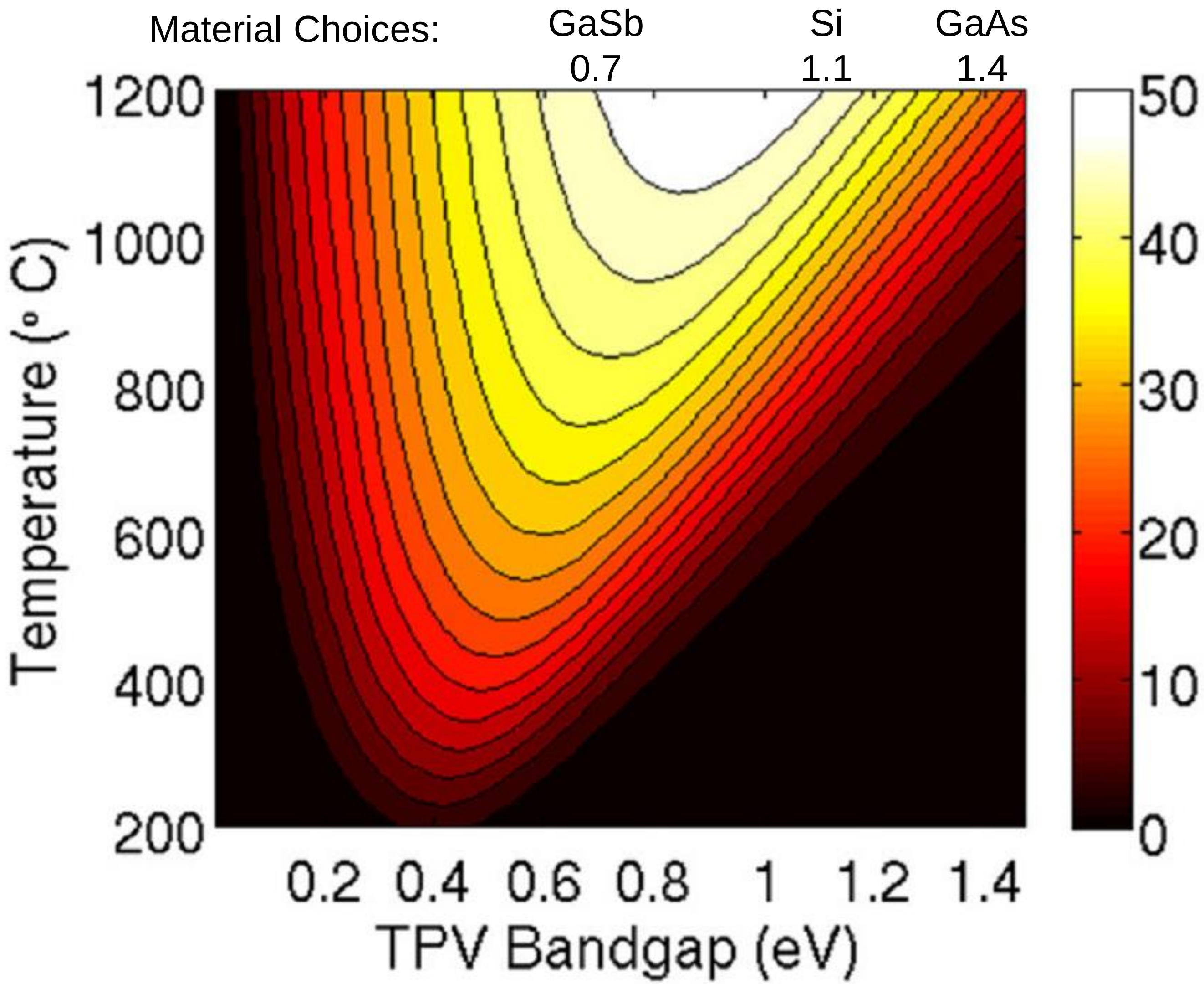


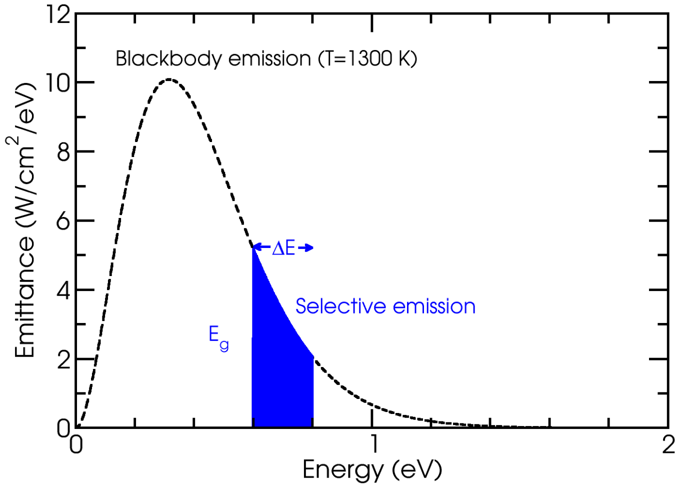
Ilic, Bermel *et al.*, *Nature Nanotechnol.* (2016)





TPV Efficiencies May Approach 52%* at Reasonable Temperatures†



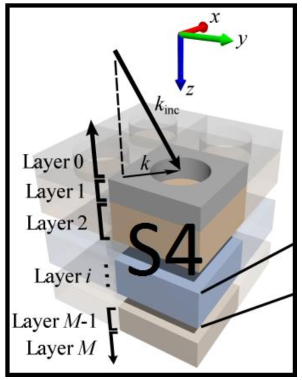


*Using highly selective emitters shown above, with MOVPE-grown GaSb TPV cells

† World record $\eta = 23\%$ at 1050 °C

B. Wernsman *et al.*, *IEEE Trans. Electron Dev.* **51**, 512 (2004)

PHYSICS AND MATH



Kirchoff's Law:

(Emissivity = Absorptivity)

$e_\lambda = a_\lambda$

$$J(V) = \underbrace{\int_0^\infty d\lambda \left[\frac{2qc}{\lambda^4}\frac{\varepsilon(\lambda)\mathrm{EQE}(\lambda)}{\exp(hc/\lambda kT)-1}\right]}_{\text{PV current}} - \underbrace{\left[\frac{q(n^2+1)E_g^2kT_d}{4\pi^2\hbar^3c^2}e^{-E_g/mkT_d}+J_{nr}\right](e^{qV/mkT_d}-1)}_{\text{Dark Current}}, \quad (1)$$

PV current

Dark Current

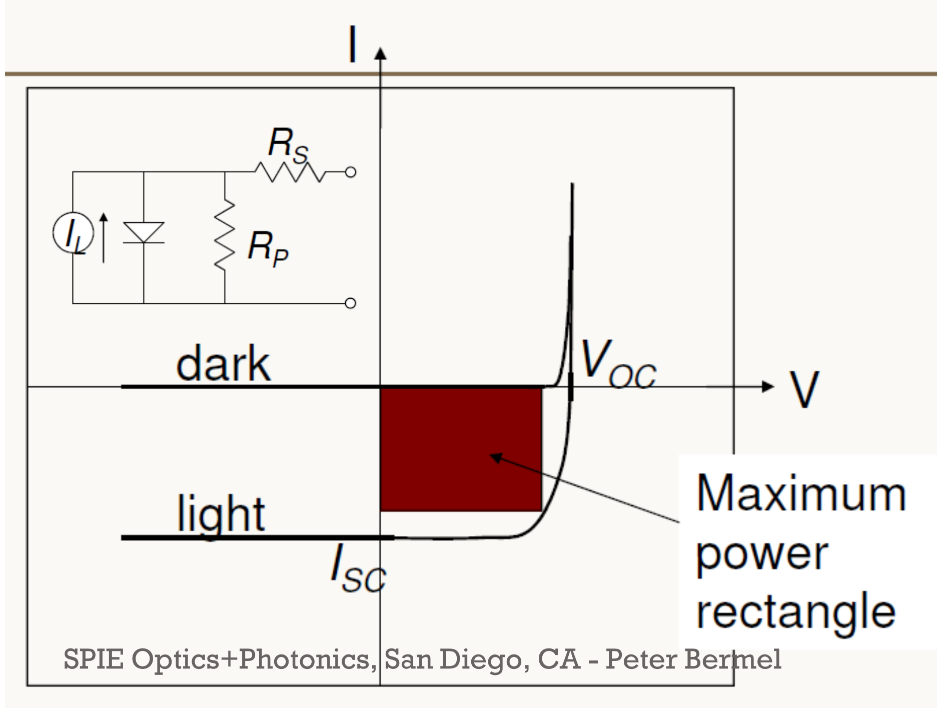
$$\eta_E \equiv \frac{\text{useful radiated power}}{\text{total radiated power}} = \frac{\int_0^{\lambda_\ell} q_\lambda(\mathrm{d})\mathrm{d}\lambda}{\int_0^\infty q_\lambda(\mathrm{d})\mathrm{d}\lambda}$$

$$= \frac{\int_0^{\lambda_\ell} \varepsilon_\lambda e_{bs}(\lambda, T_s)\mathrm{d}\lambda}{\int_0^\infty \varepsilon_\lambda e_{bs}(\lambda, T_s)\mathrm{d}\lambda}$$

Radiation Efficiency

$$\overline{\varepsilon} = \frac{\int_0^\infty d\lambda\, \varepsilon(\lambda)/\{\lambda^5[\exp(hc/\lambda kT)-1]\}}{\int_0^\infty d\lambda/\{\lambda^5[\exp(hc/\lambda kT)-1]\}}.$$

Average Emissivity



V_{OC}, open circuit voltage

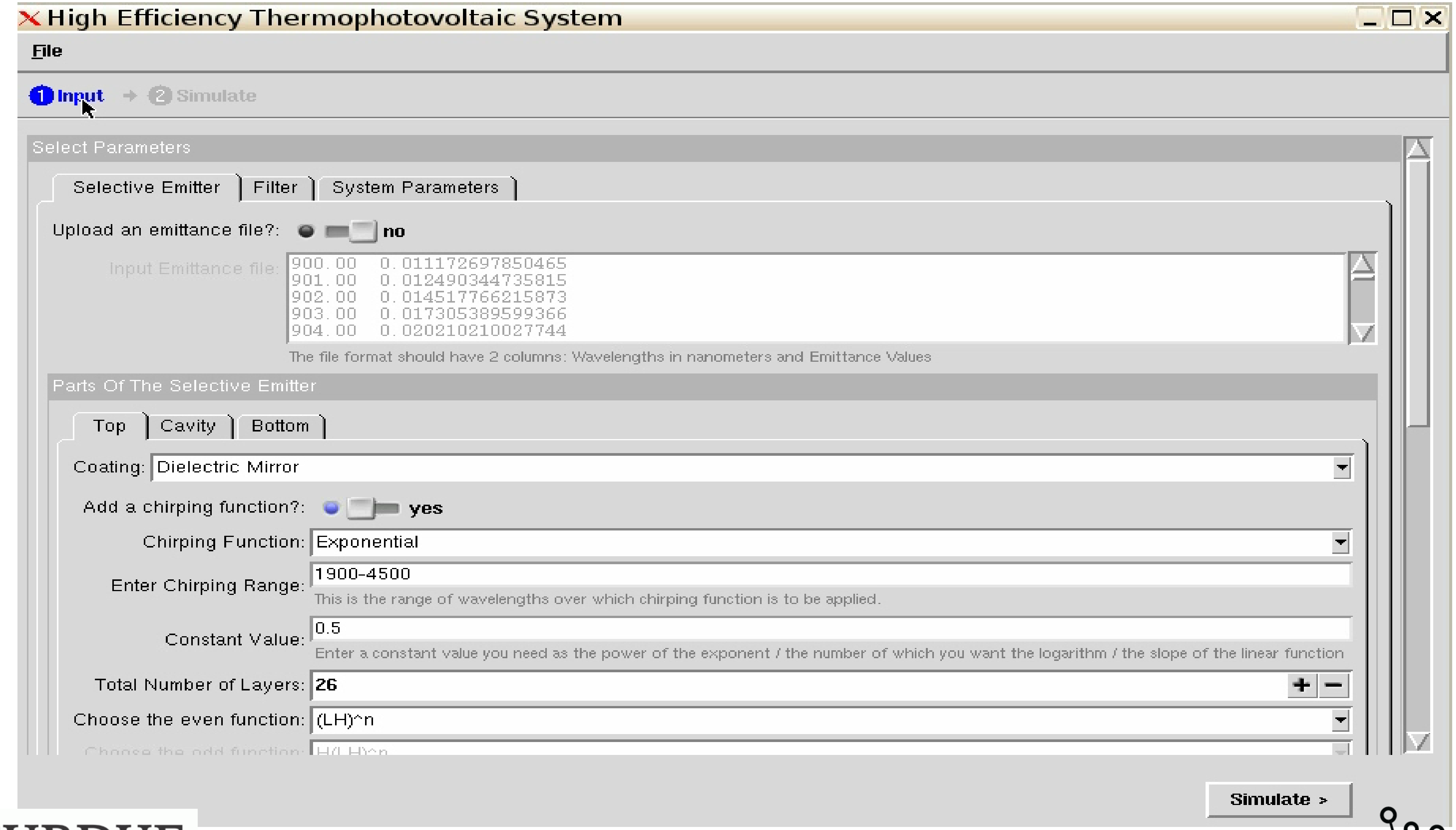
I_{SC}, short circuit current

$$\text{FF, fill factor} = \frac{\text{max. power rectangle}}{V_{OC}\cdot I_{SC}}$$

Power conversion efficiency

$$\eta = \frac{V_{OC} \times I_{SC} \times FF}{P_{inc}}$$

TPXSIM: A SYSTEM-LEVEL MODELING TOOL



Upload an emittance file?: ● no

Input Emittance file:

```
900.00   0.011172697850465
901.00   0.012490344735815
902.00   0.014517766215873
903.00   0.017305389599366
904.00   0.020210210027744
```

The file format should have 2 columns: Wavelengths in nanometers and Emittance Values

Coating: Dielectric Mirror

Add a chirping function?: ● yes

Chirping Function: Exponential

Enter Chirping Range: 1900-4500

This is the range of wavelengths over which chirping function is to be applied.

Constant Value: 0.5

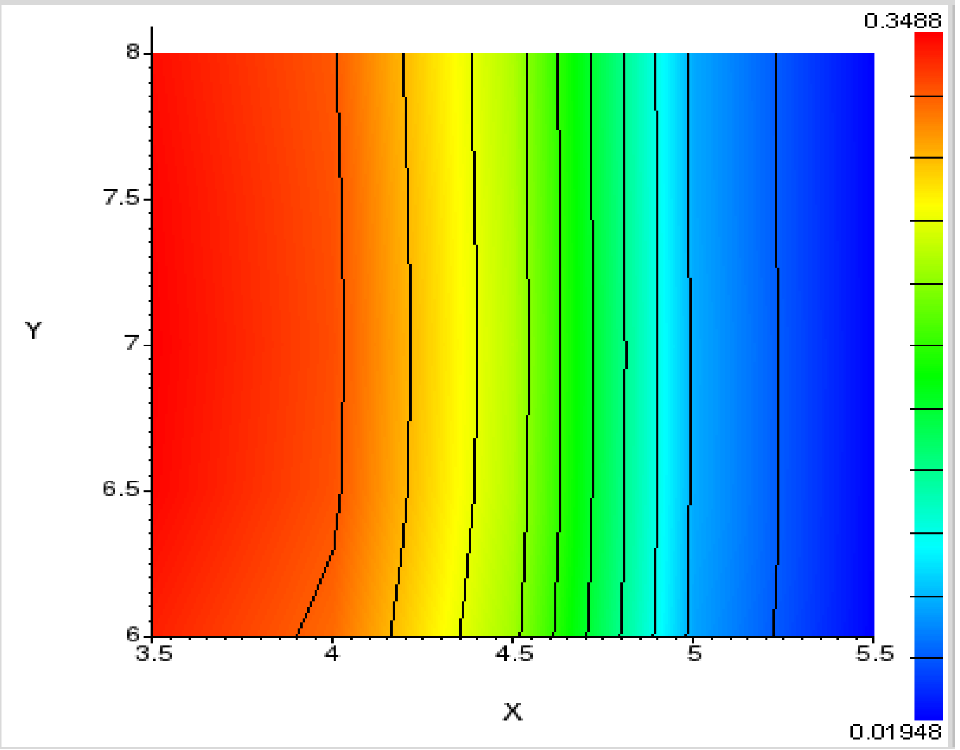
Enter a constant value you need as the power of the exponent / the number of which you want the logarithm / the slope of the linear function

Total Number of Layers: 26

Choose the even function: (LH)^n

Choose the odd function: H(LH)^n

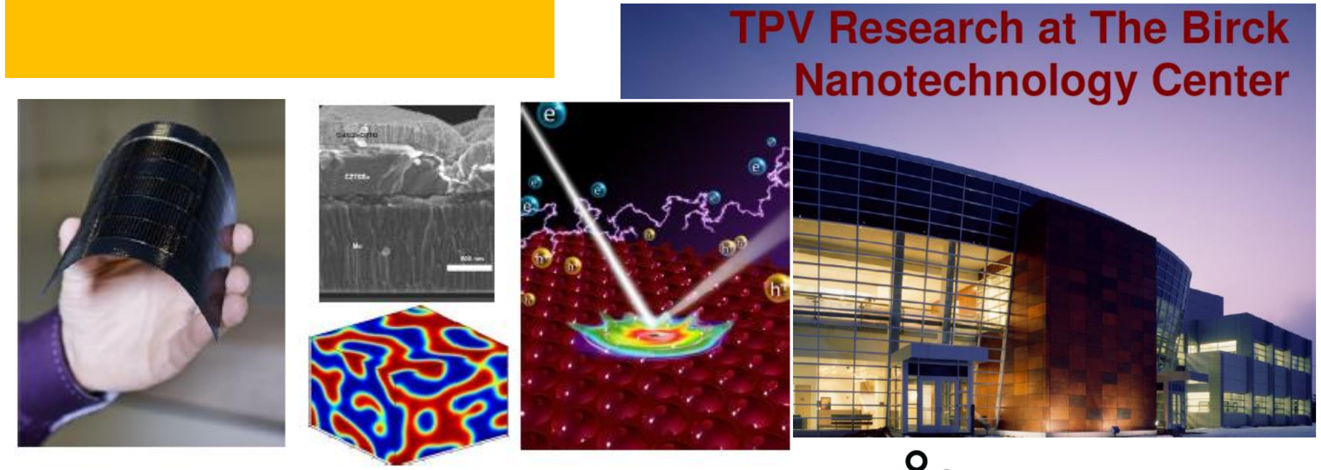
WHAT ARE THE BEST CASE EFFICIENCIES?



Contour plot showing the combination of filter bandgap and PV bandgap leading to maximum efficiency Or, just an emittance plot

- Unprecedented Efficiency of 33.89% is achievable for a filter band gap of 0.37 eV and PV band gap of 0.75 eV

Why is this meaningful?
Ongoing Research in Birck Nanotechnology center will use these predictions to experimentally fabricate and characterize these structures

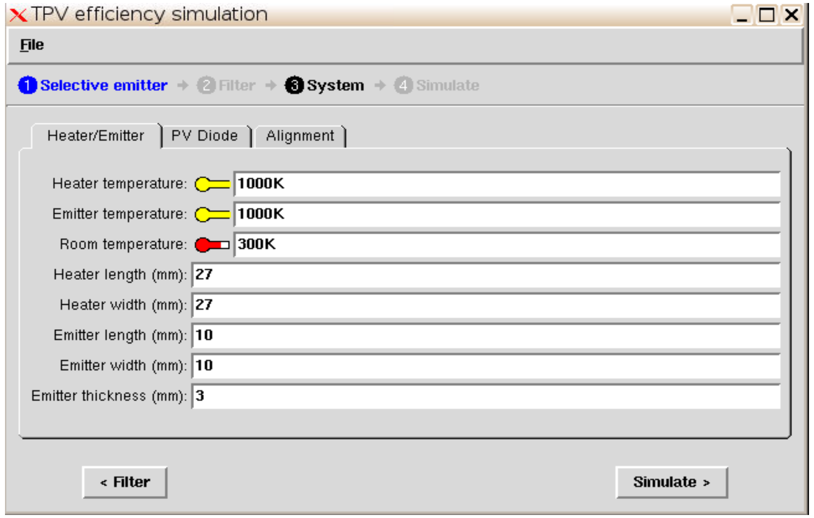


PURDUE UNIVERSITY

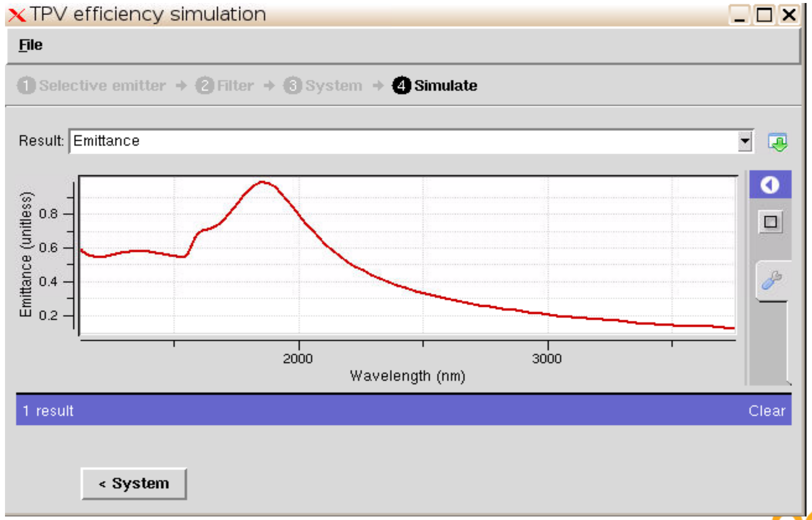
nanoHUB

TPVexpt

- Based on TPVtest
- Considers complex rectangular geometries for heater, emitter, and PV diode
- Considers non-idealities (e.g., series/shunt resistance)
- Phased GUI with overhauled “System” tab



Heater temperature: 1000K
Emitter temperature: 1000K
Room temperature: 300K
Heater length (mm): 27
Heater width (mm): 27
Emitter length (mm): 10
Emitter width (mm): 10
Emitter thickness (mm): 3



Result: Emittance

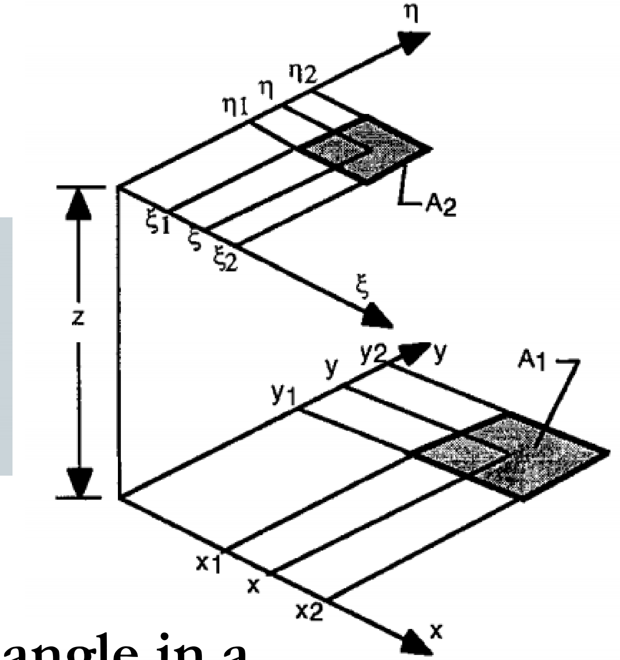
View Factor/Geometry

- **View factor:** $\boldsymbol{F_{A\rightarrow B}}$ is the proportion of the radiation which leaves surface $\boldsymbol{A}$ that strikes surface $\boldsymbol{B}$
- View factor from cell to emitter for power calculations

Definitions: $X = x/z;\ N = \eta/z;\ Y = y/z;$
$S = \xi/z;\ \alpha_{li} = S_l - X_i;\ \beta_{kj} = N_k - Y_j$

$$F_{1-2} = \frac{1}{(X_2 - X_1)(Y_2 - Y_1)} \sum_{l=1}^{2} \sum_{k=1}^{2} \sum_{j=1}^{2} \sum_{i=1}^{2} \left[(-1)^{(i+j+k+l)} G(\alpha_{li}, \beta_{jk}) \right]$$

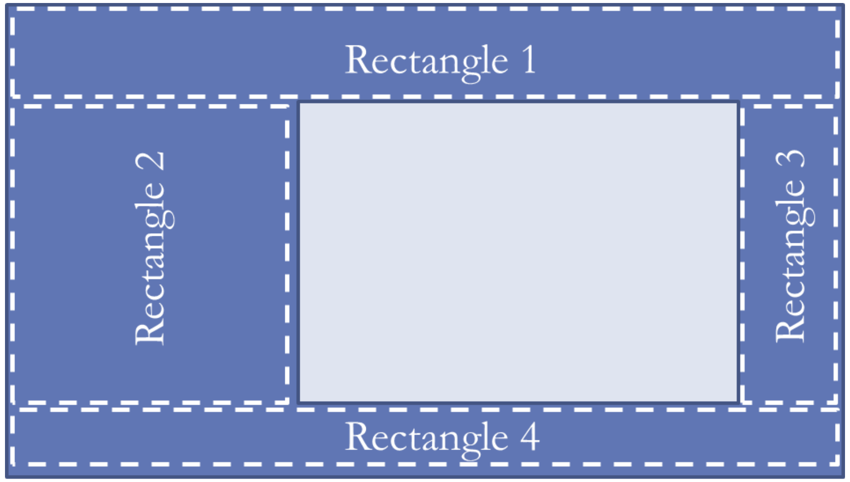
$$\text{where } G(\alpha_{li}, \beta_{jk}) = \frac{1}{2\pi} \left\{ \alpha_{li}(1 + \beta_{kj}^2)^{1/2} \tan^{-1}\left[\frac{\alpha_{li}}{(1 + \beta_{kj}^2)^{1/2}} \right] - \beta_{kj} \tan^{-1} \beta_{kj} \right.$$



View factor calculation for rectangle to rectangle in a parallel plane. All boundaries are parallel or perpendicular to x and ξ boundaries [2].

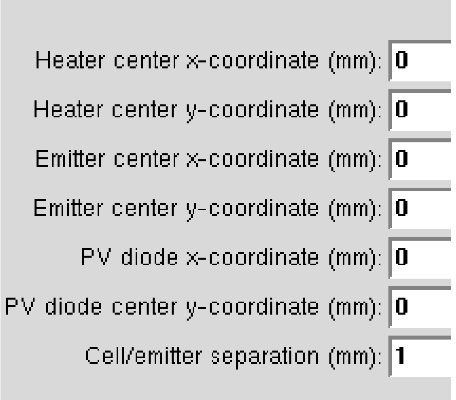
View Factor Implementation

- Heater, emitter, and cell modeled as rectangles
- Emitter physically attached to heater
- Heater area broken up into four rectangles for calculations
- Sum of rectangle view factors is equal to heater view factor
- Accounts for thickness of emitter and heater radiation



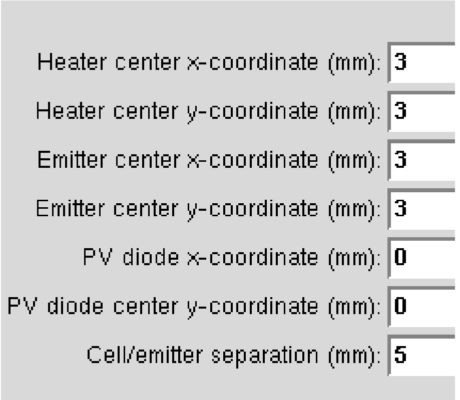
Method of calculating heater view factor. The back rectangle represents the heater (dark blue). The light blue rectangle represents the emitter.

View Factor Effect on Output



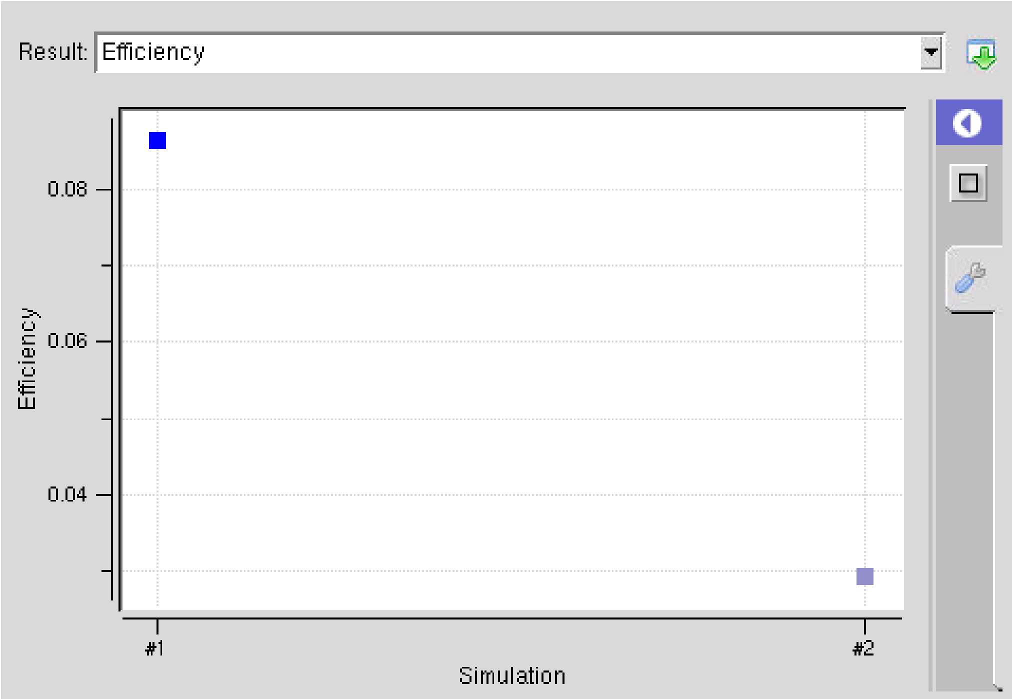
Heater center x-coordinate (mm): 0
Heater center y-coordinate (mm): 0
Emitter center x-coordinate (mm): 0
Emitter center y-coordinate (mm): 0
PV diode x-coordinate (mm): 0
PV diode center y-coordinate (mm): 0
Cell/emitter separation (mm): 1

Simulation 1



Heater center x-coordinate (mm): 3
Heater center y-coordinate (mm): 3
Emitter center x-coordinate (mm): 3
Emitter center y-coordinate (mm): 3
PV diode x-coordinate (mm): 0
PV diode center y-coordinate (mm): 0
Cell/emitter separation (mm): 5

Simulation 2

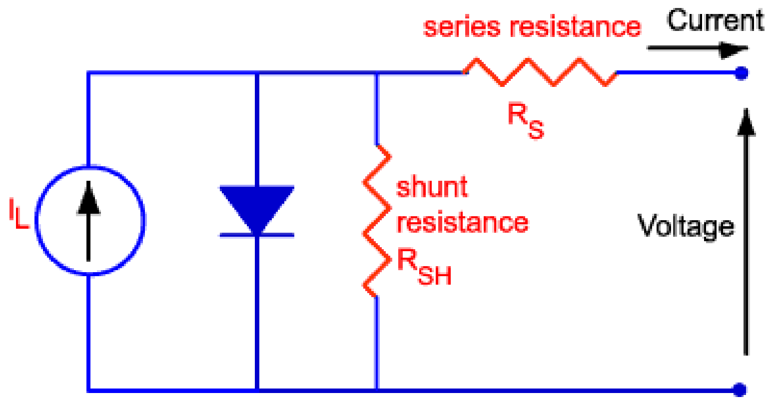


Result: Efficiency

Efficiency results. Simulation 1 results in higher efficiency due to a greater view factor (better alignment)

Shunt/Series Resistance

- Fill factor (FF) determines the efficiency of PV cell
- Ideal cell has series resistance of 0 Ω and shunt of ∞ Ω
- Non-idealities decrease FF [6]



Parasitic series and shunt resistances in PV cell model [6].

$$\eta = \frac{V_{OC} I_{SC} FF}{P_{in}} \qquad FF = \frac{V_{OC} - \ln(V_{OC} + 0.72)}{V_{OC} + 1} \qquad r_S = \frac{R_S}{R_{CH}} \qquad r_{SH} = \frac{R_{SH}}{R_{CH}}$$

$$FF = FF_0 \left\{ (1 - 1.1 r_S) + \frac{r_S^2}{5.4} \right\} \left\{ 1 - \frac{V_{OC} + 0.7}{V_{OC}} \frac{FF_0}{r_{SH}} \left[(1 - 1.1 r_S) + \frac{r_S^2}{5.4} \right] \right\}$$

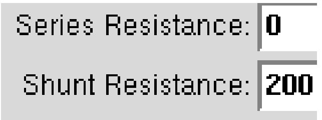
Shunt/Series Effect on Output

Series Resistance: 0
Shunt Resistance: 0

Ideal case (simulation 1)

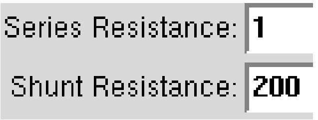
Series Resistance: 1
Shunt Resistance: 0

Series only (simulation 2)



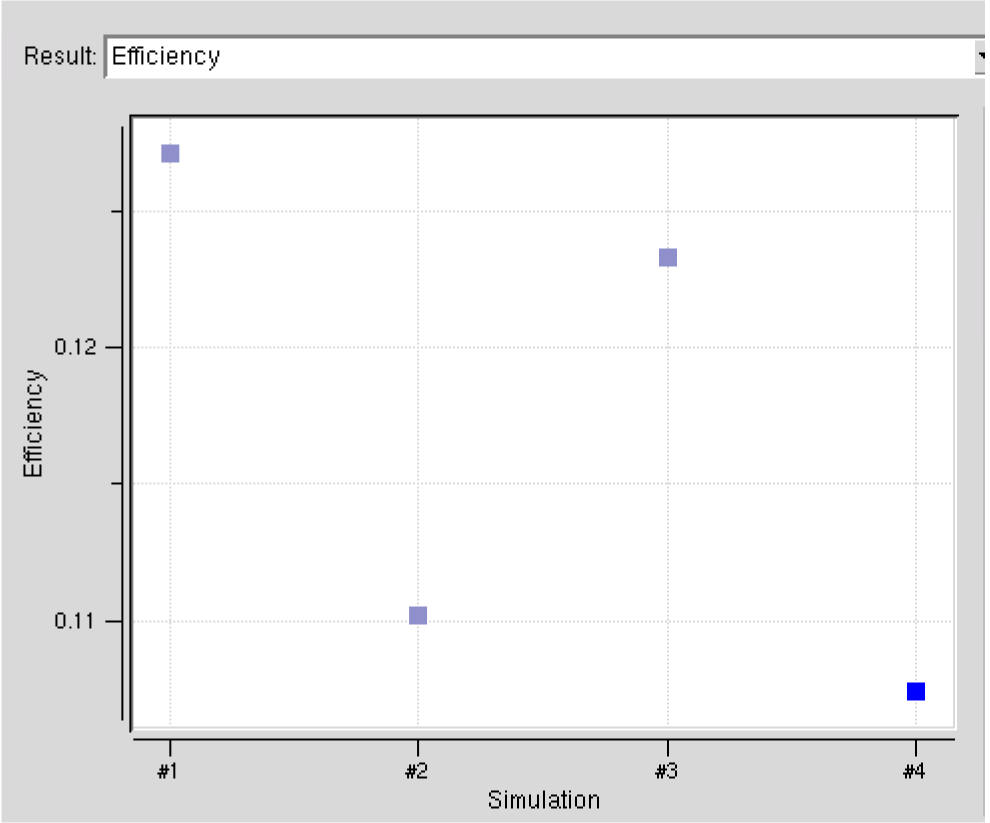
Series Resistance: 0
Shunt Resistance: 200

Shunt only (simulation 3)



Series Resistance: 1
Shunt Resistance: 200

Series and shunt (simulation 4)



Result: Efficiency

Efficiency values with varying series and shunt resistances. Default program values with emitter-cell distance of 0.1 mm.

Step 4: Improving Low-Bandgap Photovoltaic Cells

Key tool(s):

- ADEPT
- MEEPPV

Drift-Diffusion Model

- Electrostatics (Poisson's equation):

$$\nabla \cdot \varepsilon \nabla V = -\left(p - n + N_D^+ - N_A^- \right)$$

- Charge conservation:

$$\frac{\partial n}{\partial t} = \frac{1}{q} \nabla \cdot \mathbf{J}_n + U_n$$

$$\frac{\partial p}{\partial t} = -\frac{1}{q} \nabla \cdot \mathbf{J}_p + U_p$$

- Current from drift & diffusion terms:

$$J_n = qn(x)\mu_n E(x) + qD_n \frac{dn}{dx}$$

$$J_p = qp(x)\mu_p E(x) - qD_p \frac{dn}{dx}$$

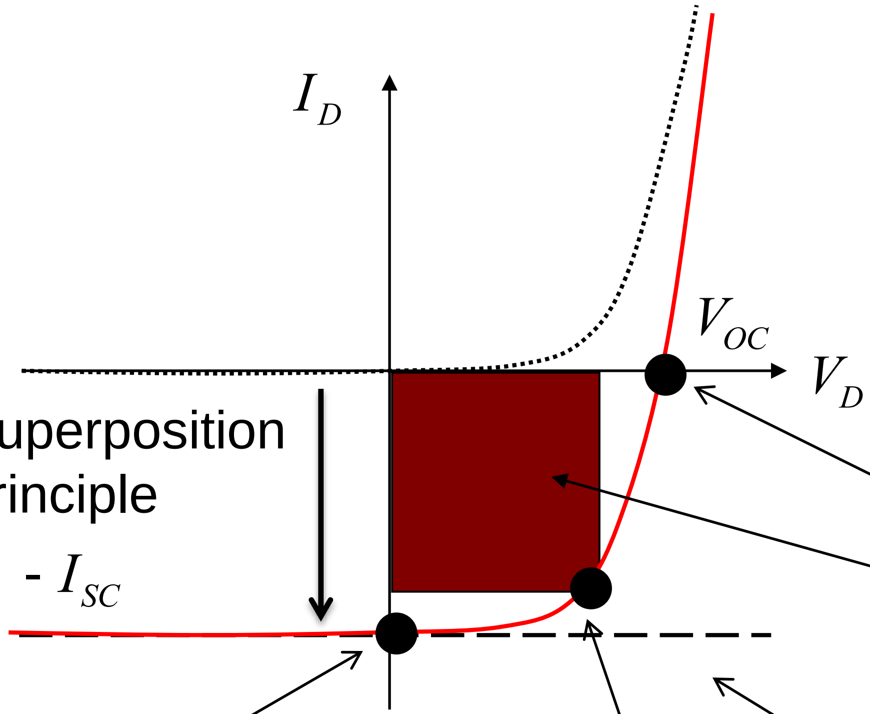
S. Selberherr: "Analysis and Simulation of Semiconductor Devices", Springer, 1984.

Solar Cells: Ideal IV Characteristics

$$I_D = I_0\left(e^{qV_D/k_BT} - 1\right)$$

$$I_{TOT} = I_0\left(e^{qV_D/k_BT} - 1\right) - I_{SC}$$

$$h = \frac{P_{out}}{P_{in}} = \frac{I_{SC}V_{OC}FF}{P_{in}}$$



Superposition principle

$$P_{out} = I_{TOT}V_{OC} = 0$$

Maximum power rectangle

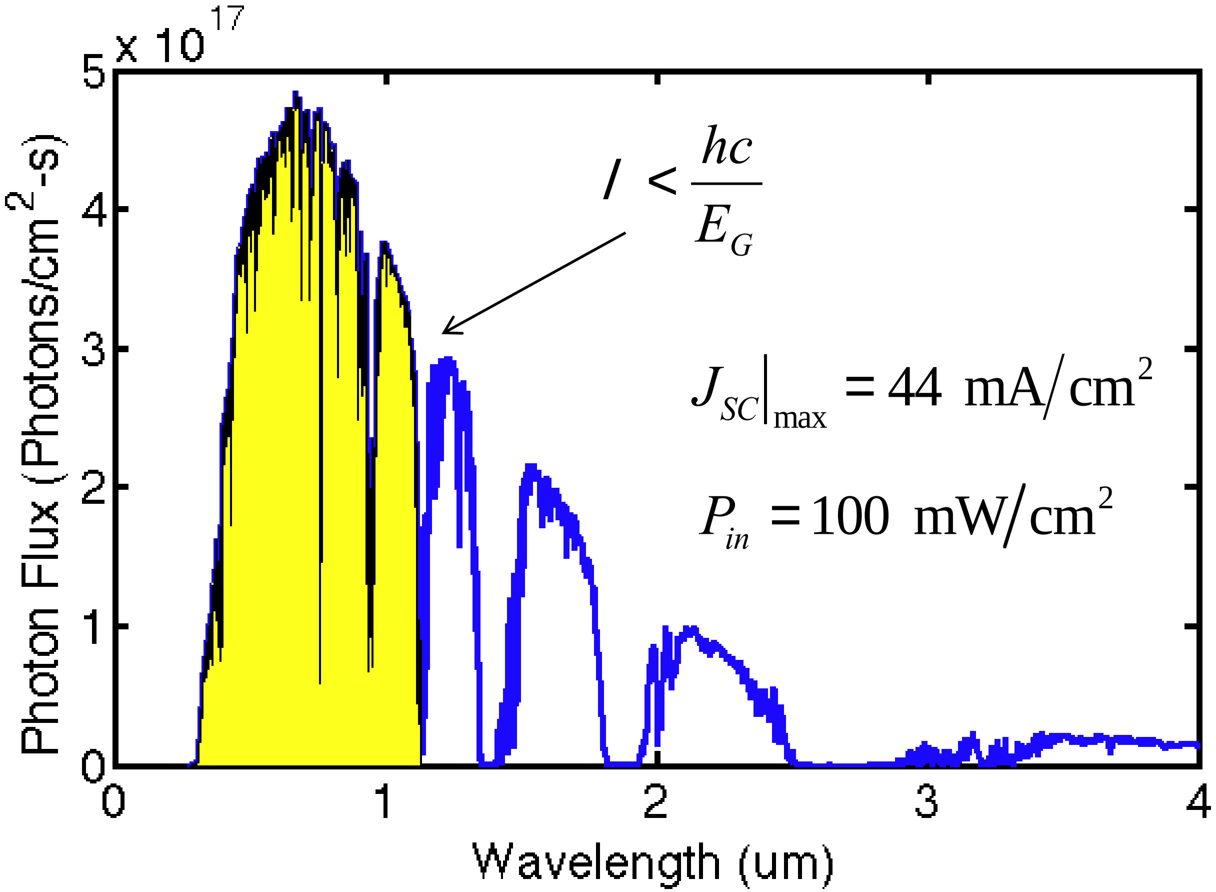
$$P_{out} = -I_{SC}V_D = 0$$

$$P_D = I_{TOT}V_D < 0$$

$$\left|P_{out}\right| = I_{mp}V_{mp} = -I_{SC}V_{OC}FF$$

Maximum Short Circuit Current

Example: Silicon E_g = 1.1eV. Only photons with a wavelength < 1.12 μm will be absorbed.



$$\lambda < \frac{hc}{E_G}$$

$$J_{SC}\big|_{\max} = 44 \ \mathrm{mA/cm^2}$$

$$P_{in} = 100 \ \mathrm{mW/cm^2}$$

solar spectrum (AM1.5G)

Open-circuit Voltage and Efficiency

$$I_{TOT} = I_0\left(e^{qV/k_BT} - 1\right) - I_{SC} \qquad V_{OC} = \frac{k_BT}{q}\ln\left(\frac{I_{SC}}{I_0}\right) \qquad \eta = \frac{P_{out}}{P_{in}} = \frac{I_{SC}V_{OC}FF}{P_{in}}$$

Example for silicon photovoltaics:

$$I_0 = 1 \times 10^{-12}\ \mathrm{A}$$

$$\eta = \frac{P_{out}}{P_{in}} = \frac{40 \times 0.63 \times 0.8}{100} = 0.20$$

$$I_{SC} = 0.90 \times 44 \times 10^{-3} = 40\ \mathrm{mA}$$

$$V_{OC} = 0.026\ln\left(\frac{40\times10^{-3}}{1\times10^{-12}}\right) = 0.63$$

Increasing the Efficiency

$$h = \frac{P_{out}}{P_{in}} = \frac{I_{SC} V_{OC} FF}{P_{in}}$$

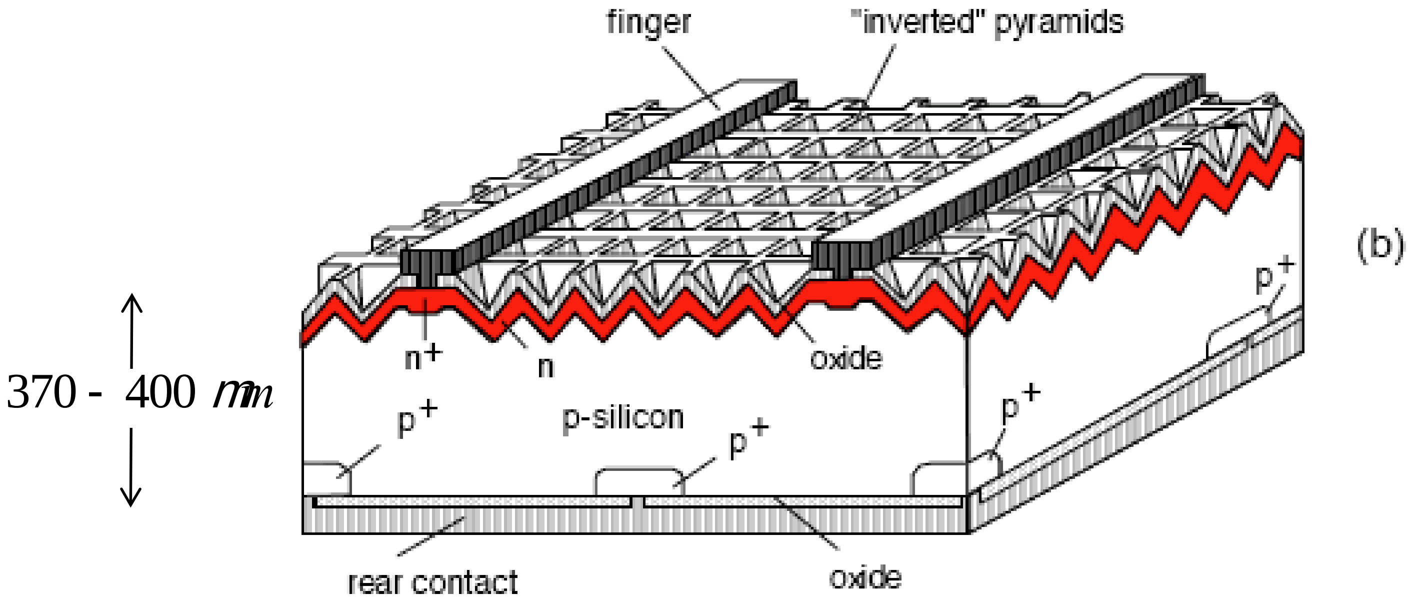
1) Increase the short circuit current from 40 towards 44

2) Increase V_{OC} (decrease I_0)

$$V_{OC} = \frac{k_B T}{q} \ln\left(\frac{I_{SC}}{I_0}\right)$$

$$I_0 = qA\left(\frac{D_n}{W_P}\frac{n_i^2}{N_A}\right)$$

Efficiency of Silicon Solar Cells (PERL Architecture)



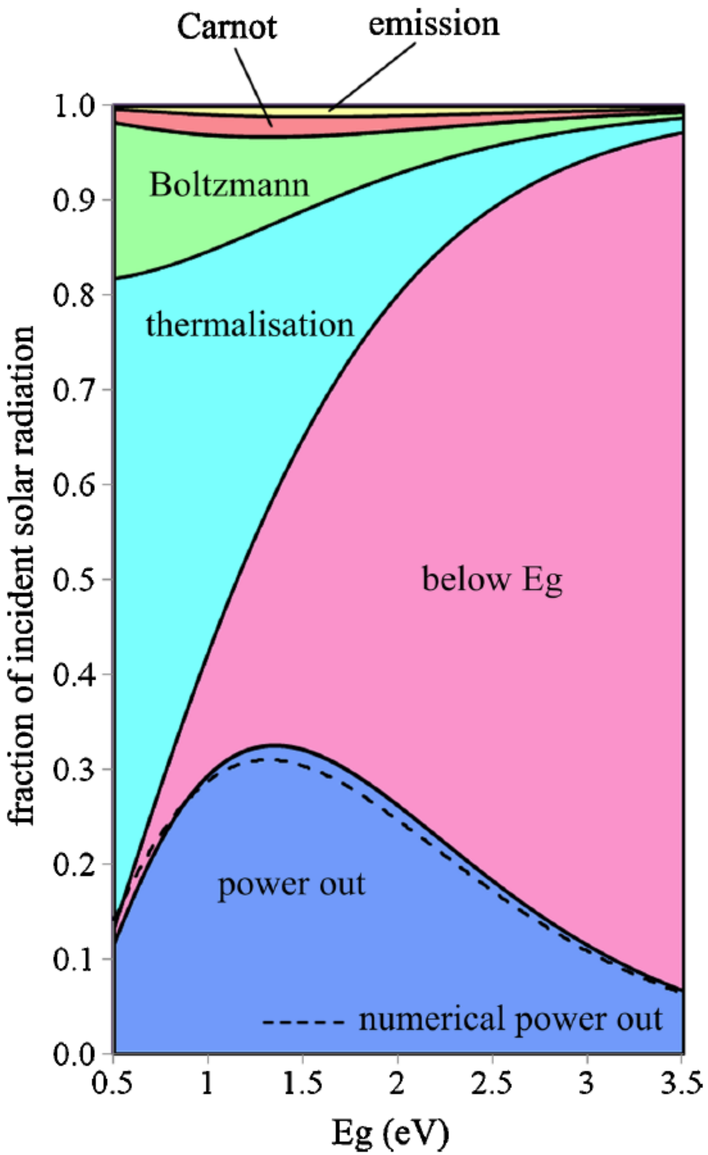
$$J_{SC} = 41.5\ \text{mA/cm}^2 \quad (94\%)$$

$$V_{OC} = 0.703 \qquad FF = 0.81$$

$$I_0 = 0.075 \times 10^{-12}\ \text{A}$$

Martin Green Group UNSW – Zhao *et al*., 1998 (25% at 1 sun)

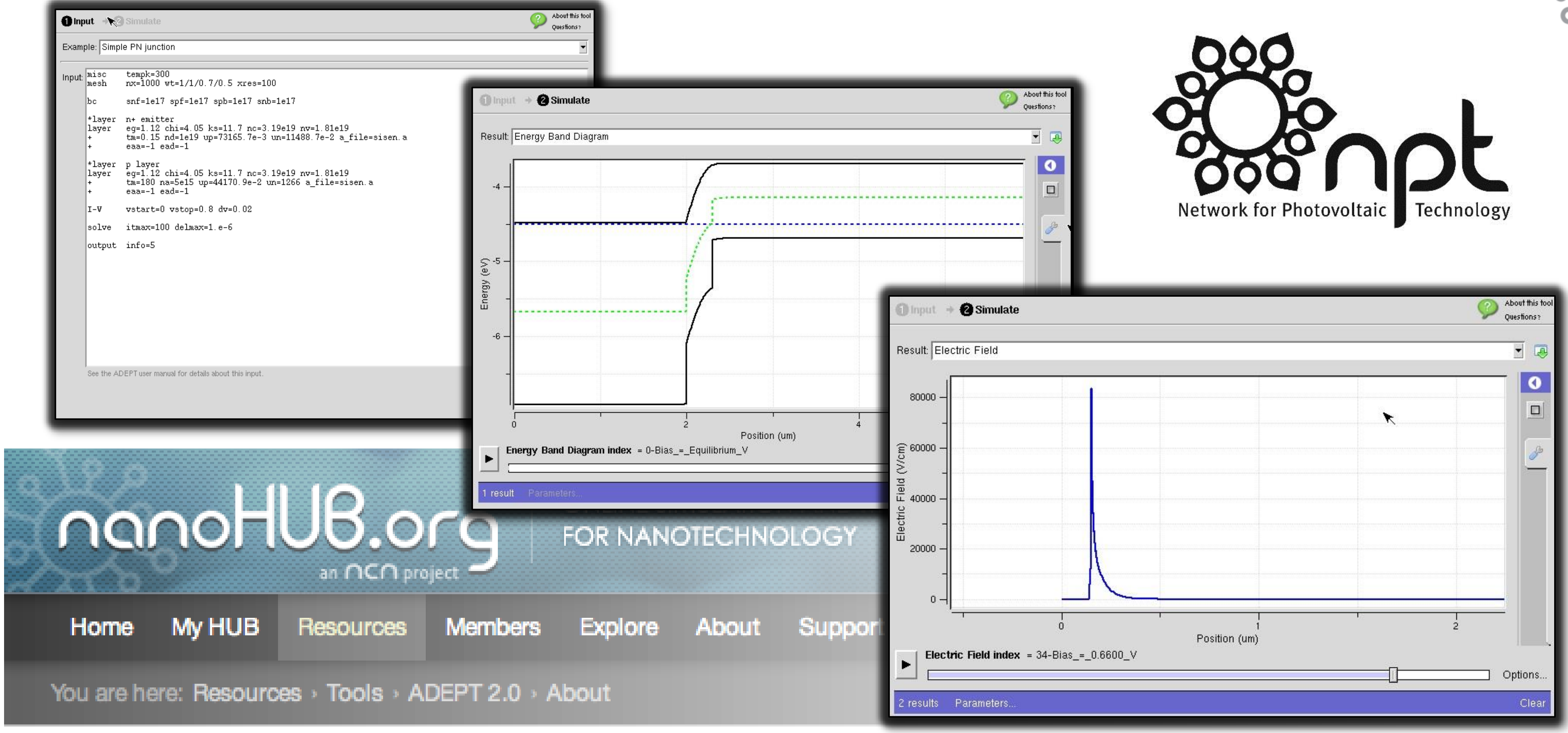
J_{SC} – V_{OC} trade-off



1) Smaller bandgaps give higher short circuit current
2) Larger bandgaps give higher open-circuit voltage
3) For the given solar spectrum, an optimum bandgap exists.

“Shockley-Queisser Limit”

ADEPT 2



Example: Simple PN junction

Input:
```
misc     tempk=300
mesh     nx=1000 wt=1/1/0.7/0.5 xres=100

bc       snf=1e17 spf=1e17 spb=1e17 snb=1e17

*layer   n+ emitter
layer    eg=1.12 chi=4.05 ks=11.7 nc=3.19e19 nv=1.81e19
+        tm=0.15 nd=1e19 up=73165.7e-3 un=11488.7e-2 a_file=sisen.a
+        eaa=-1 ead=-1

*layer   p layer
layer    eg=1.12 chi=4.05 ks=11.7 nc=3.19e19 nv=1.81e19
+        tm=180 na=5e15 up=44170.9e-2 un=1266 a_file=sisen.a
+        eaa=-1 ead=-1

I-V      vstart=0 vstop=0.8 dv=0.02

solve    itmax=100 delmax=1.e-6

output   info=5
```

See the ADEPT user manual for details about this input.

Result: Energy Band Diagram

Energy Band Diagram index = 0-Bias_=_Equilibrium_V

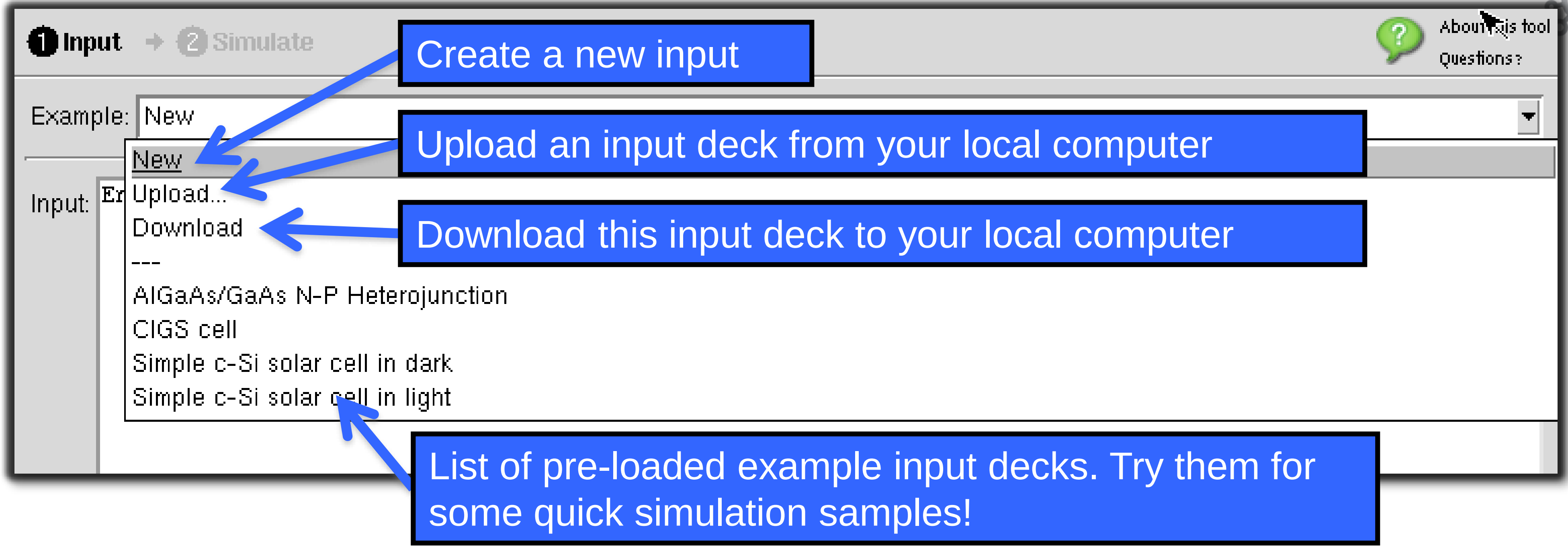
Result: Electric Field

Electric Field index = 34-Bias_=_0.6600_V

Available on nanoHUB.org via:

https://nanohub.org/tools/adeptnpt/

ADEPT: Input deck



Create a new input

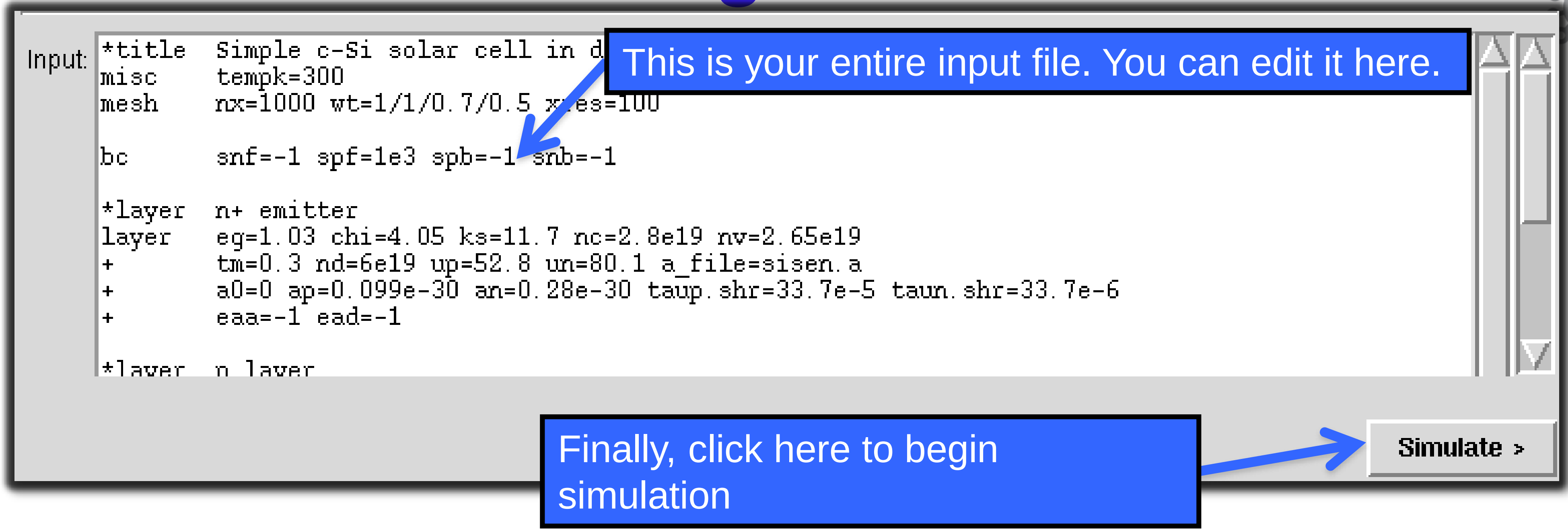
Upload an input deck from your local computer

Download this input deck to your local computer

List of pre-loaded example input decks. Try them for some quick simulation samples!

- Upon opening ADEPT 2, a blank input page will appear, awaiting your input file.
- If upload/download does not work, one reason could be “pop-up” blocking by your internet browser.

ADEPT: Running a simulation



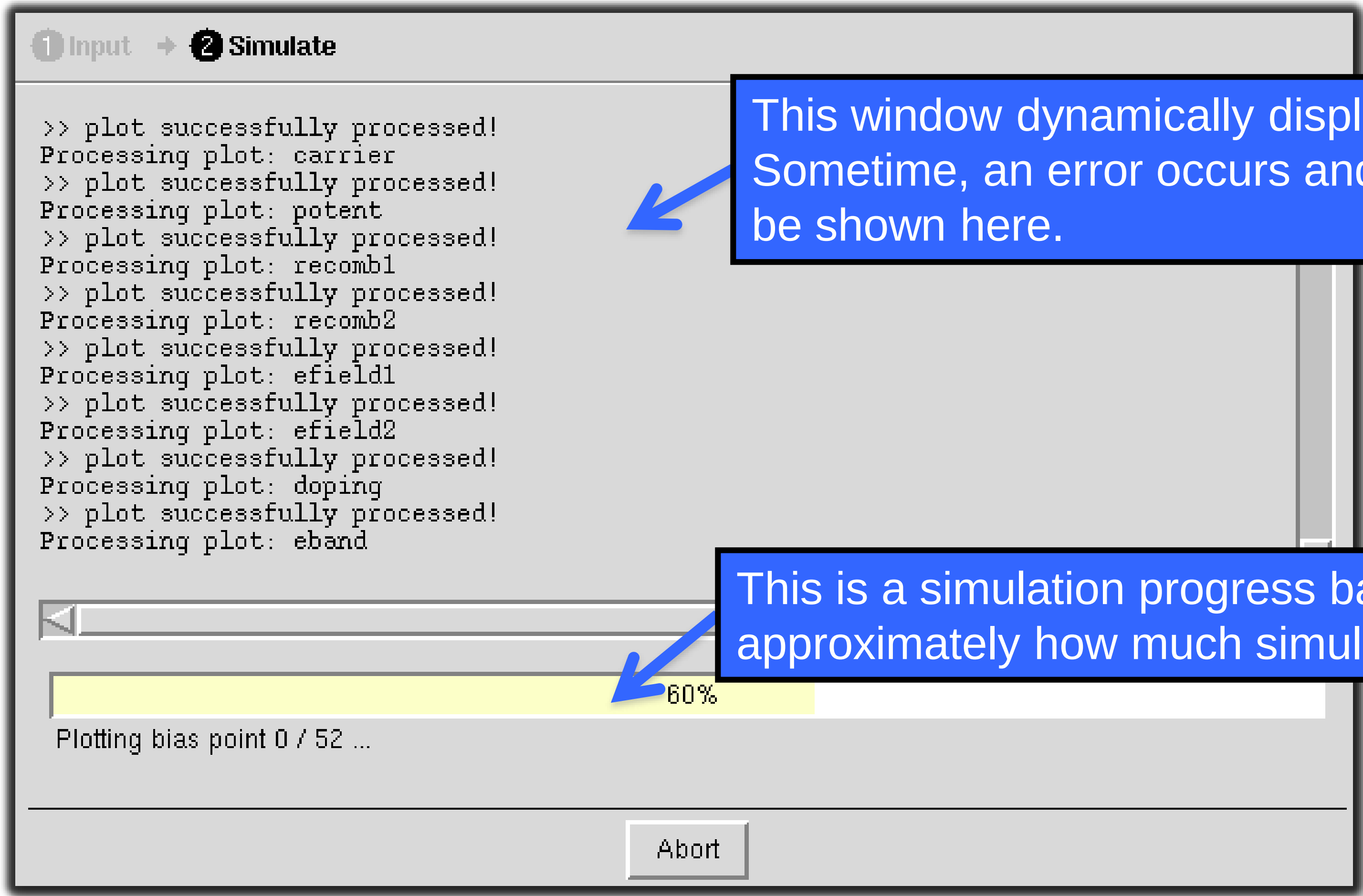
```
*title   Simple c-Si solar cell in d
misc     tempk=300
mesh     nx=1000 wt=1/1/0.7/0.5 xres=100

bc       snf=-1 spf=1e3 spb=-1 snb=-1

*layer   n+ emitter
layer    eg=1.03 chi=4.05 ks=11.7 nc=2.8e19 nv=2.65e19
+        tm=0.3 nd=6e19 up=52.8 un=80.1 a_file=sisen.a
+        a0=0 ap=0.099e-30 an=0.28e-30 taup.shr=33.7e-5 taun.shr=33.7e-6
+        eaa=-1 ead=-1

*layer   p layer
```

This is your entire input file. You can edit it here.

Finally, click here to begin simulation

- Keep in mind that ADEPT 2 is FORTRAN 77 based. The format of certain input may cause unexpected error.
- Please refer to “ADEPT 2 User Manual” for more information regarding how to write an ADEPT input deck.

ADEPT: While simulation is running



```
>> plot successfully processed!
Processing plot: carrier
>> plot successfully processed!
Processing plot: potent
>> plot successfully processed!
Processing plot: recomb1
>> plot successfully processed!
Processing plot: recomb2
>> plot successfully processed!
Processing plot: efield1
>> plot successfully processed!
Processing plot: efield2
>> plot successfully processed!
Processing plot: doping
>> plot successfully processed!
Processing plot: eband
```

60%

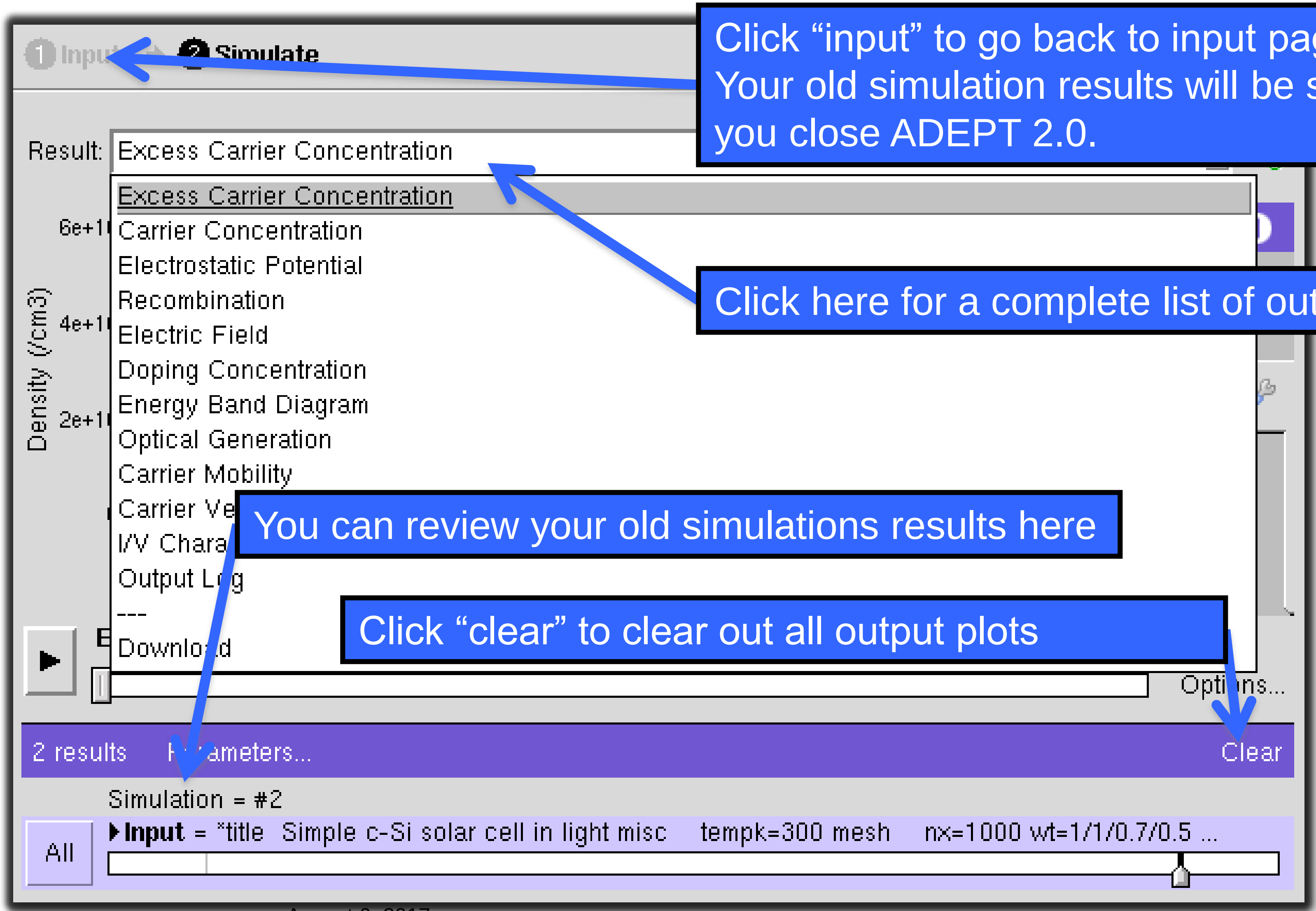
Plotting bias point 0 / 52 ...

This window dynamically displays output. Sometime, an error occurs and a notification will be shown here.

This is a simulation progress bar. It shows approximately how much simulation is done.

- In ADEPT, an entire simulation consists of two parts: ADEPT simulation and PLOTA output generation.

ADEPT: Output



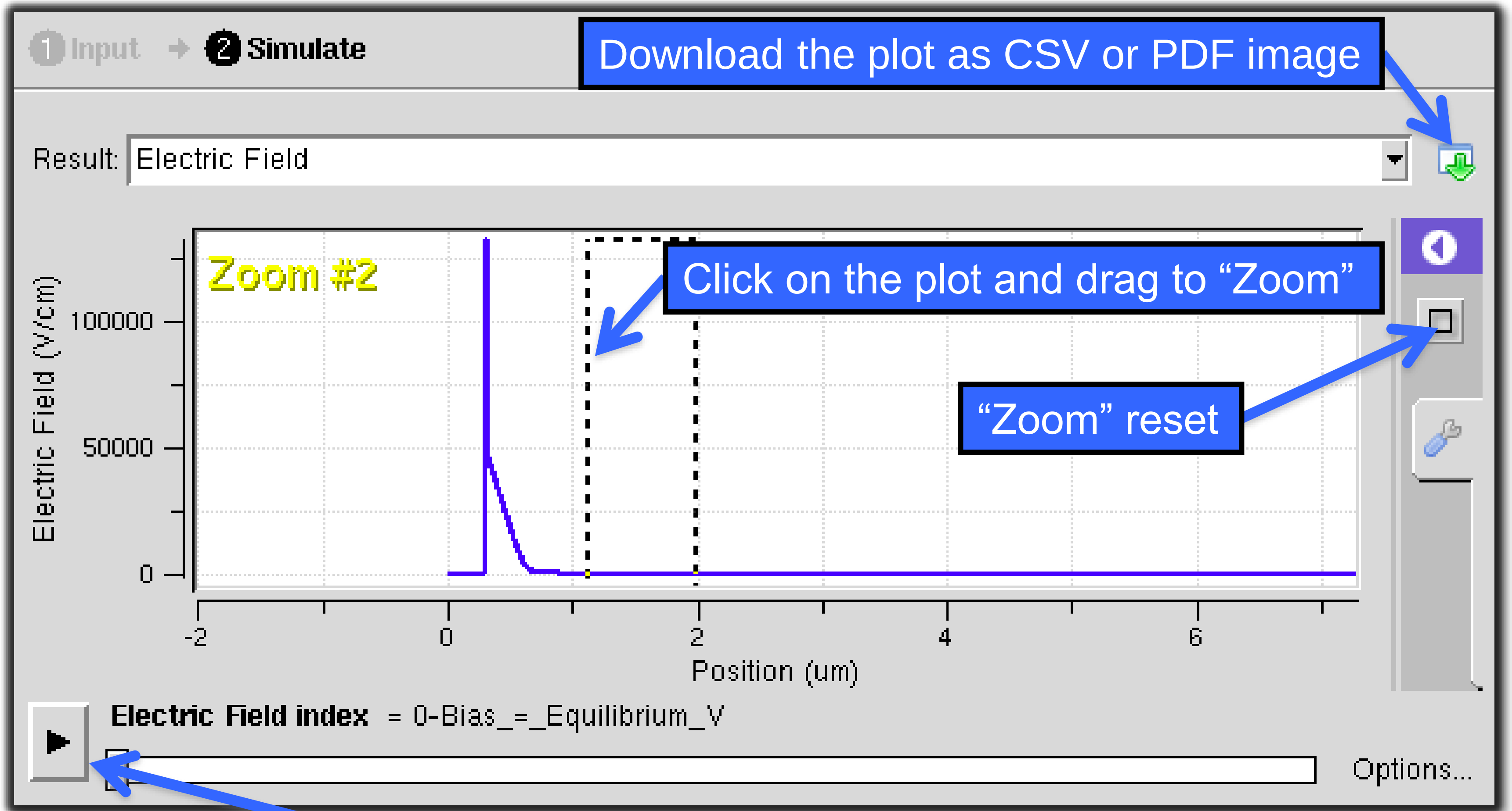
Click “input” to go back to input page. Worry not! Your old simulation results will be saved until you close ADEPT 2.0.

Click here for a complete list of output plots

You can review your old simulations results here

Click “clear” to clear out all output plots

ADEPT: Output



Electric Field index = 0-Bias_=_Equilibrium_V

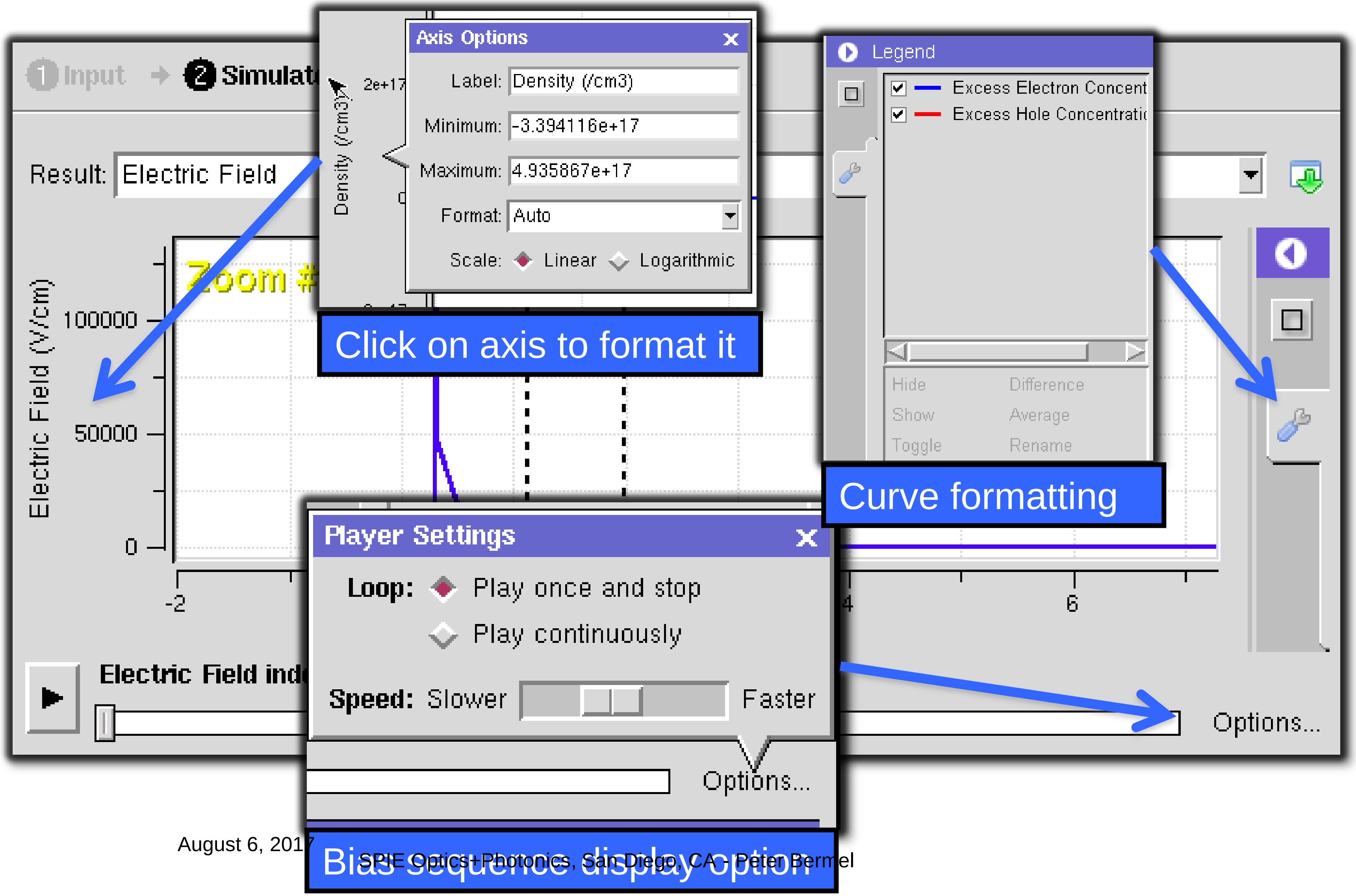
Download the plot as CSV or PDF image

Click on the plot and drag to “Zoom”

“Zoom” reset

Click “play” to look at this output quantity at different bias

ADEPT: Output



Axis Options

Label: Density (/cm3)

Minimum: -3.394116e+17

Maximum: 4.935867e+17

Format: Auto

Scale: ● Linear ○ Logarithmic

☑ Excess Electron Concent

☑ Excess Hole Concentratio

Player Settings

Loop: ● Play once and stop

○ Play continuously

Speed: Slower Faster

Options...

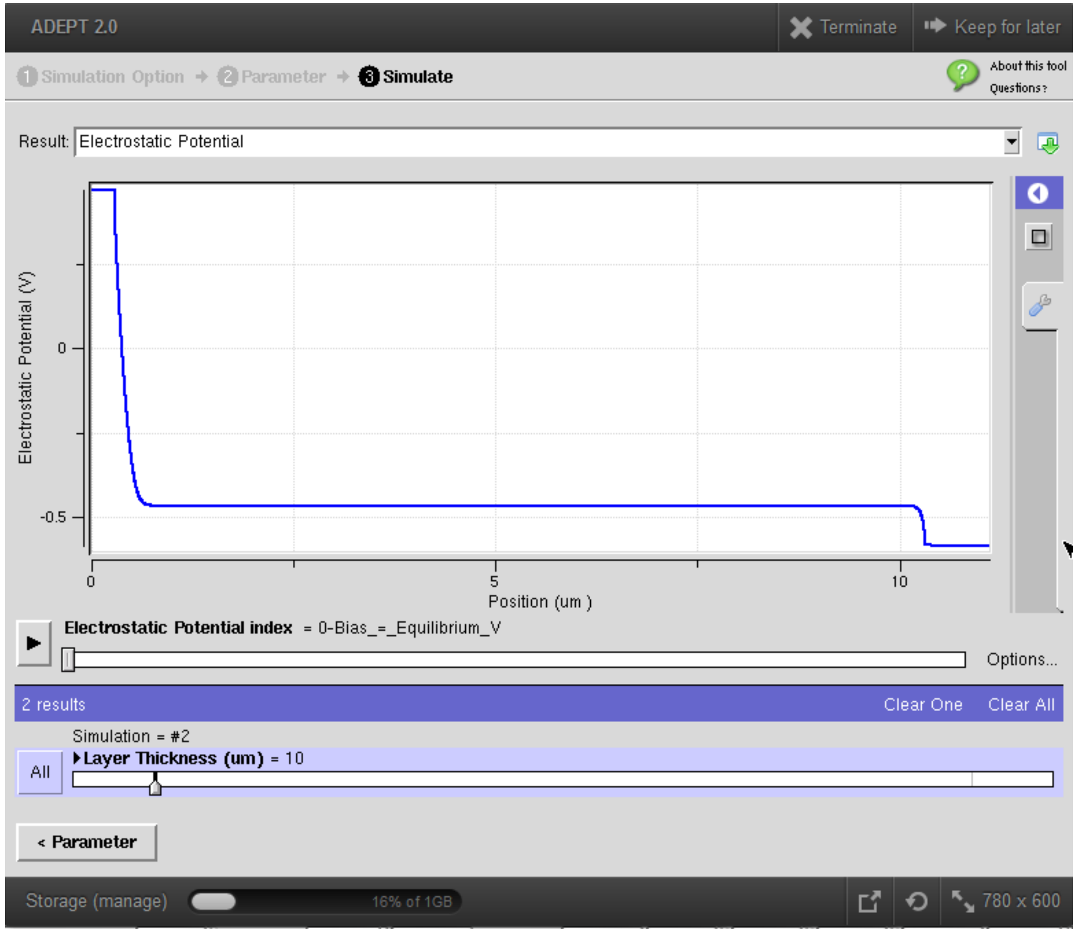
Click on axis to format it

Curve formatting

Bias sequence display option

ADEPT: Output

- Outputs include electrostatic (Poisson) solution:



Result: Electrostatic Potential

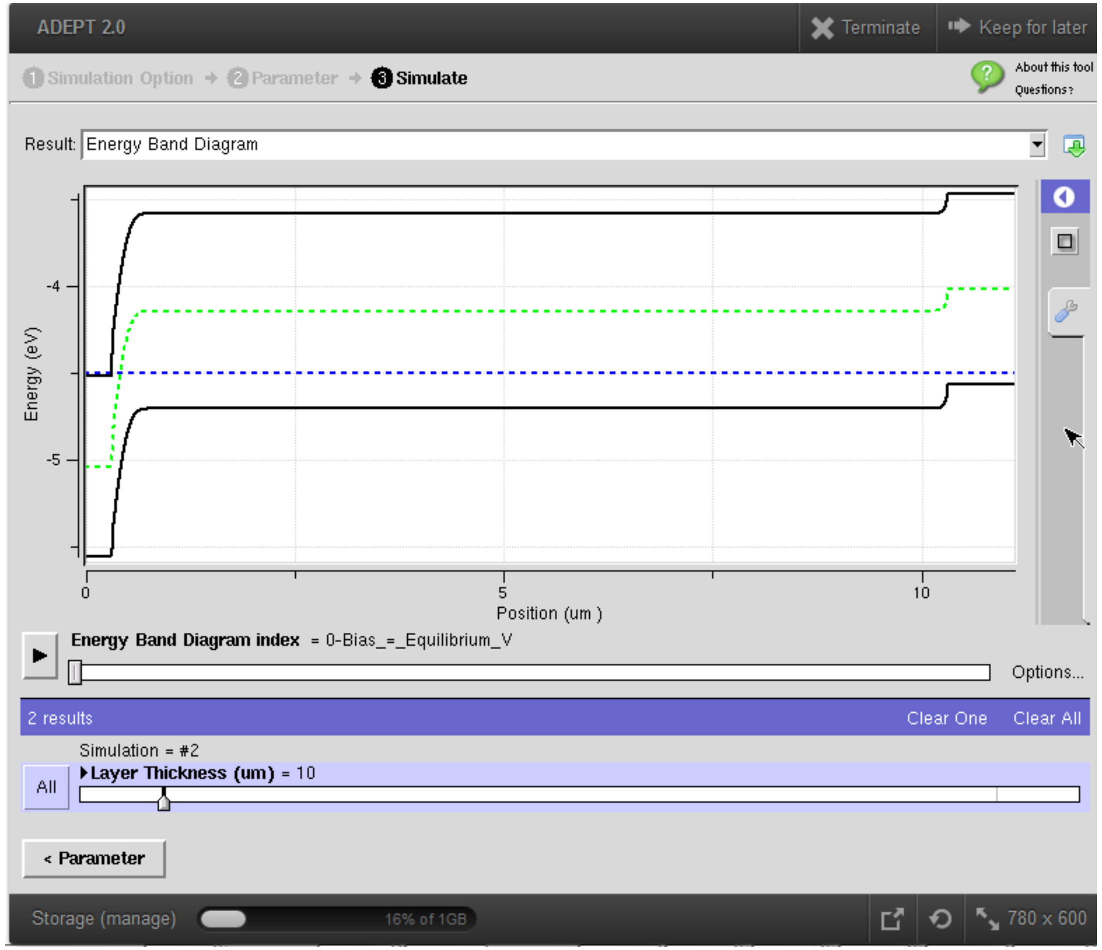
Electrostatic Potential index = 0-Bias_=_Equilibrium_V

Simulation = #2

Layer Thickness (um) = 10

ADEPT: Output

- Energy band diagram


Result: Energy Band Diagram

Energy Band Diagram index = 0-Bias_=_Equilibrium_V

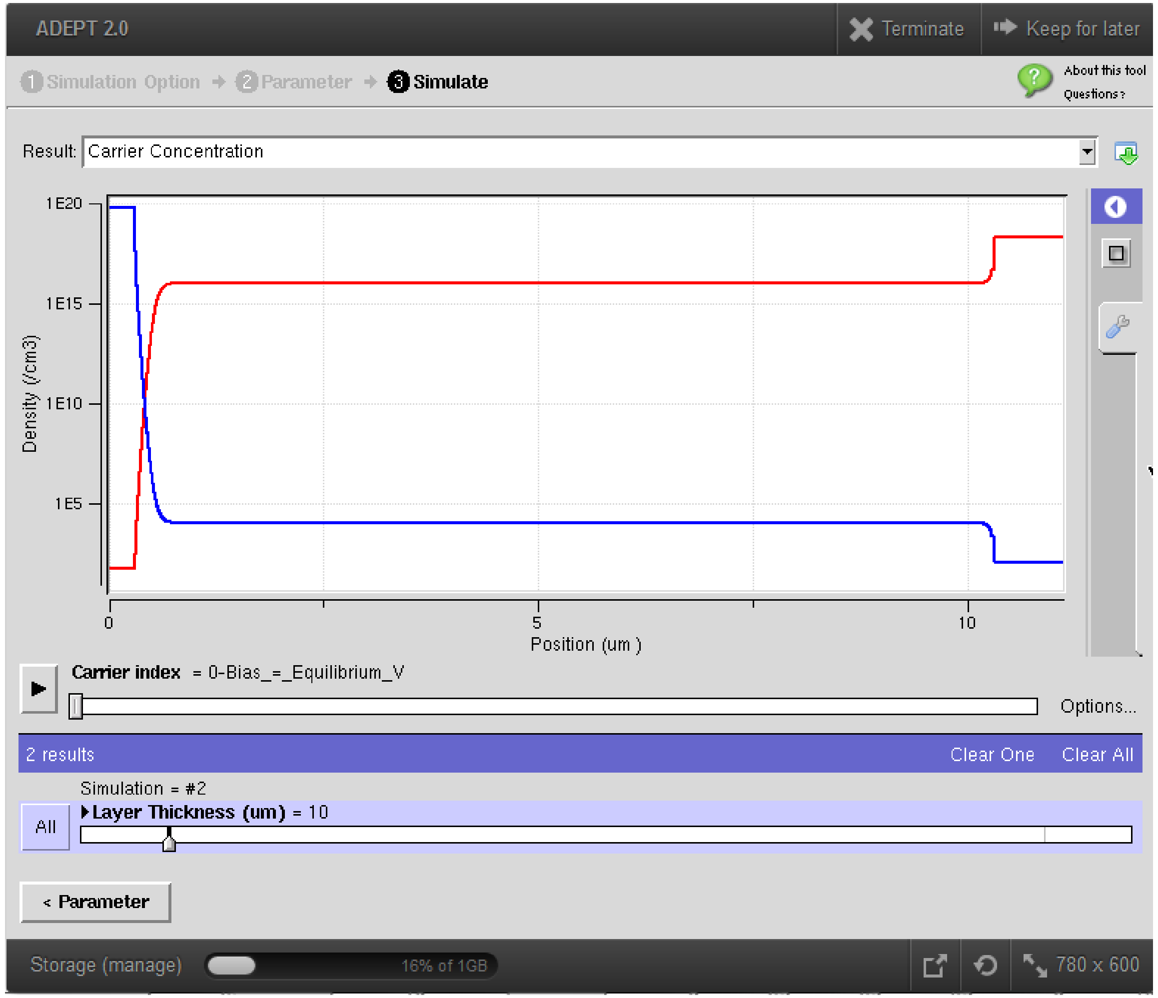
2 results

Simulation = #2

Layer Thickness (um) = 10

ADEPT: Output

- Carrier concentrations:



Result: Carrier Concentration

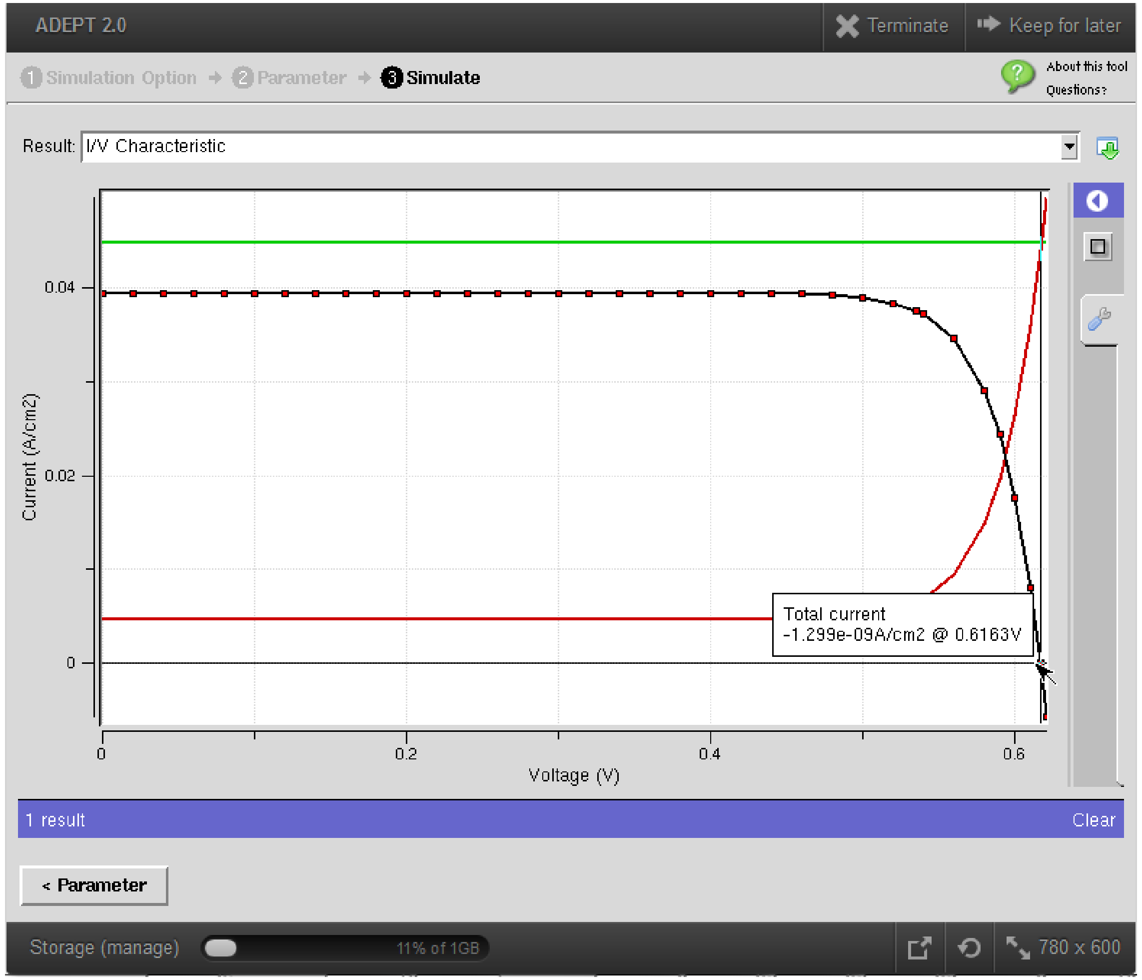
Carrier index = 0-Bias_=_Equilibrium_V

Simulation = #2

Layer Thickness (um) = 10

ADEPT: Output

- And finally, realistic I-V curves:



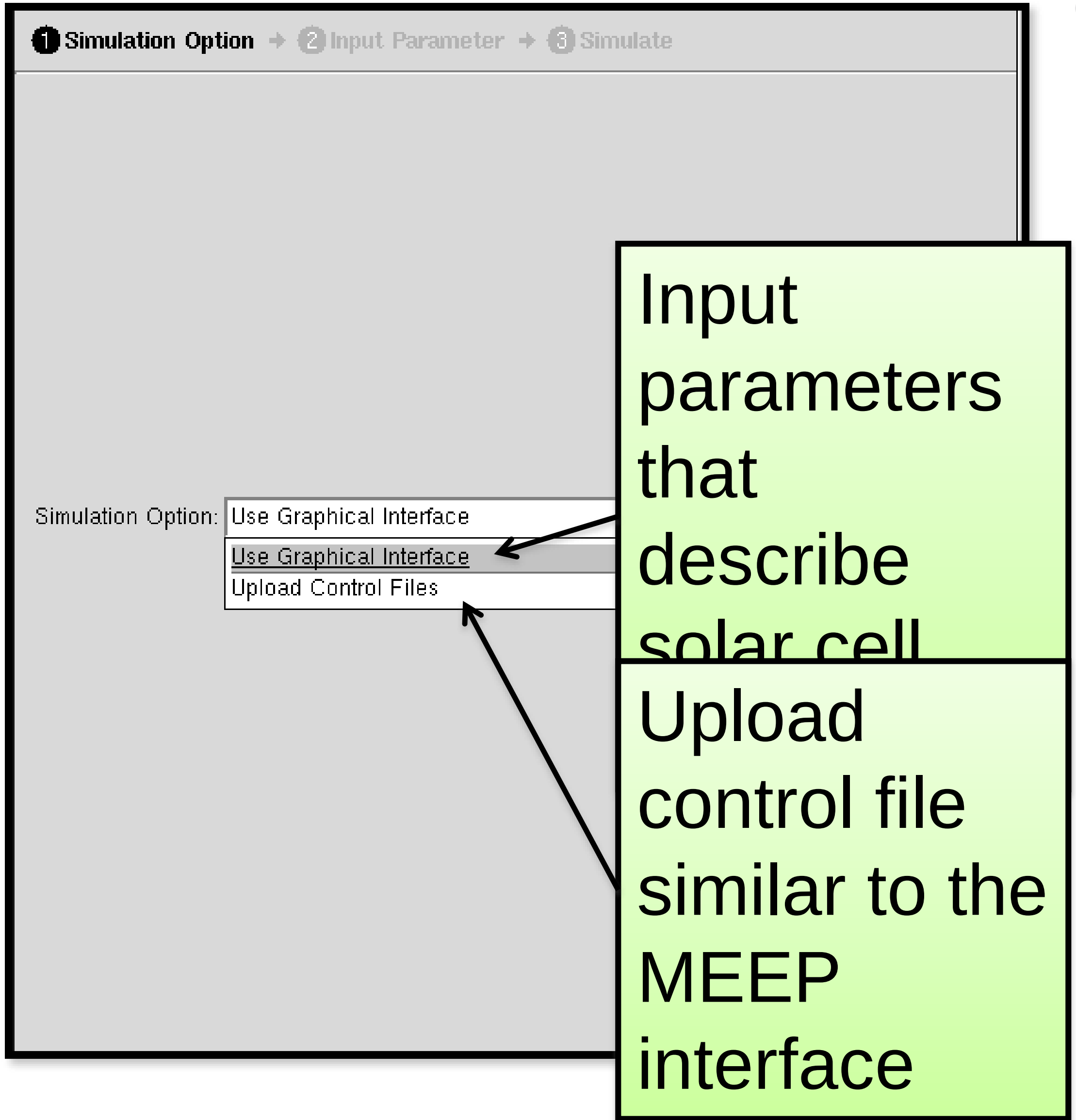
Result: I/V Characteristic

Total current
-1.299e-09A/cm2 @ 0.6163V

MEEPPV: User Interfaces

https://nanohub.org/tools/meeppv

- ❖ Upon opening MEEPPV, a simulation option page will appear, allowing users to select between using a graphical user interface and uploading a control file.
- ❖ Click on the button below to proceed to the second page.

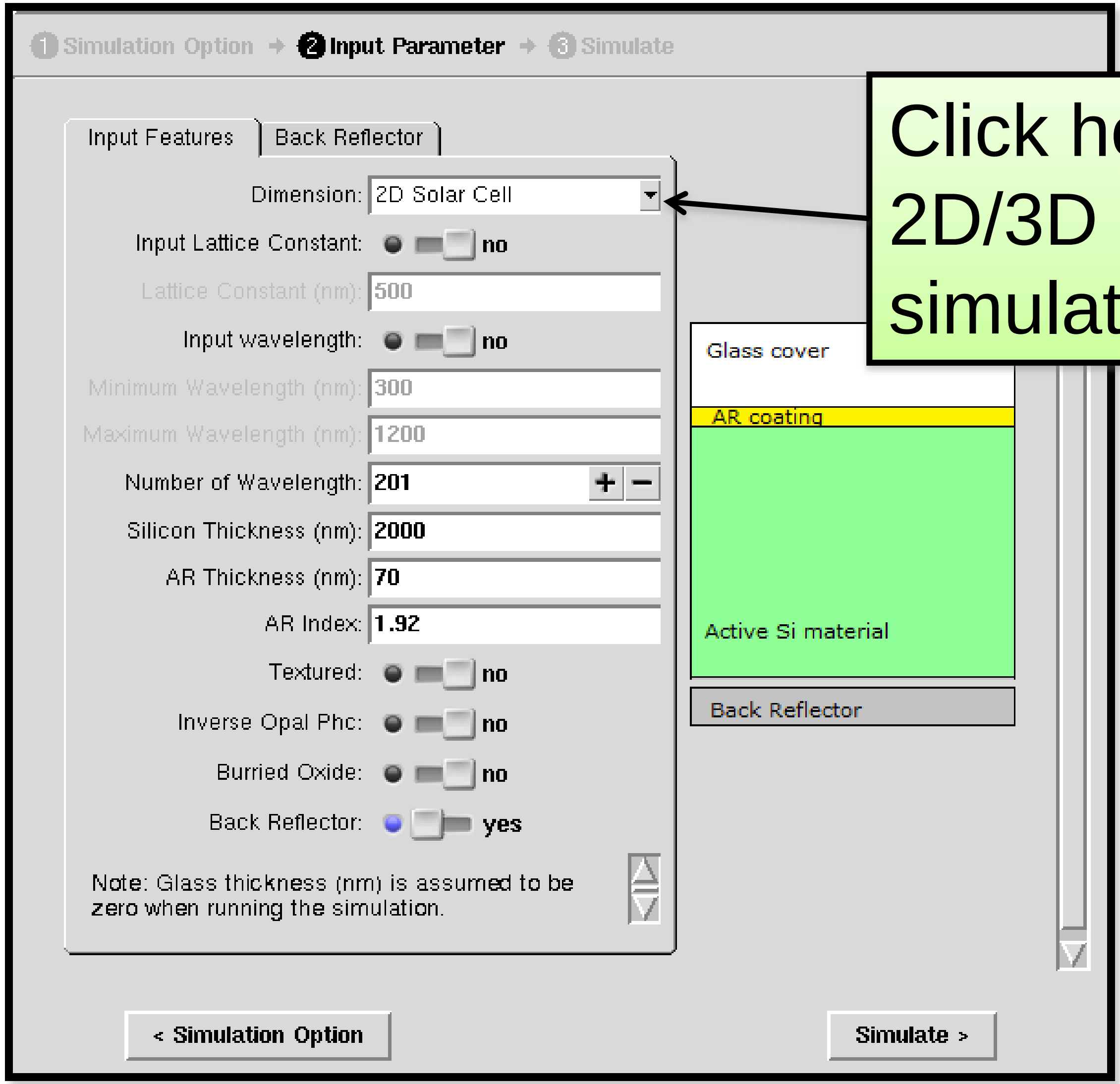


Simulation Option: Use Graphical Interface

Input parameters that describe solar cell

Upload control file similar to the MEEP interface

Graphical User Interface



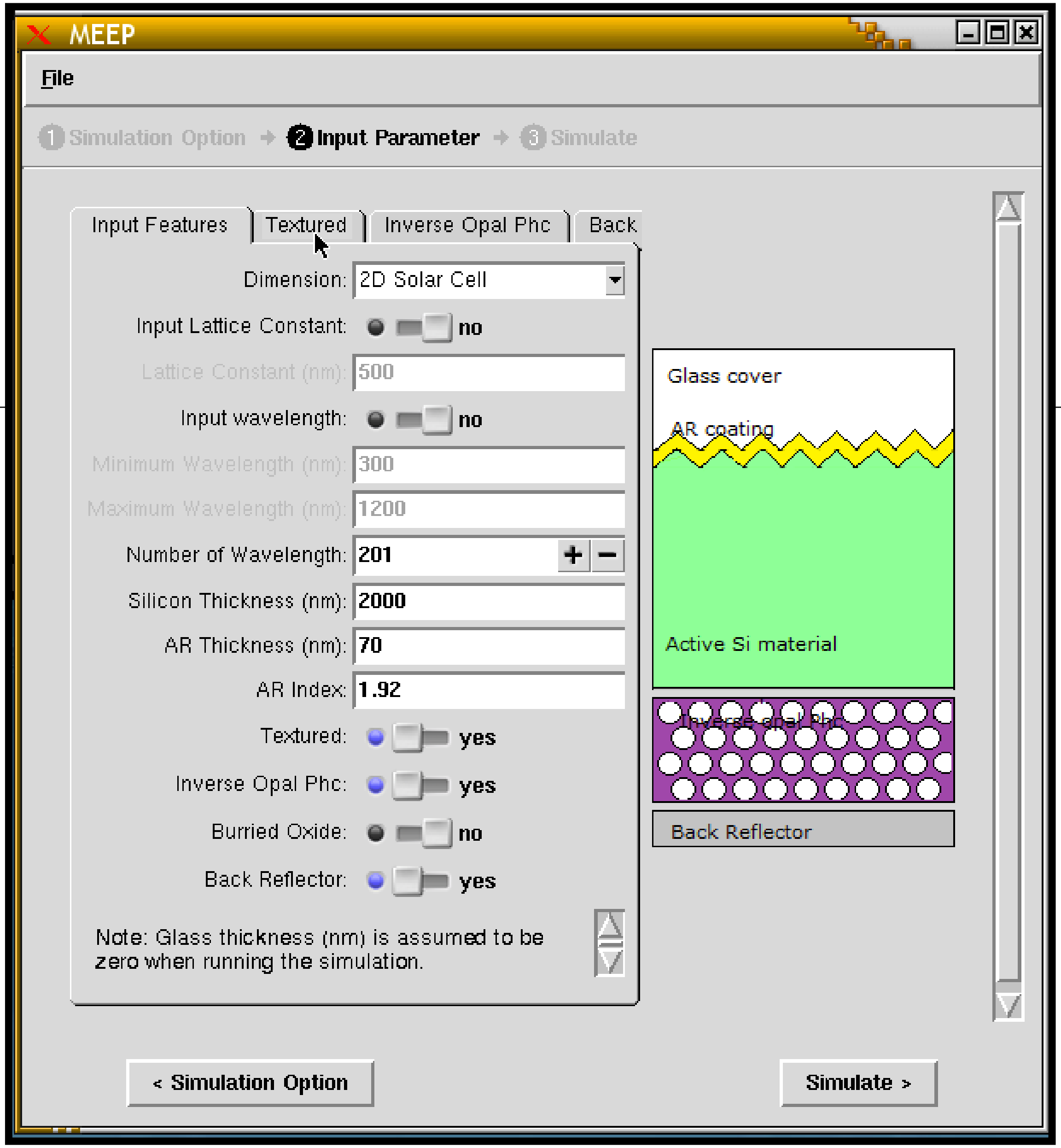
Dimension: 2D Solar Cell
Input Lattice Constant: no
Lattice Constant (nm): 500
Input wavelength: no
Minimum Wavelength (nm): 300
Maximum Wavelength (nm): 1200
Number of Wavelength: 201
Silicon Thickness (nm): 2000
AR Thickness (nm): 70
AR Index: 1.92
Textured: no
Inverse Opal Phc: no
Burried Oxide: no
Back Reflector: yes

Note: Glass thickness (nm) is assumed to be zero when running the simulation.

Click here to select 2D/3D solar cell for simulation

- You will be directed to this page if the graphical user interface (first option) is selected.
- Users can input parameters that describe the solar cell features as well as the simulation domain.

MEEPPV Input



Dimension: 2D Solar Cell

Input Lattice Constant: ● no

Lattice Constant (nm): 500

Input wavelength: ● no

Minimum Wavelength (nm): 300

Maximum Wavelength (nm): 1200

Number of Wavelength: 201

Silicon Thickness (nm): 2000

AR Thickness (nm): 70

AR Index: 1.92

Textured: ● yes

Inverse Opal Phc: ● yes

Burried Oxide: ● no

Back Reflector: ● yes

Note: Glass thickness (nm) is assumed to be zero when running the simulation.

Solar cell schematic

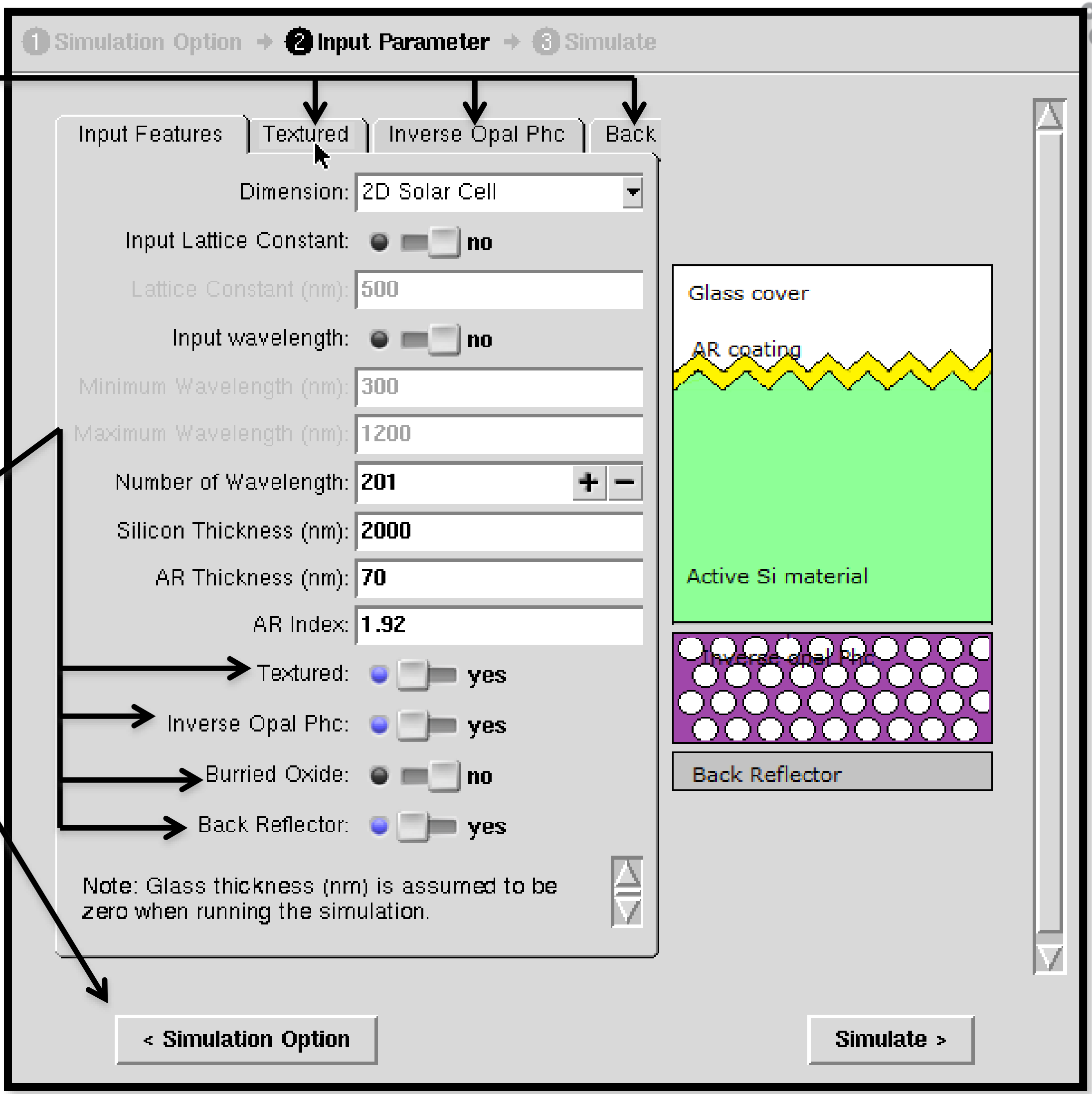
Graphical User Interface

Feature tabs will appear when the on/off button is turned on. Click on each tab to input more solar cell's features.

Click on the on/off button to include the features to the solar

Click here to go back to the first page.

shown on the left changes with respect to feature's on/off button.



Dimension: 2D Solar Cell

Input Lattice Constant: ● no

Lattice Constant (nm): 500

Input wavelength: ● no

Minimum Wavelength (nm): 300

Maximum Wavelength (nm): 1200

Number of Wavelength: 201

Silicon Thickness (nm): 2000

AR Thickness (nm): 70

AR Index: 1.92

Textured: ● yes

Inverse Opal Phc: ● yes

Burried Oxide: ● no

Back Reflector: ● yes

Note: Glass thickness (nm) is assumed to be zero when running the simulation.

Graphical User Interface

- ❖ More input parameters under each feature tab

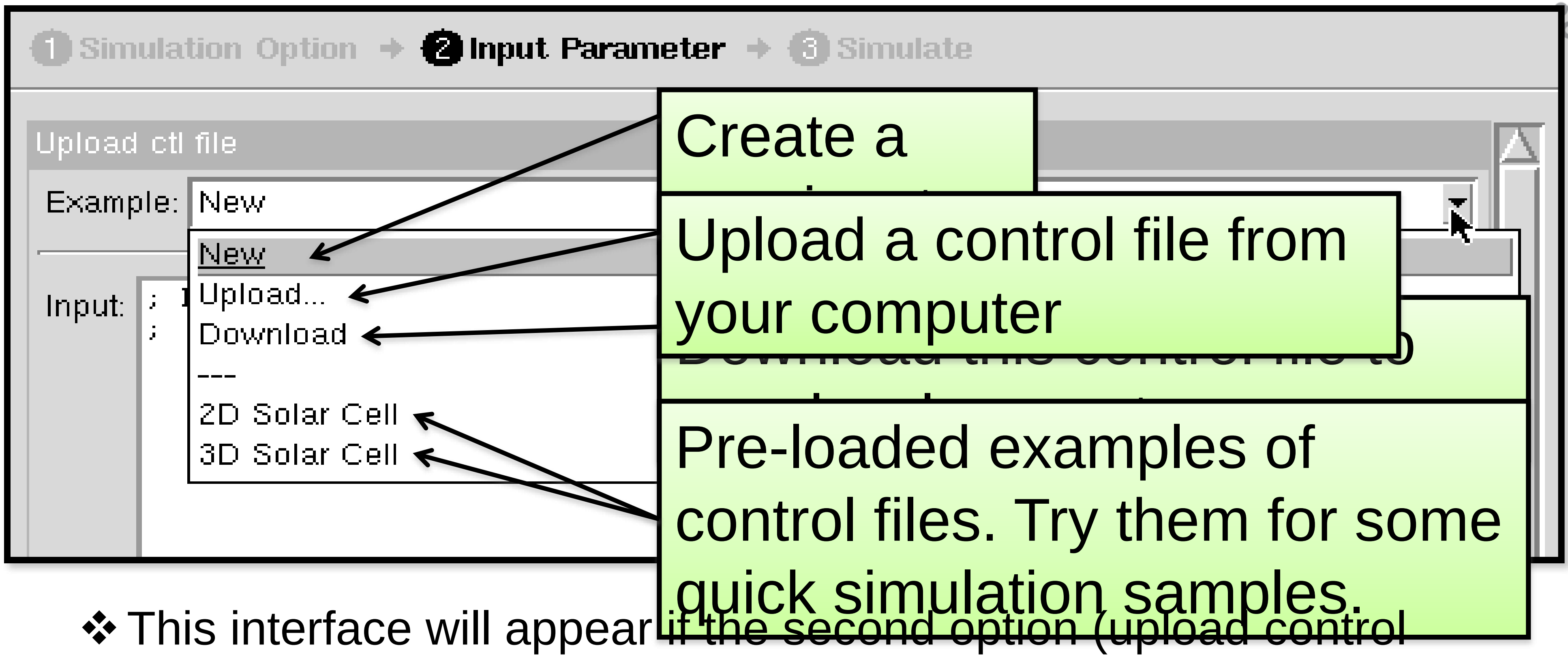
Textured Thickness (nm): 250
Width of random feature (nm): 50

Radius (nm): 250
Epsilon within the Phc: 1
Number of Opal Layers: 8

Back Reflector Material: Perfect Metal
Grating: yes
Grating thickness (nm): 60
Grating Period (nm): 600
Duty Cycle: 0.5

Finally, click here to begin simulation

Text-Based (Scheme) Interface



Create a

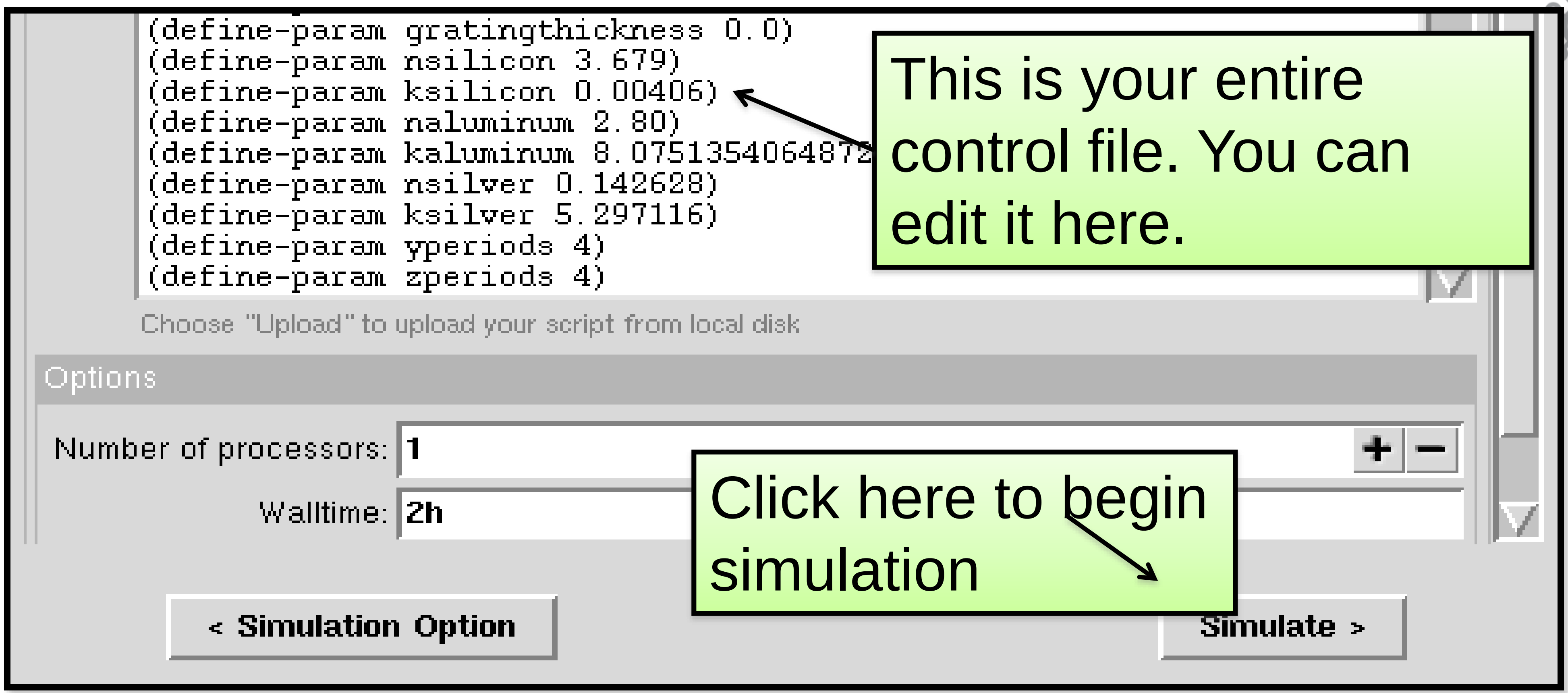
Upload a control file from your computer

Download this control file to

Pre-loaded examples of control files. Try them for some quick simulation samples.

- ❖ This interface will appear if the second option (upload control files) from the first page is selected.
- ❖ If upload/download does not work, one reason could be “pop-up” blocking by your internet browser.

Text-Based (Scheme) Interface



```
(define-param gratingthickness 0.0)
(define-param nsilicon 3.679)
(define-param ksilicon 0.00406)
(define-param naluminum 2.80)
(define-param kaluminum 8.0751354064872
(define-param nsilver 0.142628)
(define-param ksilver 5.297116)
(define-param yperiods 4)
(define-param zperiods 4)
```

Choose "Upload" to upload your script from local disk

Number of processors: 1

Walltime: 2h

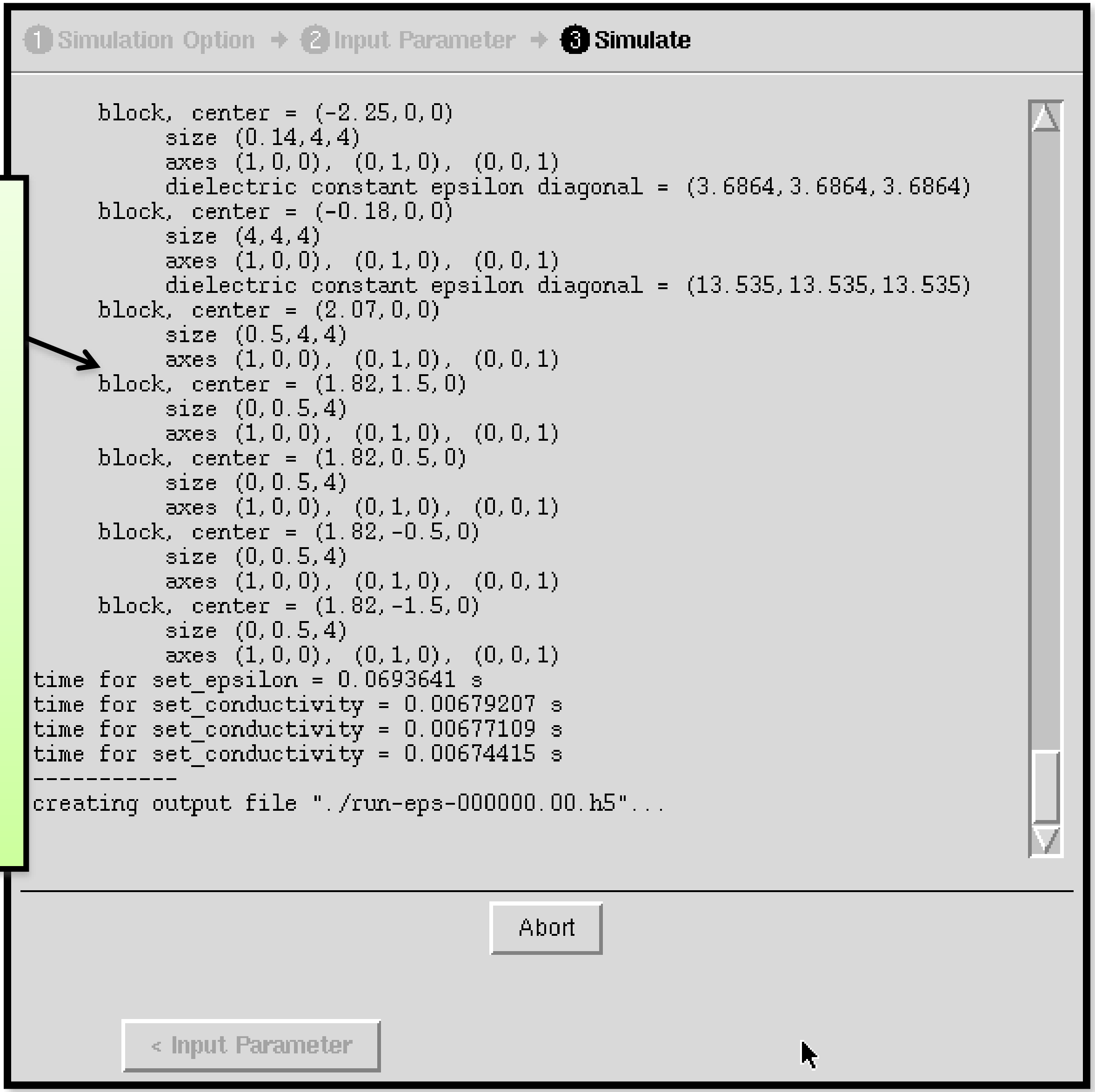
This is your entire control file. You can edit it here.

Click here to begin simulation

- ❖ Note that the input file is written in Scheme language.
- ❖ For more details and tutorial on writing control file with Scheme, please refer to: *http://ab-initio.mit.edu/wiki/index.php/Meep_Tutorial*

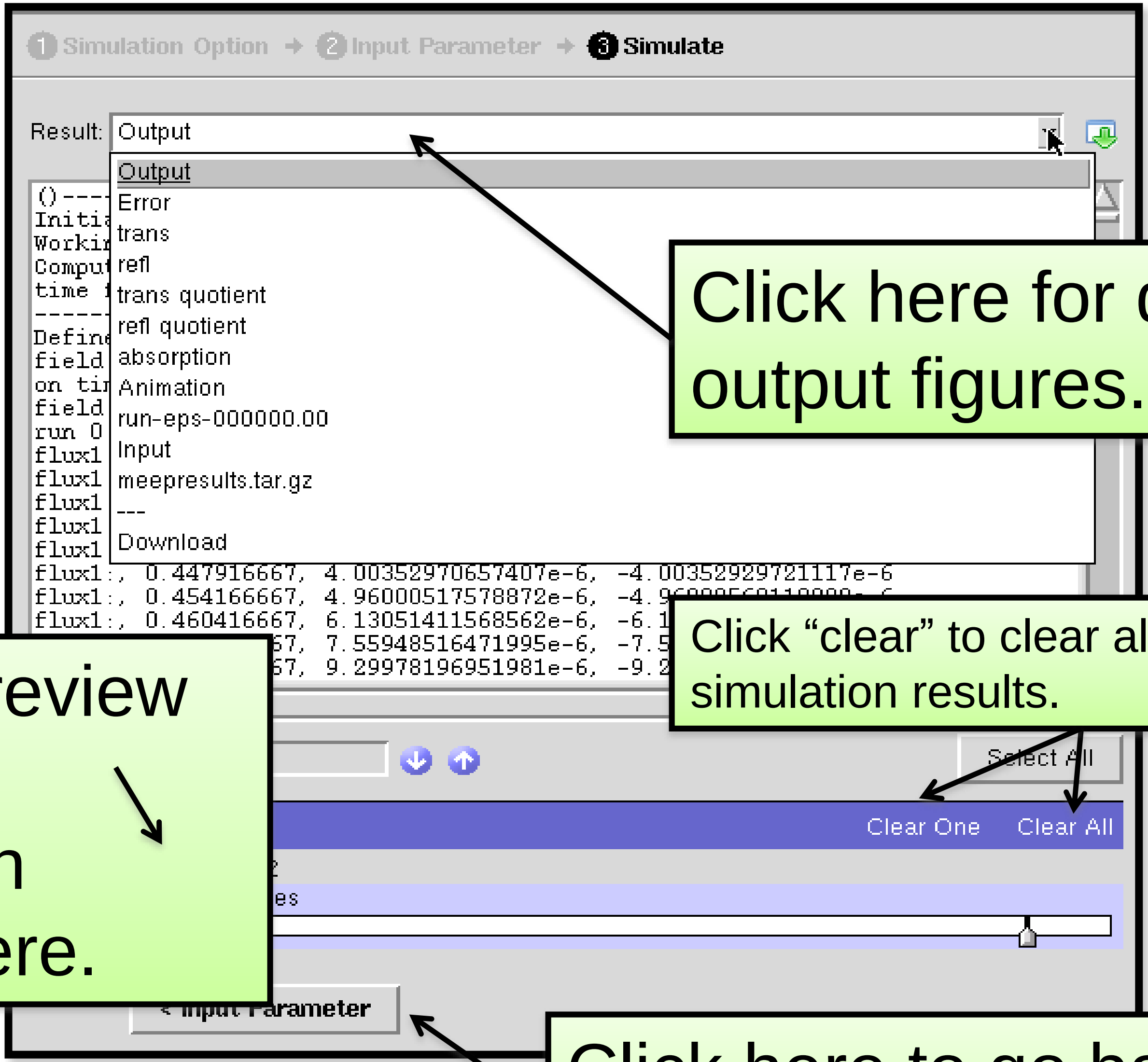
Text-Based (Scheme) Interface

This window dynamically displays output. Sometimes, an error occurs and a notification will be shown here.



```
     block, center = (-2.25,0,0)
          size (0.14,4,4)
          axes (1,0,0), (0,1,0), (0,0,1)
          dielectric constant epsilon diagonal = (3.6864,3.6864,3.6864)
     block, center = (-0.18,0,0)
          size (4,4,4)
          axes (1,0,0), (0,1,0), (0,0,1)
          dielectric constant epsilon diagonal = (13.535,13.535,13.535)
     block, center = (2.07,0,0)
          size (0.5,4,4)
          axes (1,0,0), (0,1,0), (0,0,1)
     block, center = (1.82,1.5,0)
          size (0,0.5,4)
          axes (1,0,0), (0,1,0), (0,0,1)
     block, center = (1.82,0.5,0)
          size (0,0.5,4)
          axes (1,0,0), (0,1,0), (0,0,1)
     block, center = (1.82,-0.5,0)
          size (0,0.5,4)
          axes (1,0,0), (0,1,0), (0,0,1)
     block, center = (1.82,-1.5,0)
          size (0,0.5,4)
          axes (1,0,0), (0,1,0), (0,0,1)
time for set_epsilon = 0.0693641 s
time for set_conductivity = 0.00679207 s
time for set_conductivity = 0.00677109 s
time for set_conductivity = 0.00674415 s
-----------
creating output file "./run-eps-000000.00.h5"...
```

Output



```
()----
Initia
Workin
Comput
time f
------
Define
field
on tin
field
run 0
flux1
flux1
flux1
flux1
flux1
flux1:, 0.447916667, 4.00352970657407e-6, -4.00352929721117e-6
flux1:, 0.454166667, 4.96000517578872e-6, -4.9
flux1:, 0.460416667, 6.13051411568562e-6, -6.1
               67, 7.55948516471995e-6, -7.5
               67, 9.29978196951981e-6, -9.2
```

Click here for different output figures.

Click “clear” to clear all or one of the simulation results.

You can review your old simulation results here.

Click here to go back to input page

Generating Graphics

Result: Animation

Player Settings

Loop: ◆ Play once and stop

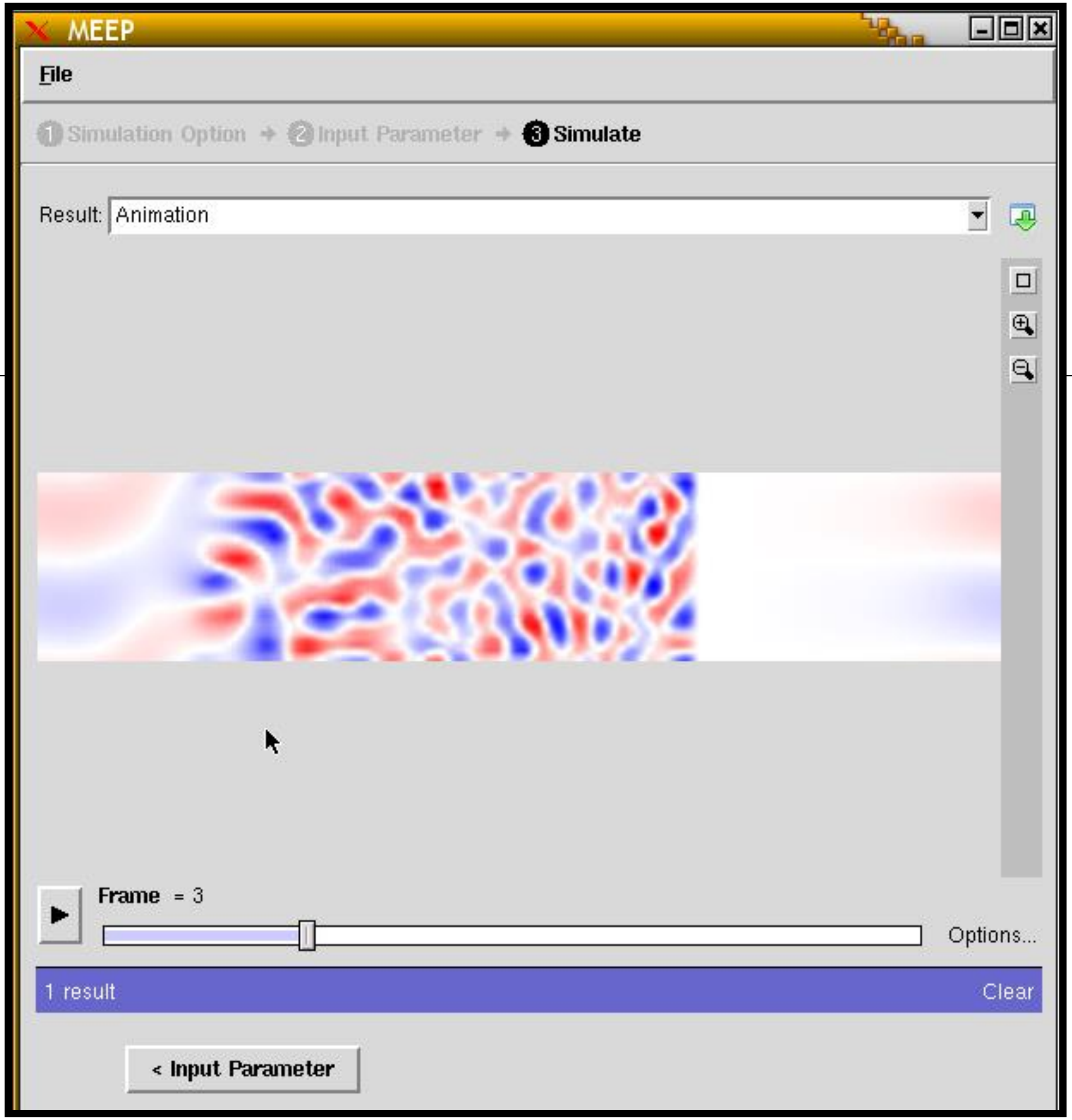
◇ Play continuously

Speed: Slower — Faster

Click play to see the animation of fields propagating through the solar cell

Image sequence display option

MEEPPV: https://nanohub.org/tools/meeppv

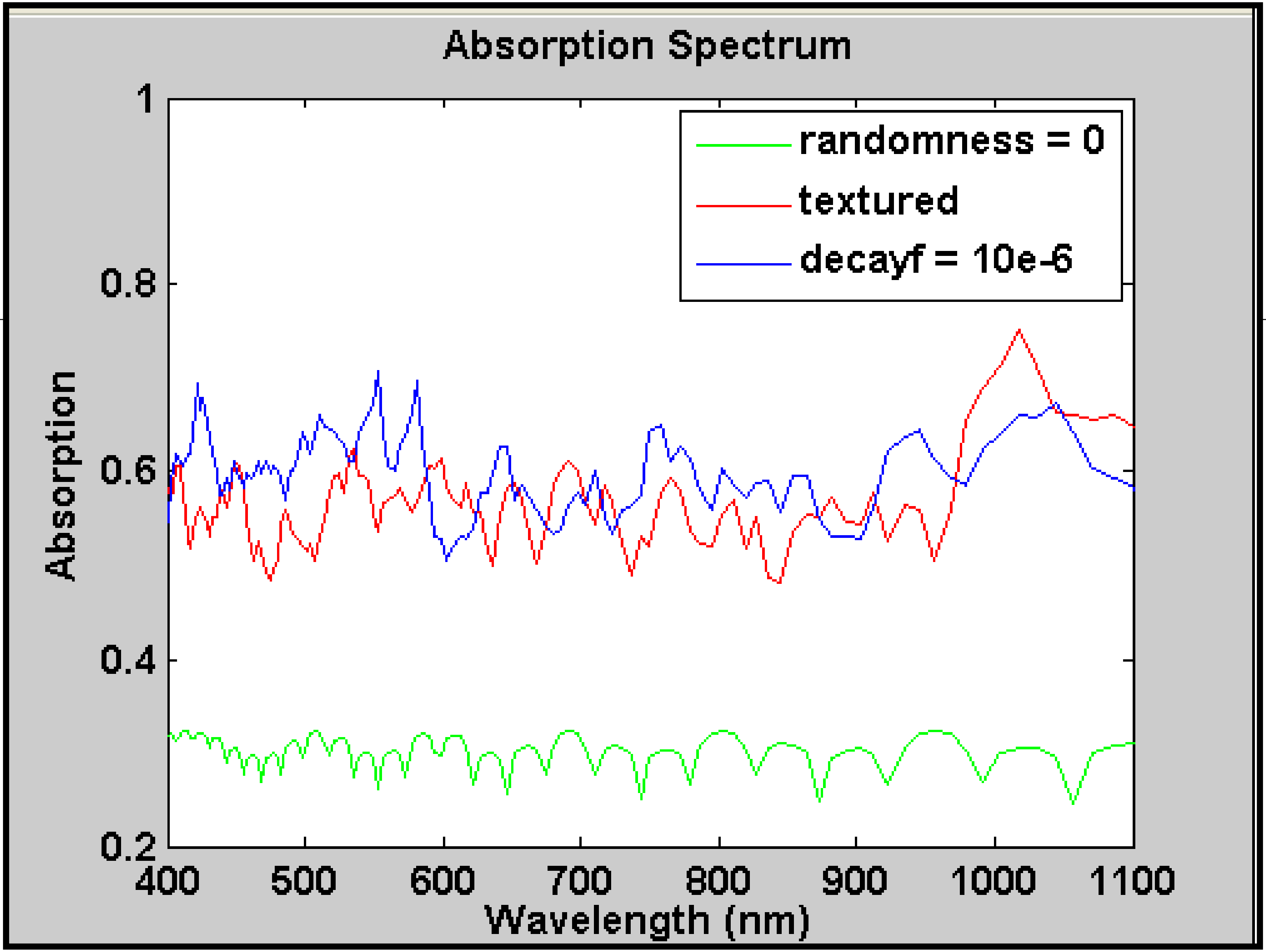


Result: Animation

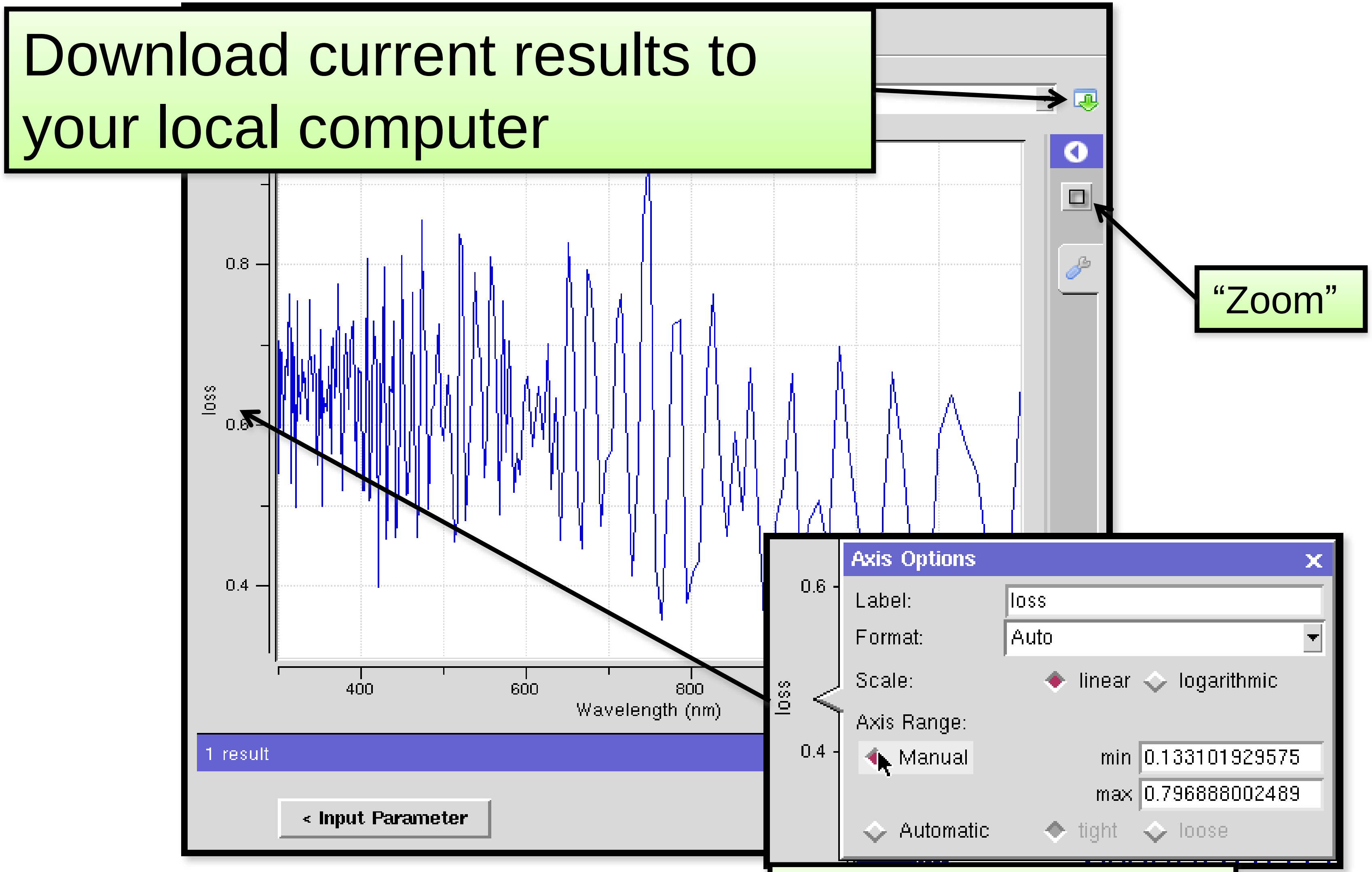
Frame = 3

Output animations

MEEPPV Output



Downloading Data



Download current results to your local computer

“Zoom”

Axis Options

Label: loss

Format: Auto

Scale: ● linear ○ logarithmic

Axis Range:

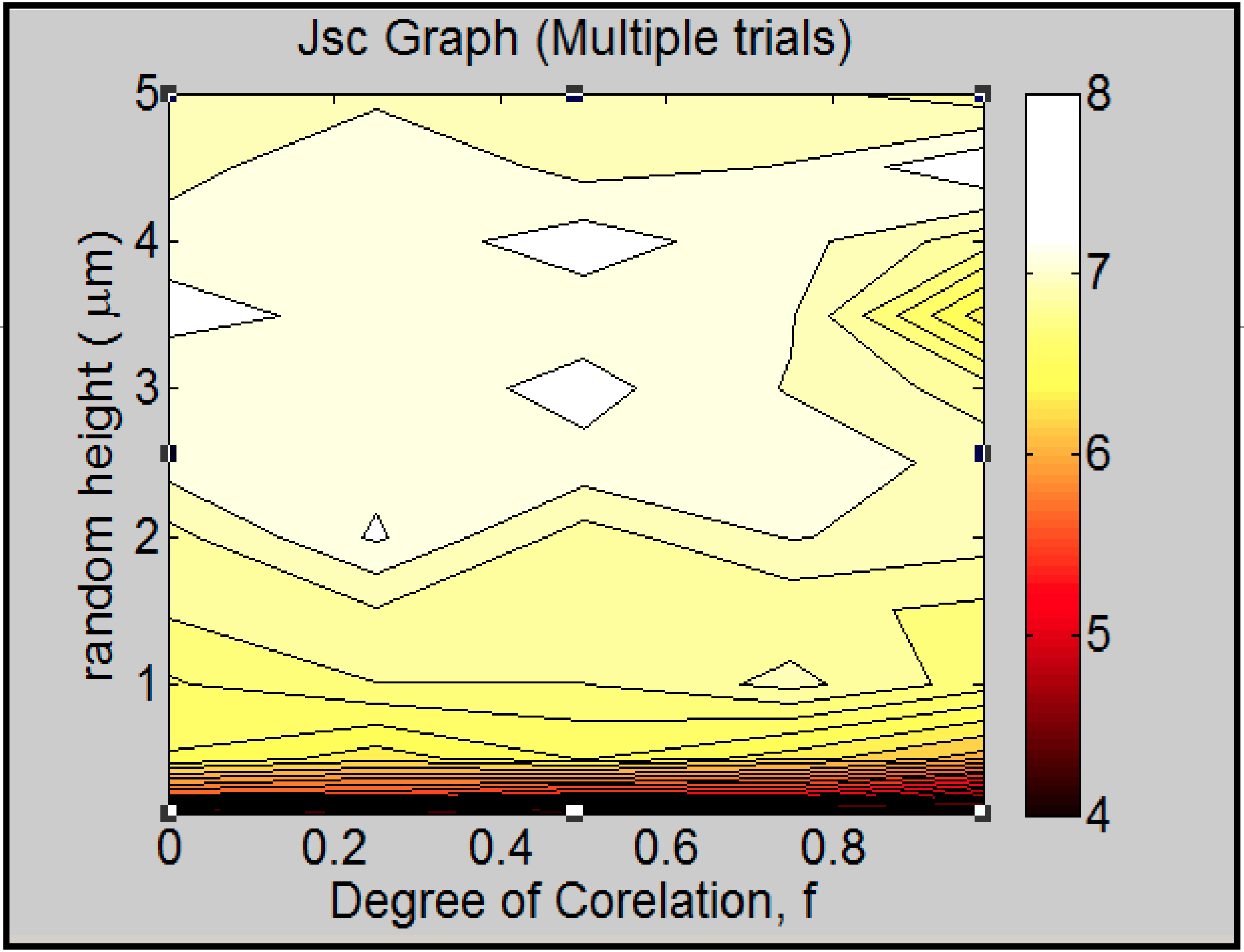
● Manual min 0.133101929575

max 0.796888002489

○ Automatic ○ tight ○ loose

Click on axis to

MEEPPV: Post-processing in MATLAB



Summary

- MEEPPV performs full-wave electromagnetics simulations of photovoltaic devices
- Two interfaces to control the input:
  - Graphical user interface – allows graphical feedback on device design
  - Text-Based (Scheme) interface – allows greatest degree of control, designed for experts
- Output
  - Can generate graphics, including line plots (with adjustable axes) and field distributions (either at a single time, or as a movie)
  - Can download raw data as text or csv for further analysis
- Any problems handled through nanoHUB help interface

Future Capabilities

- Jupyter Notebooks
- MATLAB-based version of ADEPT