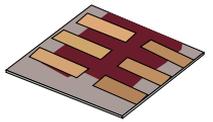


An absolute beginners guide to solar energy
and
Simulating perovskites solar cells with
OghmaNano

Dr. Roderick MacKenzie

<https://www.oghma-nano.com>

roderick.mackenzie@oghma-nano.com



•Introduction

- What is this lecture?
- Why solar?
- Why not silicon?

•New solar cell technologies

- Organic solar cells
- Dye sensitized solar cells
- Cadmium telluride solar cells
- Why Perovskites for solar?

•What is OghmaNano

- Making a new simulation

•Fundamentals

- Semiconductor fundamentals
- The anatomy of a dark current curve

•Fundamentals (cont)

- The anatomy of a light current voltage curve
- Parasitic components
- Optical materials
- Optical simulations

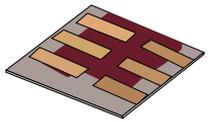
• Advanced topics

- Recombination
- Mobility
- The tau/mu product

• Mobile ions

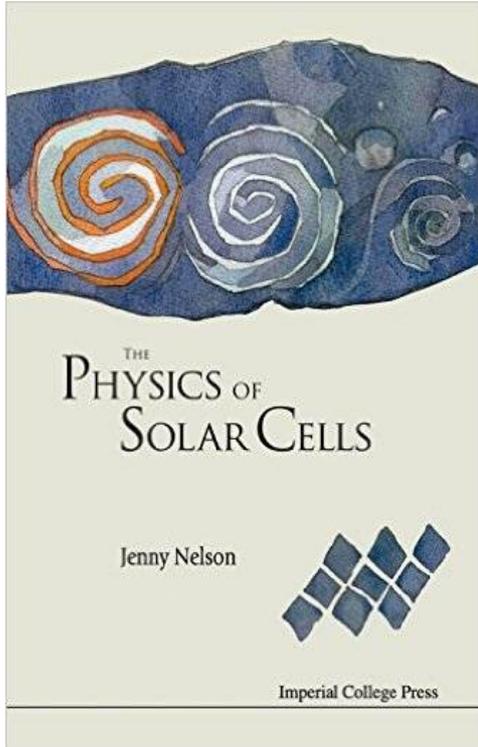
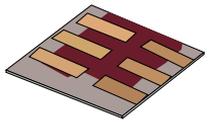
- Mobile ions
- Time domain perovskite simulation

What is this lecture?



- This lecture is designed to take you from ***no knowledge*** about solar cells to being able to simulate perovskite solar cells ***in about an hour***.
- The lecture is intended for people with backgrounds other than Engineering and Physics, you should be able to get through it even if you have a background in finance/geography.
- There will be some exercises spread through the lecture to reinforce this knowledge. These will be in blue.
- We will cover key concepts needed to understand and simulate solar cells.
- Lessons learnt here can be applied to many other classes of opto-electronic devices such as: sensors, optical filters and transistors.

Recommended book (if you like Physics)

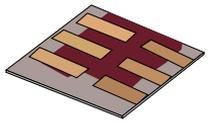


Jenny Nelson

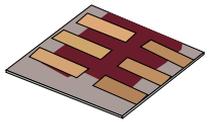
ISBN:1860943497

- This lecture is only 1.5 hours long, so I can't cover everything about solar cells and solar energy.
- The Physics of Solar Cells (Properties of Semiconductor Materials)
- If you want a deeper understanding get this book.

Download



- You can download the software used in this lecture from:
 - <https://www.oghma-nano.com/download.php>
- You can download these slides and many others from:
 - <https://www.oghma-nano.com/docs.html?page=Videos>
- You can watch more video tutorials also at:
 - <https://www.oghma-nano.com/docs.html?page=Videos>
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 - [@OghmaNano](https://twitter.com/OghmaNano)
- Or [@OghmaNano@fediscience.org](https://twitter.com/OghmaNano)



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• Advanced topics

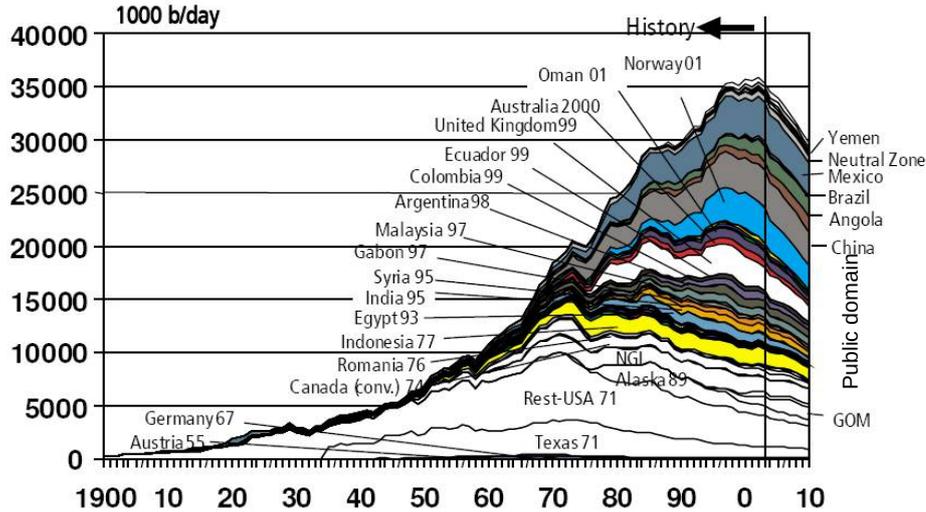
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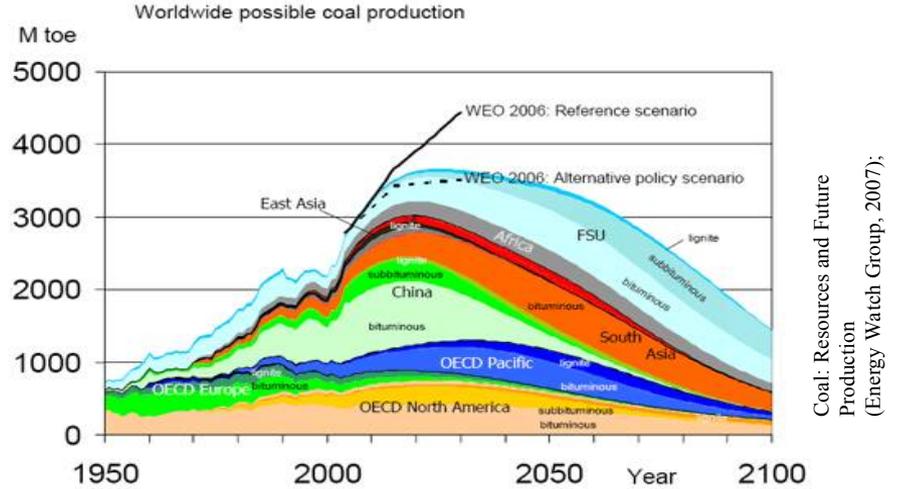
Why solar energy?

Reason 1: We are running out of oil and coal



Source: Industry database, 2003 (IHS 2003)
OGJ, 9 Feb 2004 (Jan-Nov 2003)

Oil production



(Source: Energy Watch Group)

Coal production

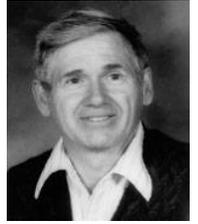
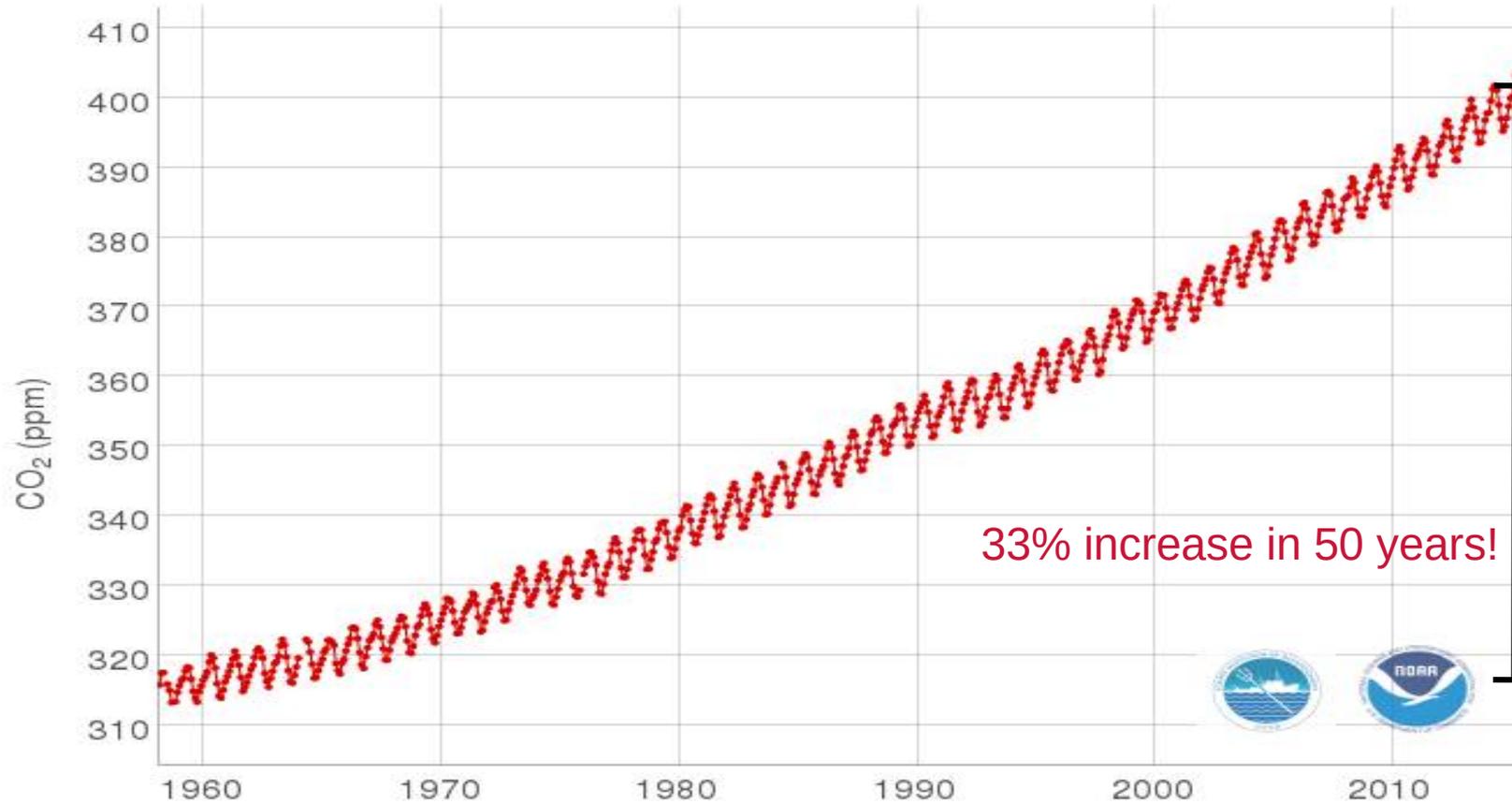
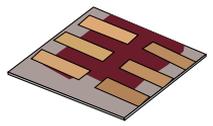
Coal: Resources and Future
Production
(Energy Watch Group, 2007);

- This will damage the economy and our standard of living, our health and well being.

Nature, January 2012, Vol 481, pp. 433-435

Why solar energy?

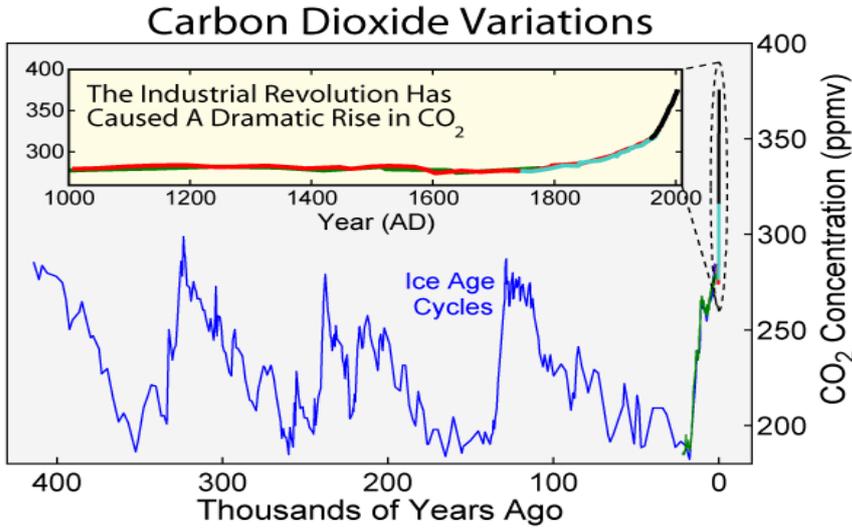
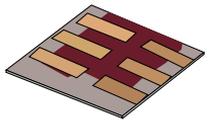
Reason 2a: CO₂ in the atmosphere Jan 1980-June 2015



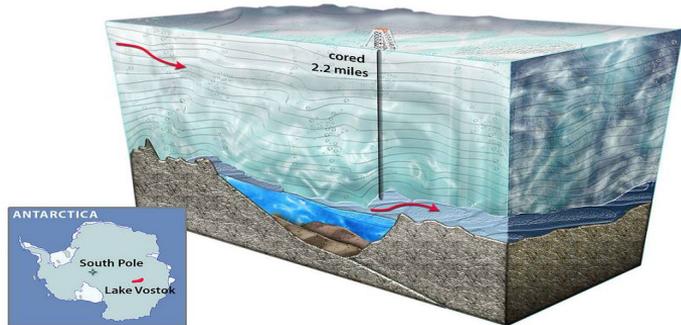
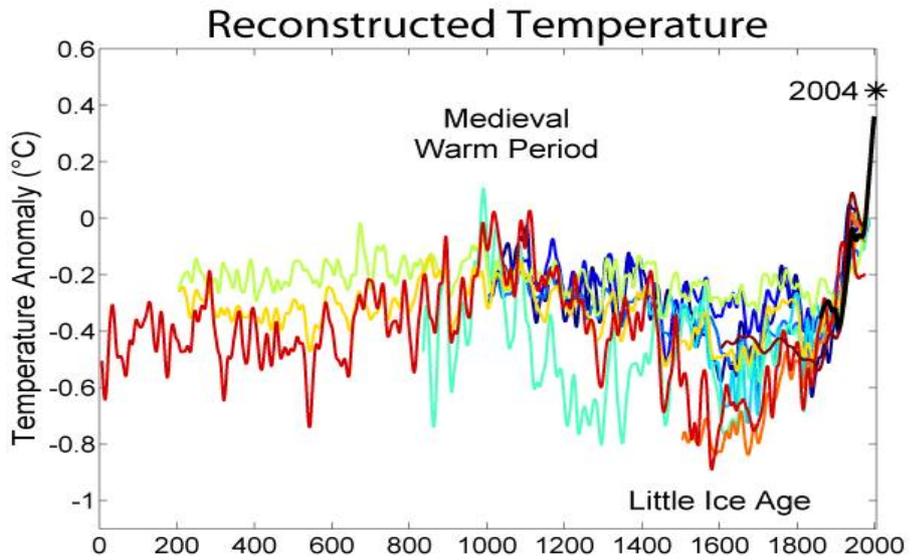
Charles Keeling

Why solar energy?

Reason 2b: Global temperature 1000 AD – 2000 AD



Robert A. Rohde



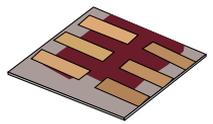
Nicolle Rager-Fuller / NSF



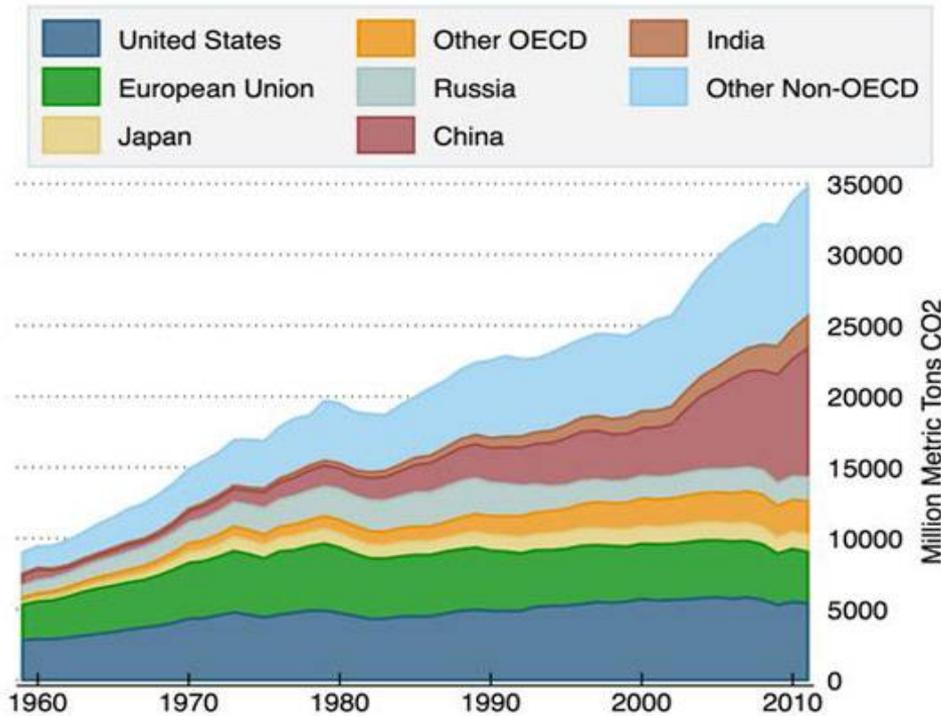
Jenski369

Why solar energy?

CO₂ Emissions by country



Global CO2 Emissions



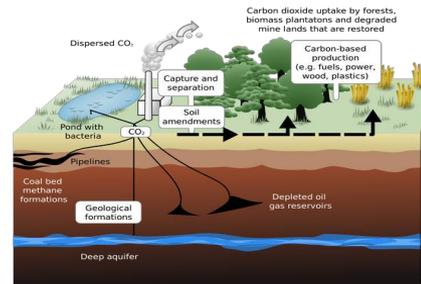
Based on data from the Global Carbon Budget for 1959-2011.

- India GDP 2,277 USD
- USA GDP 69,287 USD
- China GDP 12,556 USD

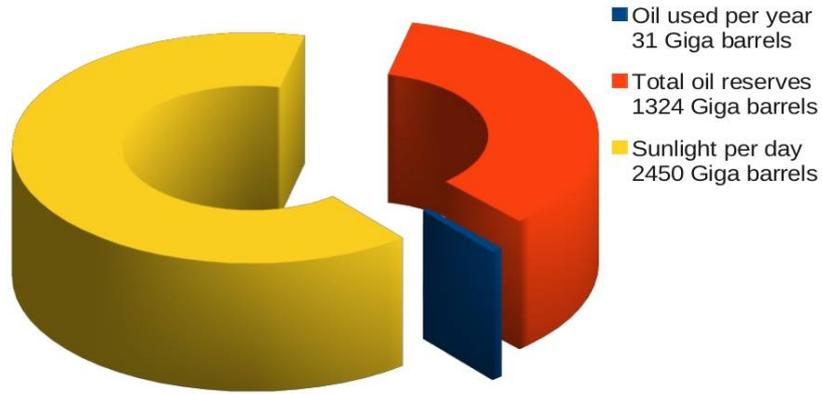
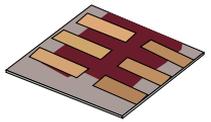
• Imagine the emissions of Indian/China once their GDP reaches that of the UK?

• The solution you propose it has to be lower cost than just burning stuff.

• So let's think the Toyota Prius as an example.



Why solar energy?

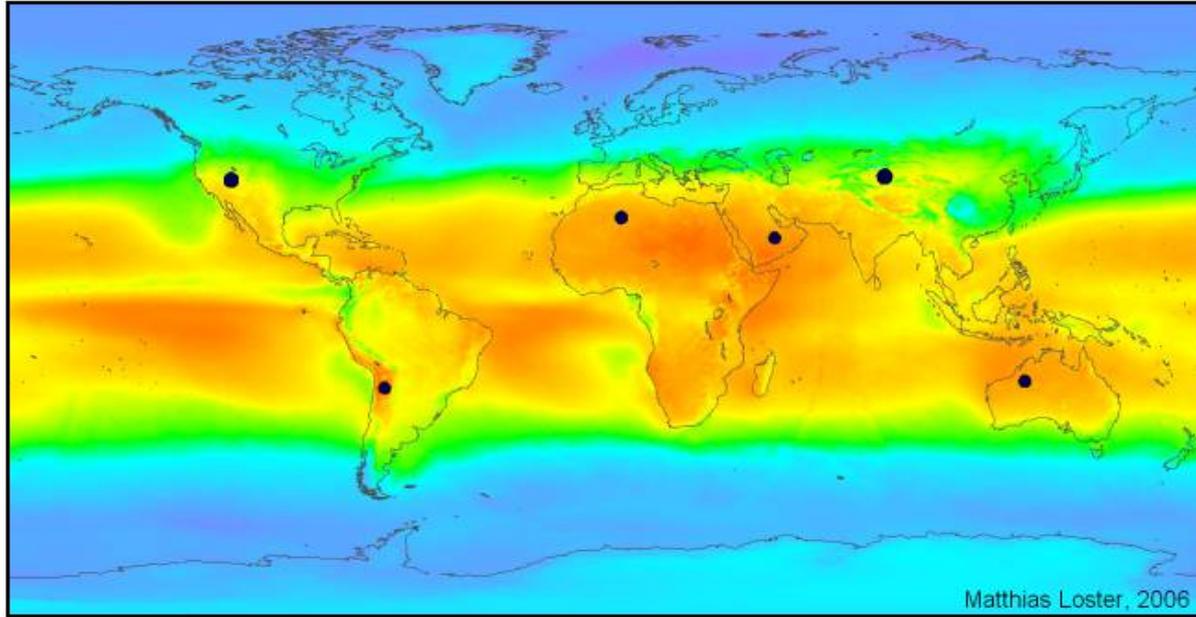
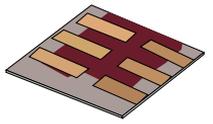


- Solar max power flux:
 $\sim 1500 \text{ W / m}^2$
- Average density over the year:
 - Sahara: $\sim 400 \text{ W / m}^2$
 - UK: $\sim 100 \text{ W / m}^2$

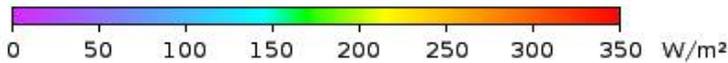
- Typical solar cell efficiency 15%
- In UK need 40 m^2 per person to supply average electricity demand (700 W)



Solar radiation map



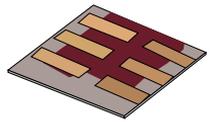
Milino76



$\Sigma \bullet = 18 \text{ TWe}$

Wiki: “Solar areas defined by the dark disks could provide more than the world's total primary energy demand (assuming a conversion efficiency of 8%). That is, all energy currently consumed, including heat, electricity, fossil fuels, etc., would be produced in the form of electricity by solar cells. The colors in the map show the local solar irradiance averaged over three years from 1991 to 1993 (24 hours a day) taking into account the cloud coverage available from weather satellites.”

Where do we find PV systems?



Andrewglaser

Building integrated



Sawu12

Solar power stations

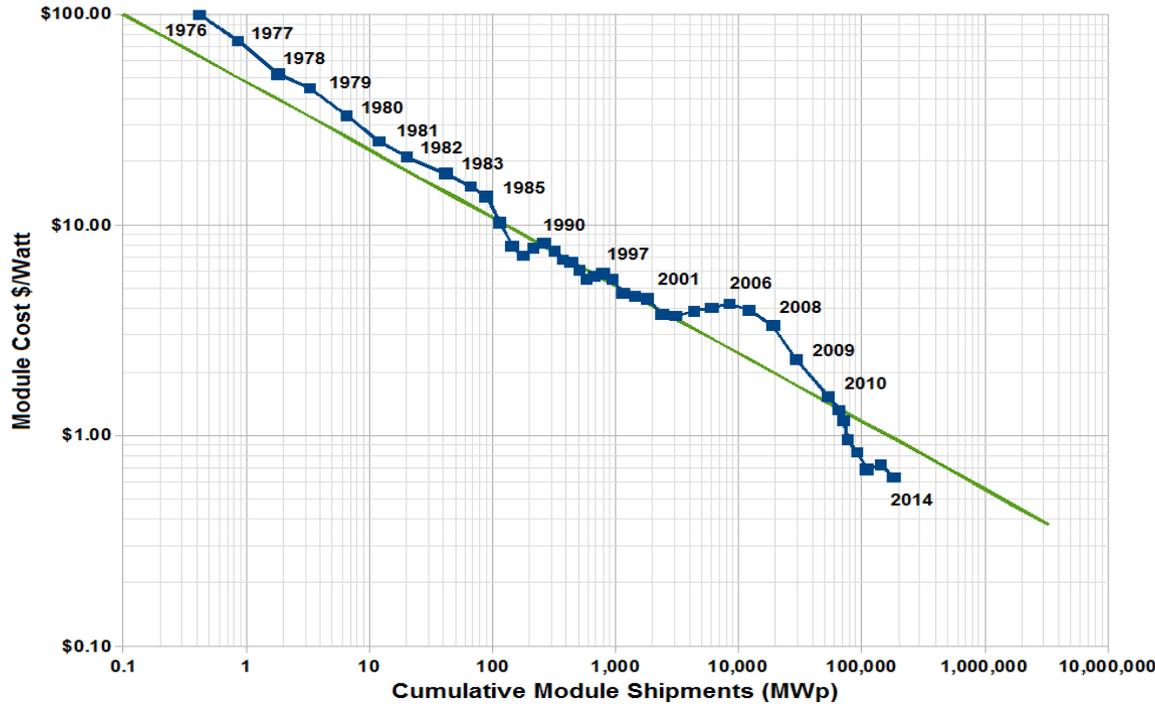
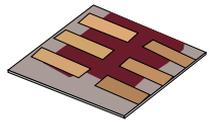


Hideki Kimura,
Kouhei Sagawa

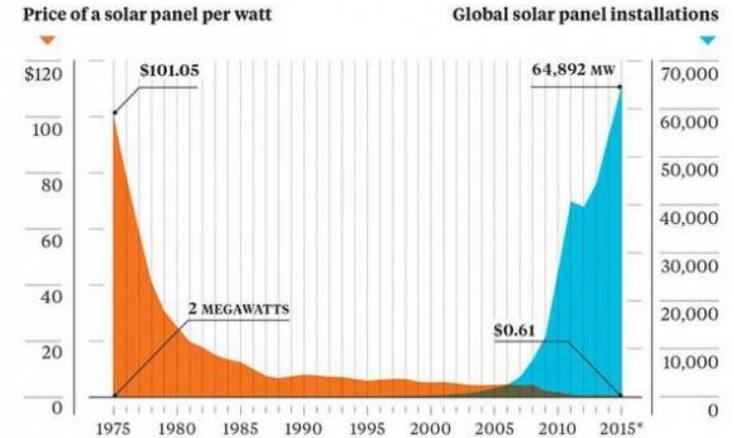
Transport integrated??

Why solar energy?

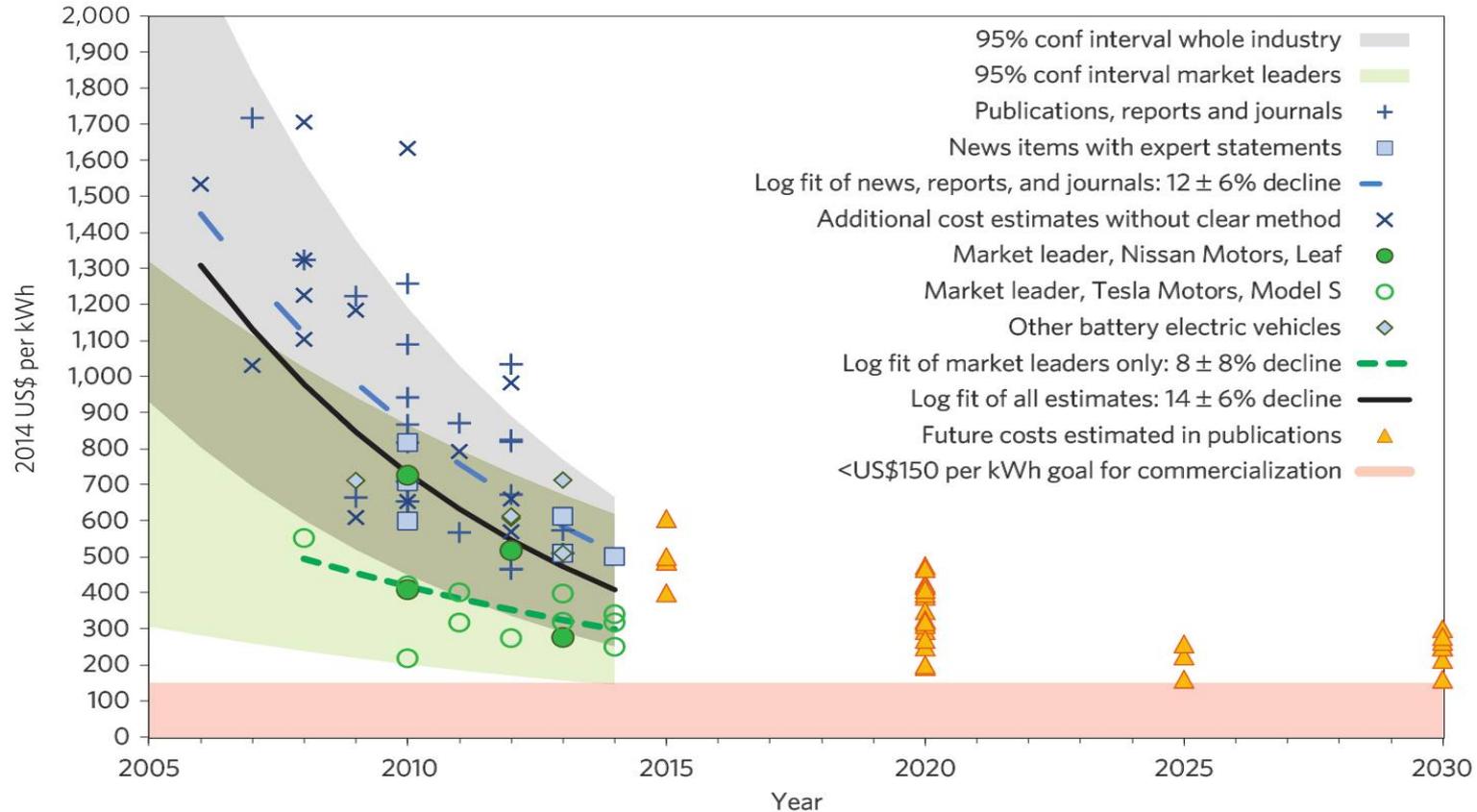
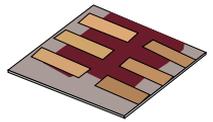
Swanson's law – production vs unit cost



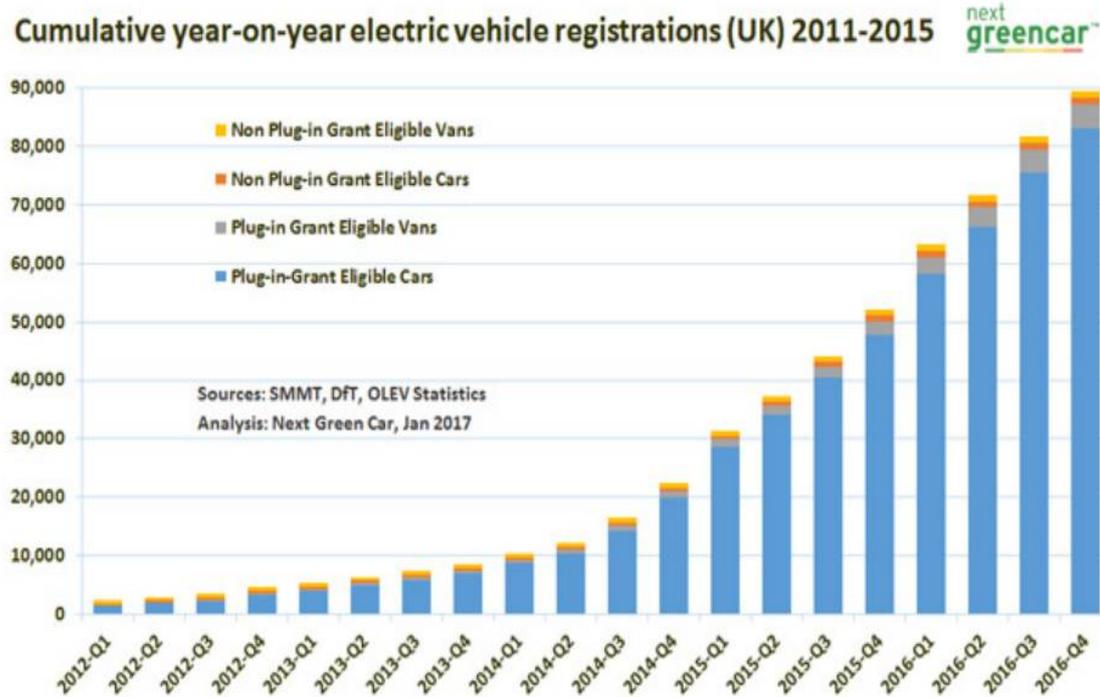
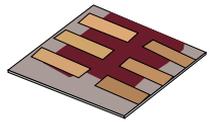
Every time solar cell production the price falls by 20%.



The same thing is happening with batteries: Cost of Li batteries

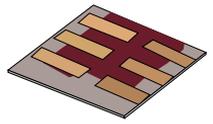


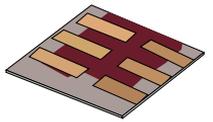
EV car registrations



Cell production – massive infrastructure investment

But we are getting off topic





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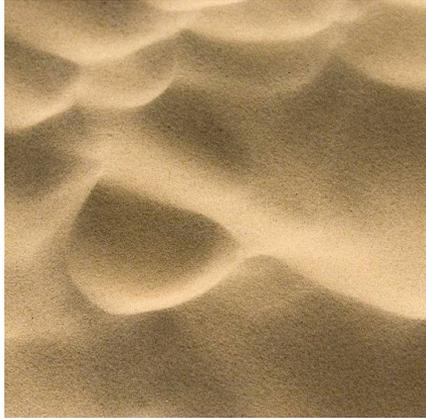
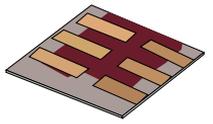
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What's wrong with silicon?



Naturally occurring silicon



Mono-crystalline silicon



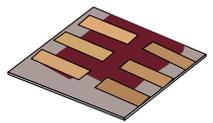
Silicon solar cell



5000 MJ per square meter!



Other classes of solar cell

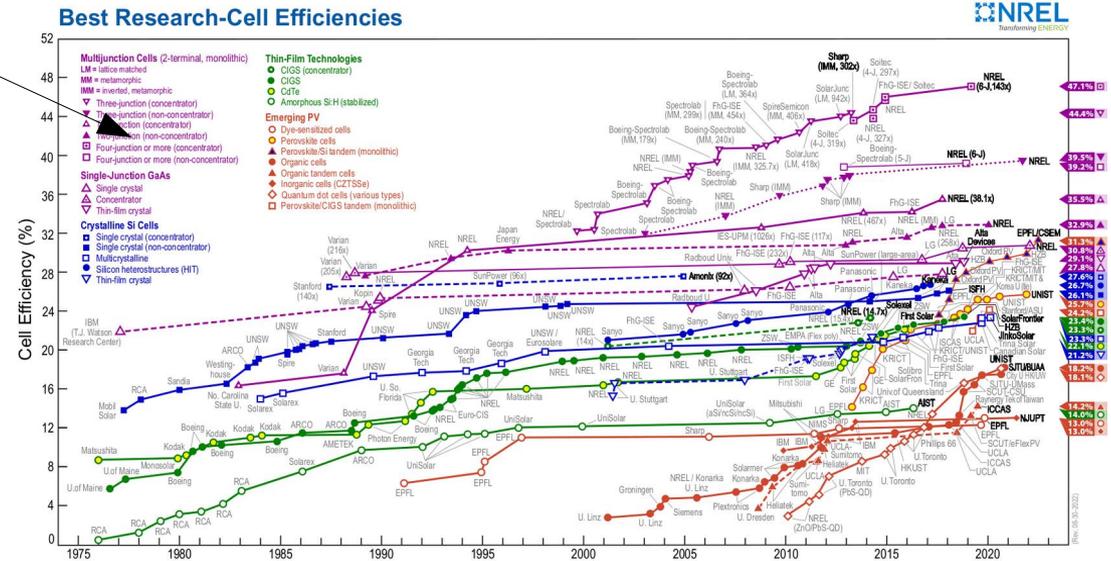


• People have been searching for alternatives to silicon solar cells for a long time

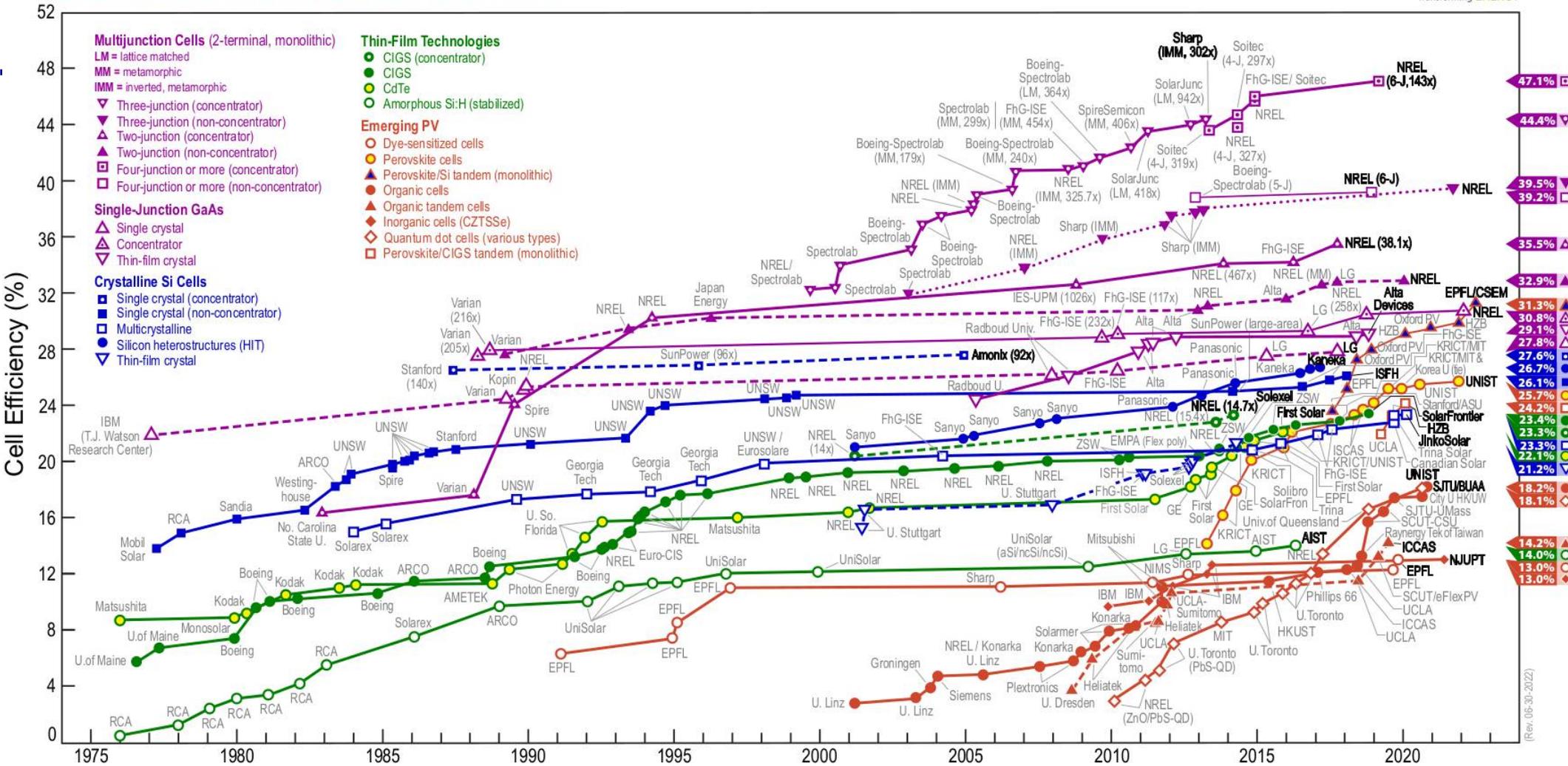
• Below is a graph of efficiency of different types of solar cell as a function of time.

• Let's have a closer look.

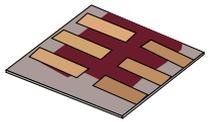
• Before we look at some of these technologies in more detail.



Best Research-Cell Efficiencies

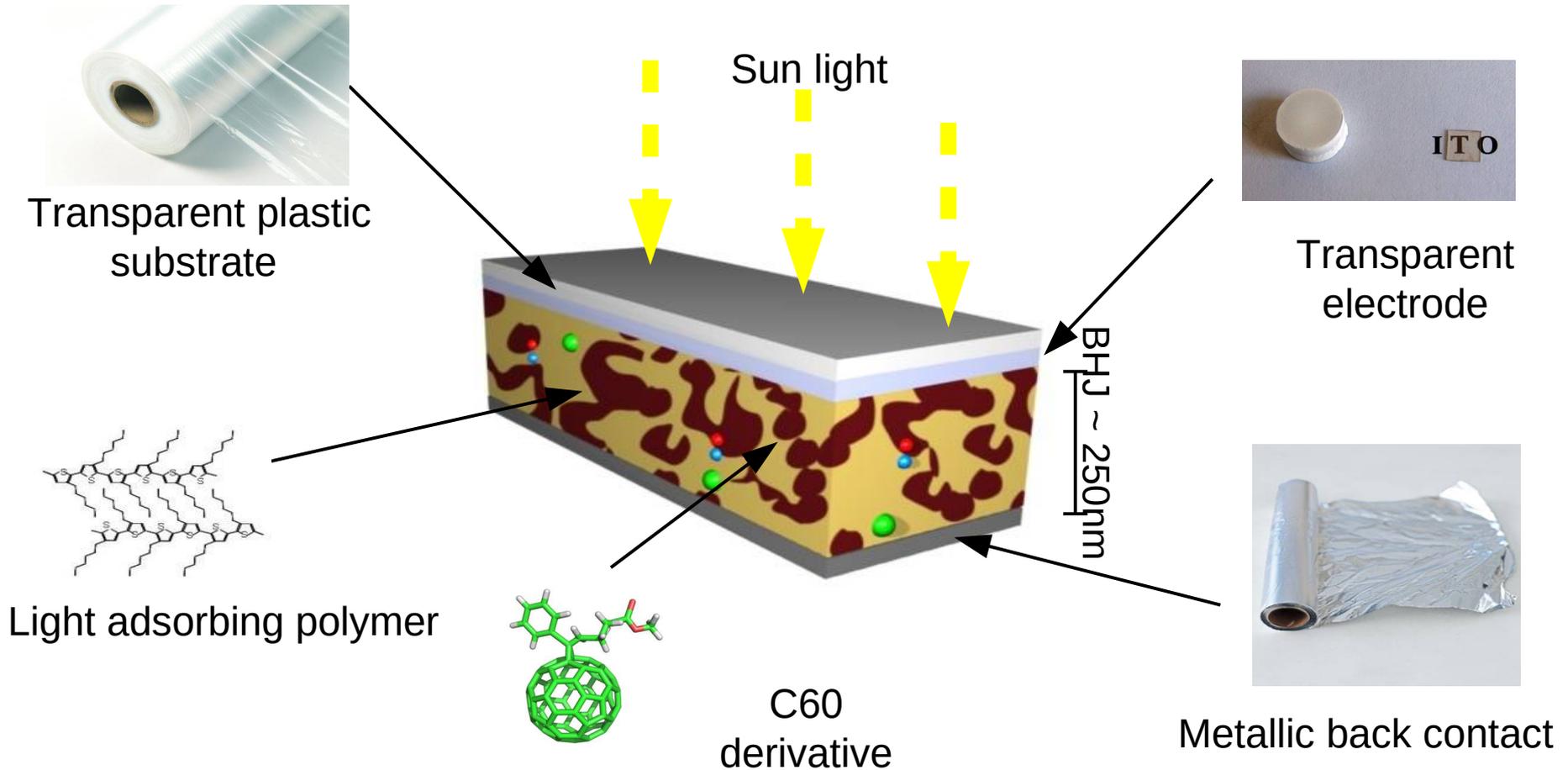
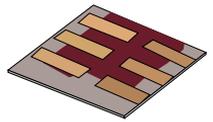


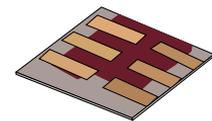
(Rev. 06-30-2022)



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One answer to this problem, the plastic solar cell.





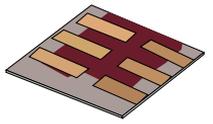
What are the advantages of organic solar cells?

- Organic molecules are cheap to make.
- They are flexible so the cells can be easily integrated into products and buildings.



Images from
www.konarka.com

Advantages of being flexible

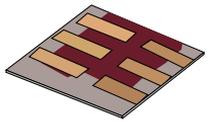


- But most importantly:
 - Organic devices can be printed onto a plastic substrate just like newspapers are printed onto paper at (100>m/min).
 - The principle is that does not matter that they are not very efficient as they are cheap to manufacture.



M. M. Voigt, R C.I. Mackenzie, et al. Solar Energy Materials and Solar Cells, 95, 2, 2011, pp. 731-734





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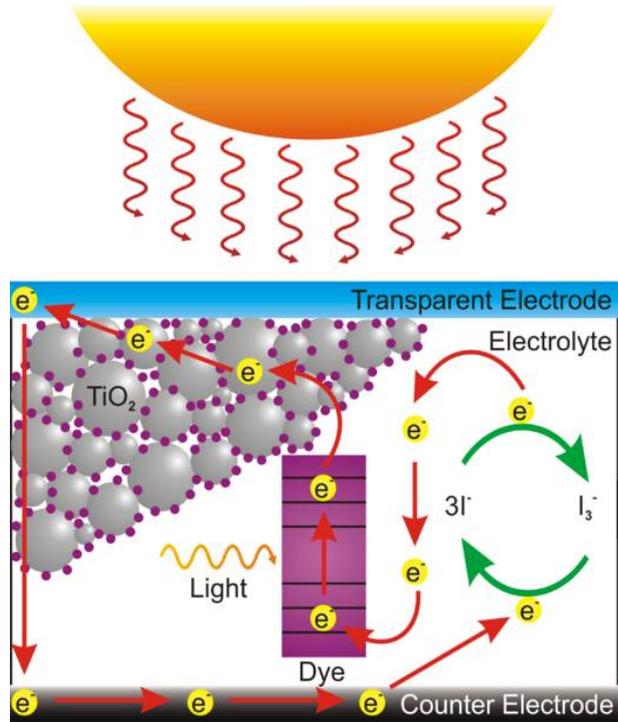
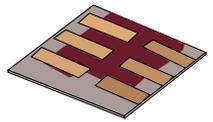
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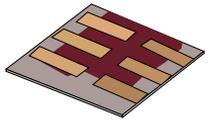
Dye sensitized solar cell



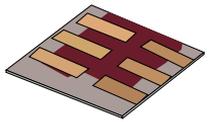
M. R. Jones



Dye sensitized solar cell



- Efficiency never really got really high.
- Over taken by perovskite solar cells.
- The liquid in them was a problem.
- Never really very successful.



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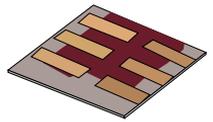
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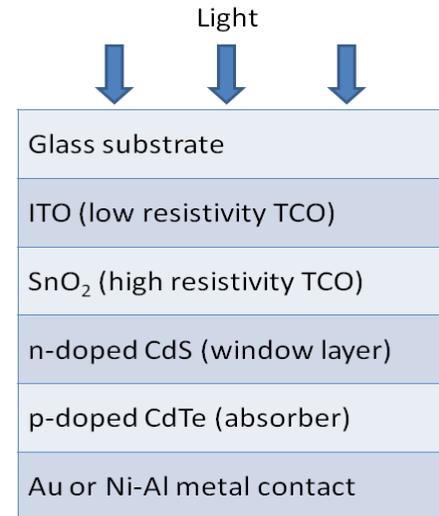
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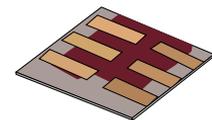
Spotting Cadmium Telluride solar cells.



- Generally a deeper blue than silicon and don't have metallic strips on the front of them.



Problems with Cadmium Telluride solar cells.



SAFETY DATA SHEET



Alchemist-hp

Environmental hazards

Hazardous to the aquatic environment, acute hazard Category 1

Hazardous to the aquatic environment, long-term hazard Category 1

OSHA defined hazards

Not classified.

Label elements



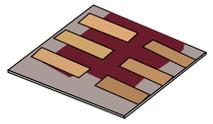
Signal word

Danger

Hazard statement

Toxic if swallowed. Fatal if inhaled. Suspected of causing genetic defects. May cause cancer. Suspected of damaging fertility. Suspected of damaging the unborn child. Causes damage to organs through prolonged or repeated exposure. Very toxic to aquatic life. Very toxic to aquatic life with long lasting effects.

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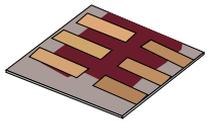
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•They fail the 'lick' test. Would you lick a Cadmium Telluride solar cell?



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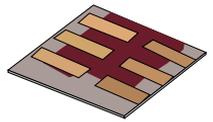
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What is the perovskite material?

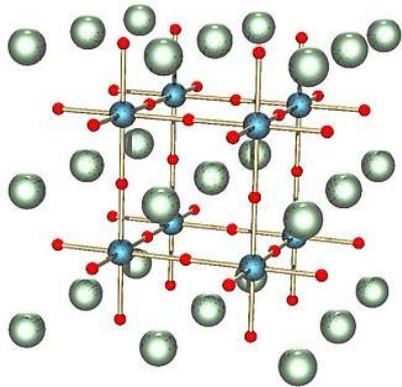


- Perovskites look like this (left), they have an ABX_3 structure (below), first discovered by the German mineralogist Gustav Rose in 1839.

- The perovskite most commonly used in solar cell is MAPbI₃ or $CH_3NH_3PbI_3$ note the CH_3NH_3 which is Methylammonium.

- They first came to prominence in 2012 when the first 10% cell was fabricated in Oxford.

- Since then there has been what I would describe as mass hysteria in the solar community with over 248,000 published on the topic.



Science

Current Issue First release papers Archive About

HOME > SCIENCE > VOL. 338, NO. 6107 > EFFICIENT HYBRID SOLAR CELLS BASED ON MESO-SUPERSTRUCTURED ORGANOMETAL HALIDE PEROVSKITES

REPORT

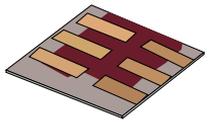


Efficient Hybrid Solar Cells Based on Meso-Superstructured Organometal Halide Perovskites

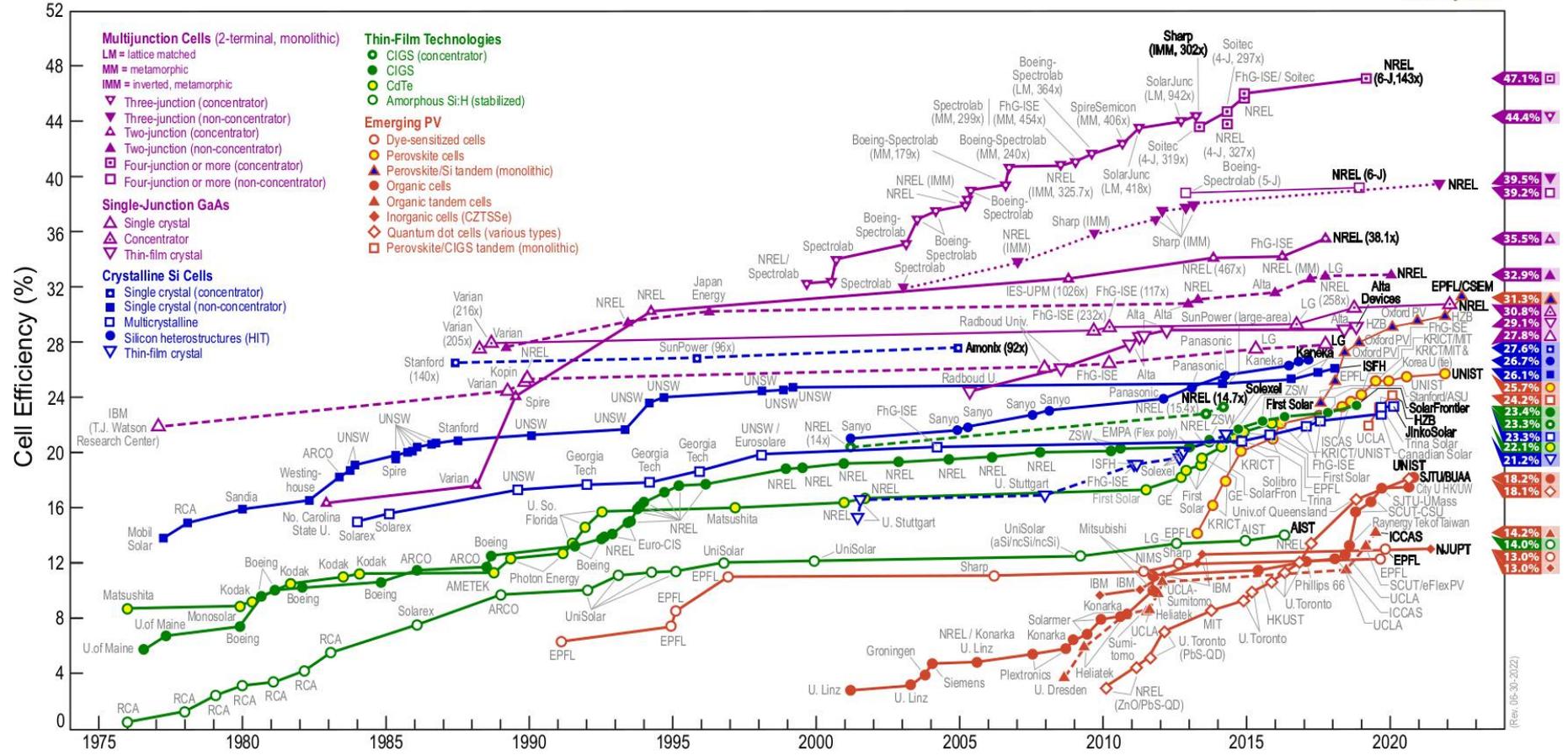
MICHAEL M. LEE, JOËL TEUSCHER, TSUTOMU MIYASAKA, TAKUROU N. MURAKAMI, AND HENRY J. SNAITH [Authors Info & Affiliations](#)

SCIENCE • 4 Oct 2012 • Vol 338, Issue 6107 • pp. 643-647 • DOI:10.1126/science.1228604

Comparison of perovskite and other solar cells

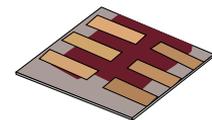


Best Research-Cell Efficiencies



(Rev. 05-30-2022)

And this is what I mean by mass hysteria: Write only journals :)



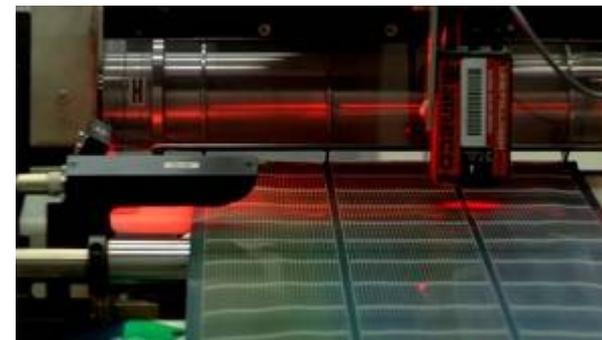
Google Scholar search results for "perovskite solar cell". The search bar contains "perovskite solar cell" and the search button is visible. The results section shows "Articles" with a red box highlighting "About 248,000 results (0.05 sec)". The top result is "Challenges for commercializing perovskite solar cells" by Y Rong, Y Hu, A Mei, H Tan, M Saidaminov, S Seok... - Science, 2018 - science.org. The abstract snippet reads: "... The road ahead for perovskites The high power conversion efficiencies of small-area perovskite solar cells (PSCs) have driven interest in the development of commercial devices. Rong ...". Below the abstract are links for "Save", "Cite", "Cited by 1019", "Related articles", and "All 13 versions".

- Perovskite cells are now going into production.

- And the Si-Perovskite tandem cells have reached 29.8% efficiency.

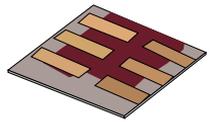
- Sounds good, and they seem a popular research topic.

Google Scholar search results for "perovskite". The search bar contains "perovskite" and the search button is visible. The results section shows "Articles" with a red box highlighting "About 1,150,000 results (0.05 sec)". The top result is "Challenges for commercializing perovskite solar cells" by Y Rong, Y Hu, A Mei, H Tan, M Saidaminov, S Seok... - Science, 2018 - science.org. The abstract snippet reads: "... Recently, a 110-m² perovskite PV system with ... perovskite absorber sensitizes a mesoporous metal oxide layer (eg, meso-TiO₂) used as a scaffold (3, 8). In planar PSCs, the perovskite ...". Below the abstract are links for "Save", "Cite", "Cited by 1019", "Related articles", and "All 13 versions".



Mark Shwartz

Why not perovskites (my personal view)?



- They contain lead $\text{CH}_3\text{NH}_3\text{PbI}_3$
 - Lead is highly toxic – let's read what the WHO says on the topic.
- In comparison to Si Perovskites are unstable in Oxygen, light and water (max lifetime of 1 year*). Key problem is getting financing for such a system.
- There are perovskites without lead but they are not as efficient in solar cells.
- So the point I am making is that they are an interesting material system but are they really such a good idea and did we need to publish 0.25 Million papers on the topic?

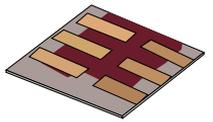


Key facts

- Lead is a cumulative toxicant that affects multiple body systems and is particularly harmful to young children.
- Lead in the body is distributed to the brain, liver, kidney and bones. It is stored in the teeth and bones, where it accumulates over time. Human exposure is usually assessed through the measurement of lead in blood.
- Lead in bone is released into blood during pregnancy and becomes a source of exposure to the developing fetus.
- There is no level of exposure to lead that is known to be without harmful effects.
- Lead exposure is preventable.



*<https://www.nature.com/articles/s41467-018-07255-1>



- Introduction

- What is this lecture?
- Why solar?
- Why not silicon?

- New solar cell technologies

- Organic solar cells
- Dye sensitized solar cells
- Cadmium telluride solar cells
- Why Perovskites for solar?

- **What is OghmaNano**

- Making a new simulation

- Fundamentals

- Semiconductor fundamentals
- The anatomy of a dark current curve

- Fundamentals (cont)

- The anatomy of a light current voltage curve
- Parasitic components
- Optical materials
- Optical simulations

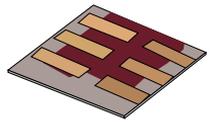
- Advanced topics

- Recombination
- Mobility
- The tau/mu product

- Mobile ions

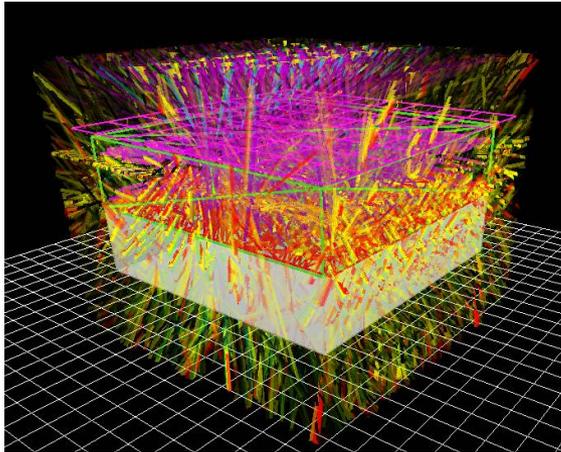
- Mobile ions
- Time domain perovskite simulation

What is OghmaNano?

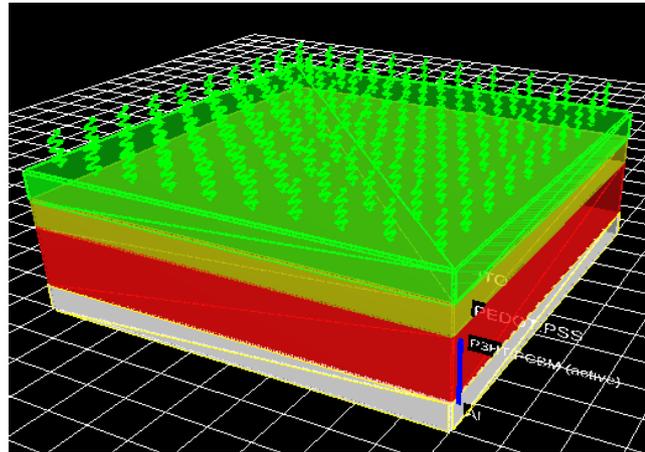


•OghmaNano is a software package which enables you to simulate:

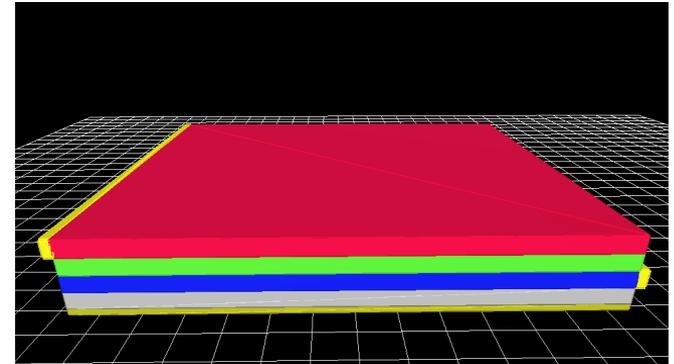
- **Solar cells, transistors, Sensors, OLEDs** (Organic Light Emitting Diodes)
- In general any device where light, electrons and heat interact.



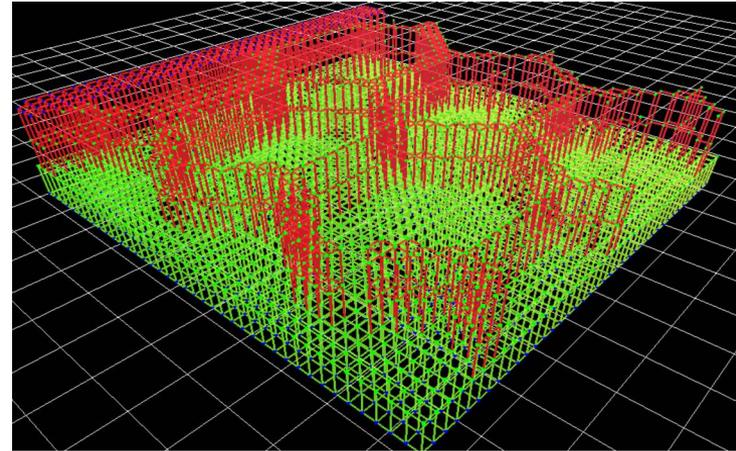
Light emission from a thin film



Solar cell simulations

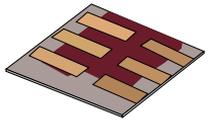


Organic Transistors (side contacts)



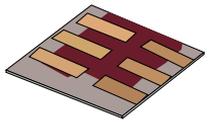
Large area devices.

What is OghmaNano?

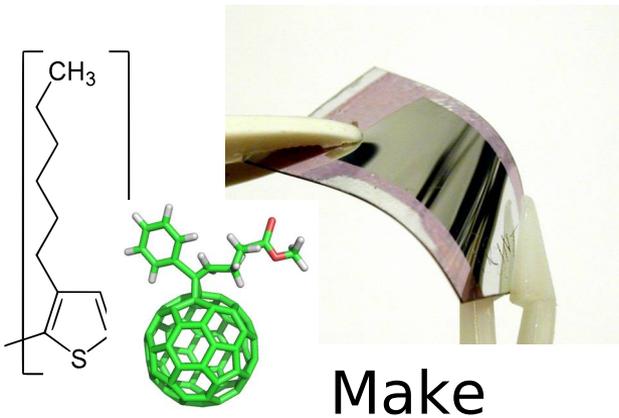


- The model can perform:
 - Electrical simulations**
 - Optical simulations**
 - Excited state simulations**
 - Simulate light emission (PL/EL)**
 - Thermal problems**
- In summary you can simulate all properties of a novel device.

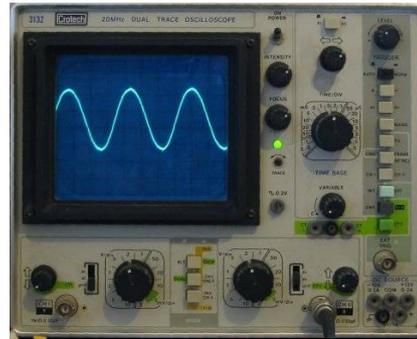
Why do device simulation?



- Results from novel devices are usually too complex and nuanced to understand without modeling
- To reach high impact journals and do really good science just demonstrating functionality is not enough you need to **model/understand** the results.



Make

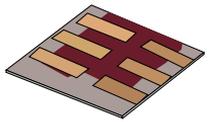


Measure



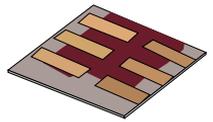
Simulate

Outline



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 - Semiconductor fundamentals
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Task 1: Make a new perovskite simulation



Organic and hybrid Material Nano Simulation tool (https://www.Oghma-Nano.com)

File Simulation type Simulation Editors Electrical Optical Thermal Databases Questions? Contact: roderick.mackenzie@durham.ac.uk About

New simulation Open simulation Export Zip Run simulation Parameter scan Fit to experimental data Optical Simulation Machine Learning Edit Probes

Information

Organic and hybrid Material Nano Simulation tool

www.Oghma-Nano.com

To make a new simulation select *Open simulation*

Documentation and tutorials

Follow updates on Twitter and YouTube

If you have questions or requests contact roderick.mackenzie@durham.ac.uk

Please consider joining the OghmaNano to be accessible in your language.

Feature requests/comments

If OghmaNano can't do exactly what you want...

/home/rod/oghma/oghma8.0/oghma_gui/gui

Which type of device would you like to simulate?

- P3HT:PCBM solar cell (PCE=4%)
- Amorphous silicon solar cell
- CIGS Solar cell
- EQE demo
- Equivalent circuit model
- Exciton domain
- Exciton device
- Fitting and
- Heterojunction tunneling example
- IS/IMPS/IMVS/ CV
- Large area PM6:Y6 solar cell
- Large area hexagonal contact
- Laser Example
- Matlab scripting demo
- Morphology
- OLED
- Optical filter
- Organic solar cells
- Perovskite solar cell
- Photonic-xtal FDTD
- Polycrystalline silicon
- Ray tracing
- Tandem solar cell
- Thermal simulation
- oled
- papers

Which type of device would you like to simulate?

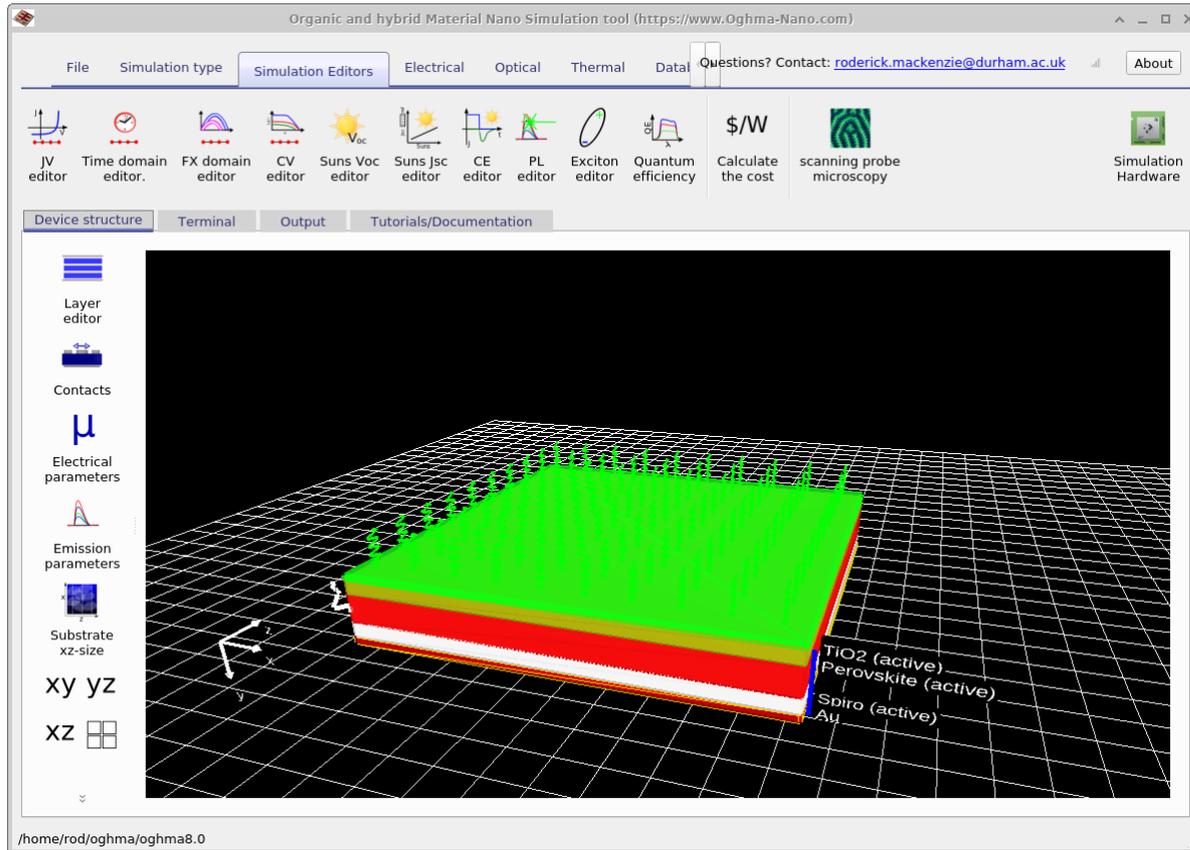
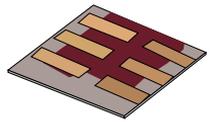
- MAPI device 10.1021/acsaem.9b00755
- Perovskite solar cell
- papers

• Double click! On 'MAPI device' and then save the simulation on your local disk, ideally not on:

• OneDrive, Dropbox, a network attached drive or a slow USB disk.

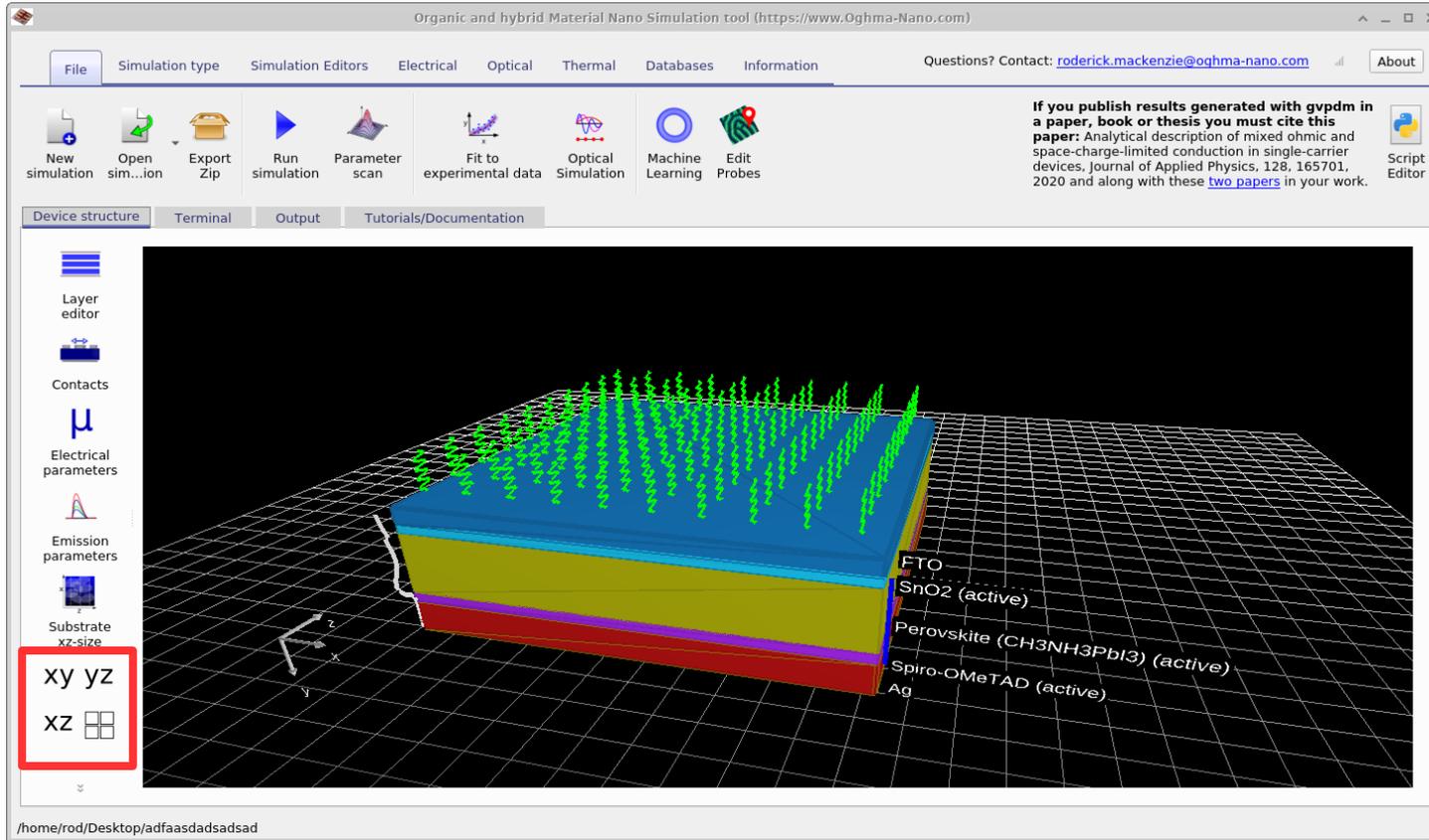
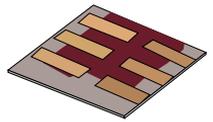
• The simulation dumps a lot of data to disk and therefore will be slow if run over a network.

Make a new perovskite simulation



- After you have saved you should get a window that looks like this.

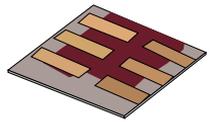
You should get a window which looks like this



- Try using the mouse to look around the picture of the cell and look at its layer structure

- Then try playing with the xy, yx, buttons.

Try hitting the play button to see what happens



Organic and hybrid Material Nano Simulation tool (<https://www.Oghma-Nano.com>)

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New simulation Open simulation Export Zip **Run simulation** Parameter scan Fit to experimental data Optical Simulation Machine Learning Edit Probes

If you publish results generated with gvpdm in a paper, book or thesis you must cite this paper: Analytical description of mixed ohmic and space-charge-limited conduction in single-carrier devices, Journal of Applied Physics, 128, 165701, 2020 and along with these [two papers](#) in your work. Script Editor

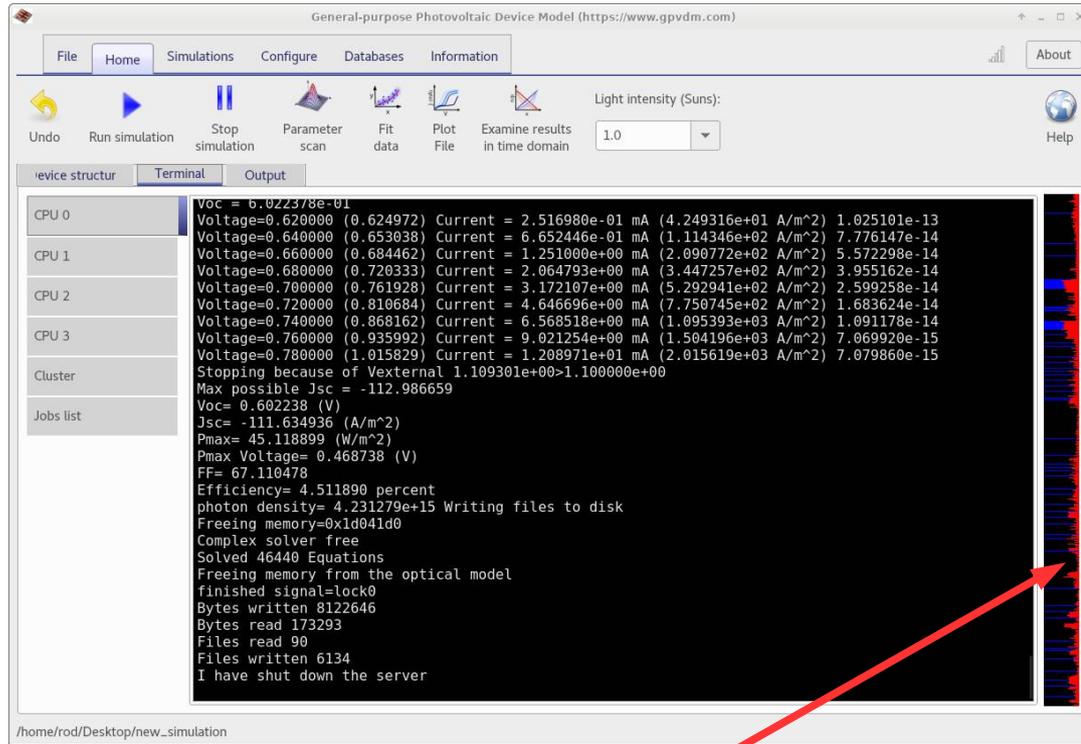
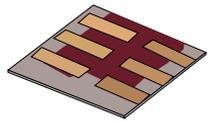
Device structure Terminal Output Tutorials/Documentation

Layer editor Contacts Electrical parameters Emission parameters Substrate xz-size xy yz XZ

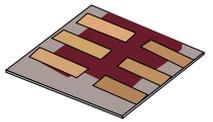
FTO
SnO₂ (active)
Perovskite (CH₃NH₃PbI₃) (active)
Spiro-OMeTAD (active)
Ag

/home/rod/Desktop/adfaasadsadsad

The core solver will be run on CPU 0

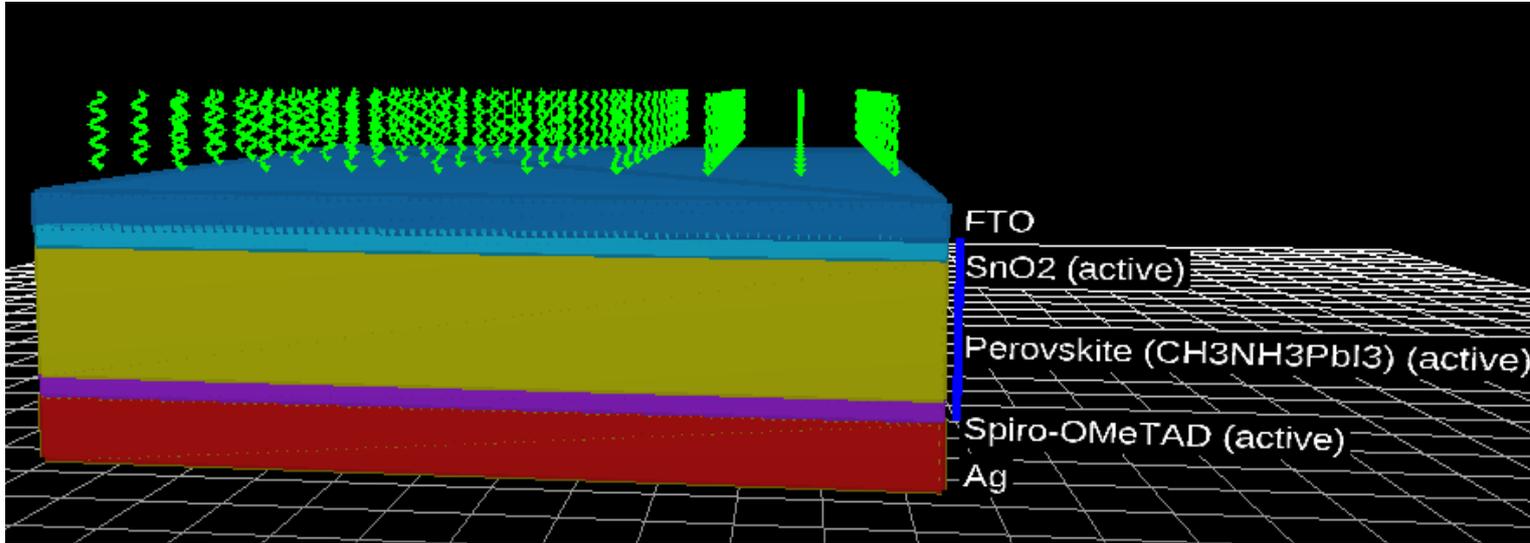
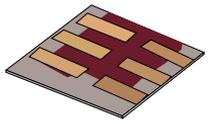


- Blue is CPU usage, red is disk usage, if you simulation is running slowly, writing to the HDD is **always** the bottleneck, SSDs highly recommended.



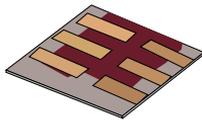
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The structure of a perovskite solar cell

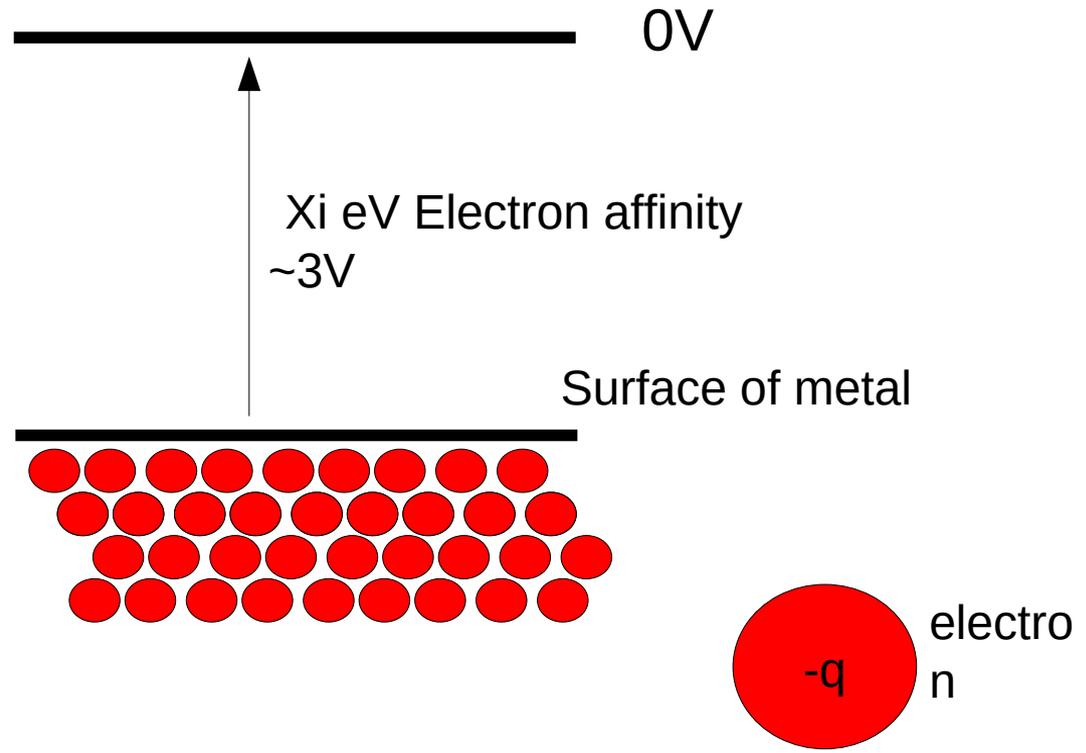


- We have various layers, FTO, SnO₂, Perovskite, Spiro and Ag
- Before we can understand this structure more we need to know what electron affinity and band gap are.
- How many of you know this already?

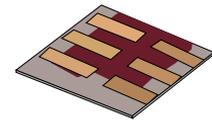
Fundamental principle of semiconductors: Electron affinity



This is how much energy is needed to remove one electron from the surface of a metal.

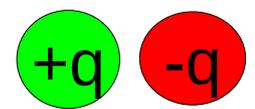
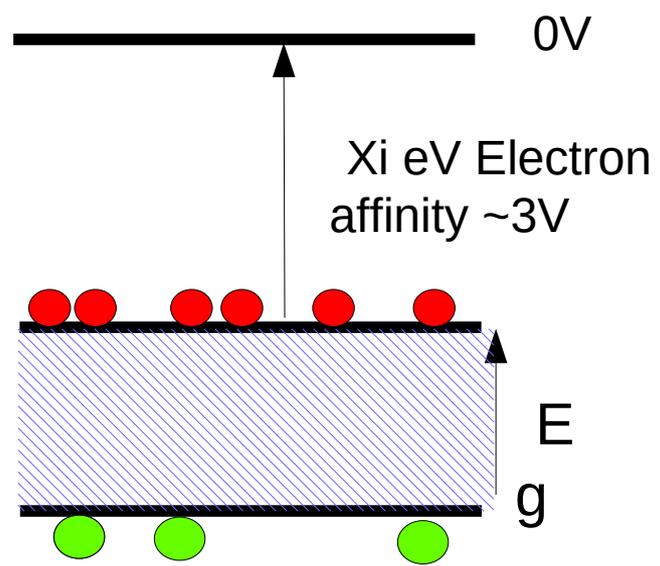


$$q = 1.60217657 \times 10^{-19} \text{ coulombs}$$



Fundamental principle of semiconductors: In semiconductors we have the concept of the band gap

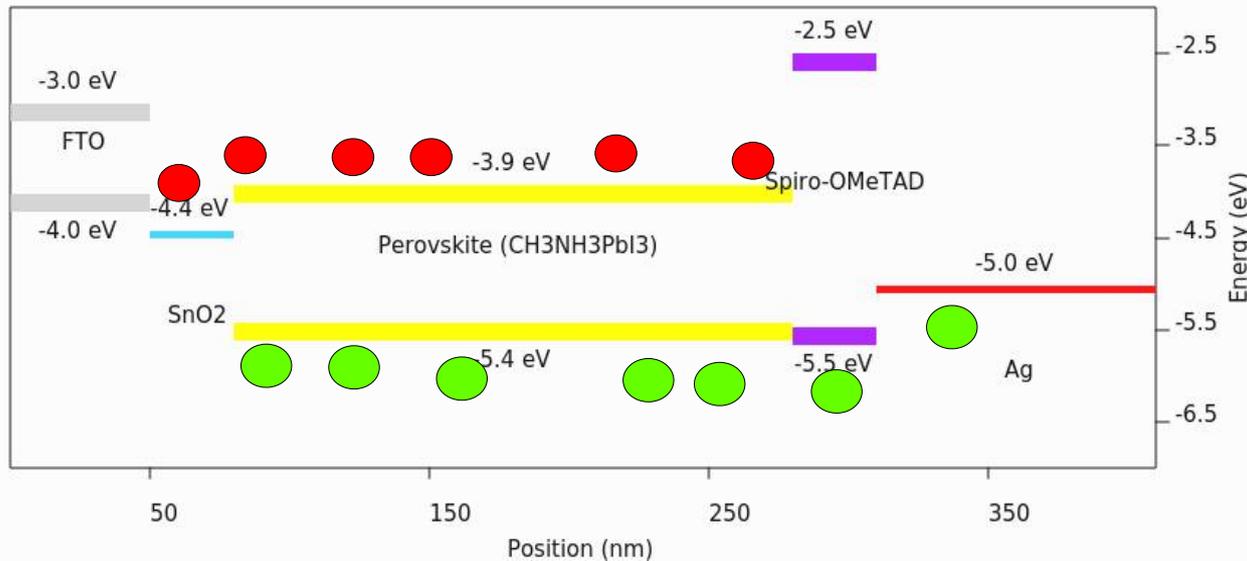
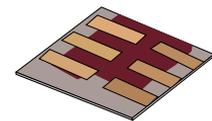
- Solar cells are made from a special type of material called a semiconductor.
- A semiconductors are a special because they have a **forbidden region** called the **band gap (Eg)** where no charge can exist.



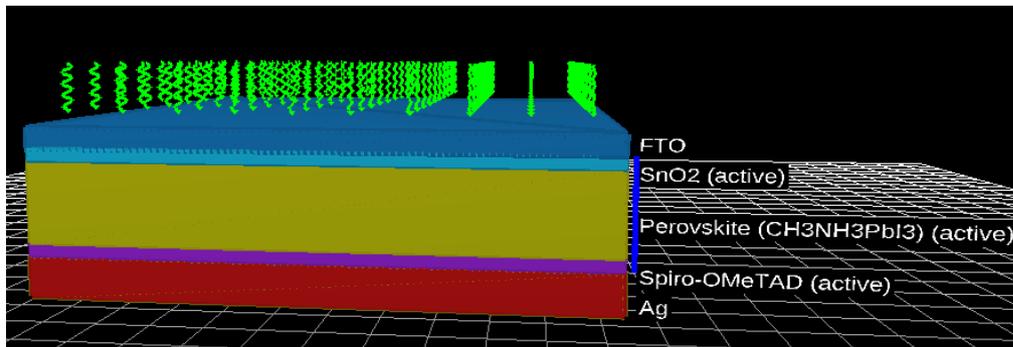
hole electron

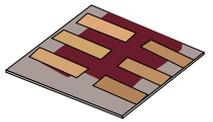
$$q=1.60217657 \times 10^{-19} \text{ coulombs}$$

With this knowledge let's now plot the 'band structure' of our solar cell



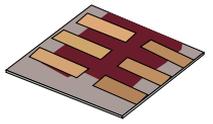
- **FTO (fluorine-doped tin oxide):** This is a conduction transparent contact material
- **SnO₂:** Only allows electrons (negative charge) to get to the FTO
- **Perovskite:** This is the semiconducting layer that adsorbs light.
- **Spiro-OmeTAD:** Is a molecule which only conducts positive charge.





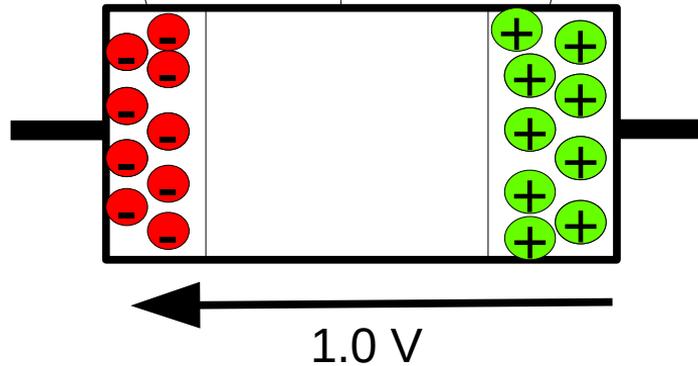
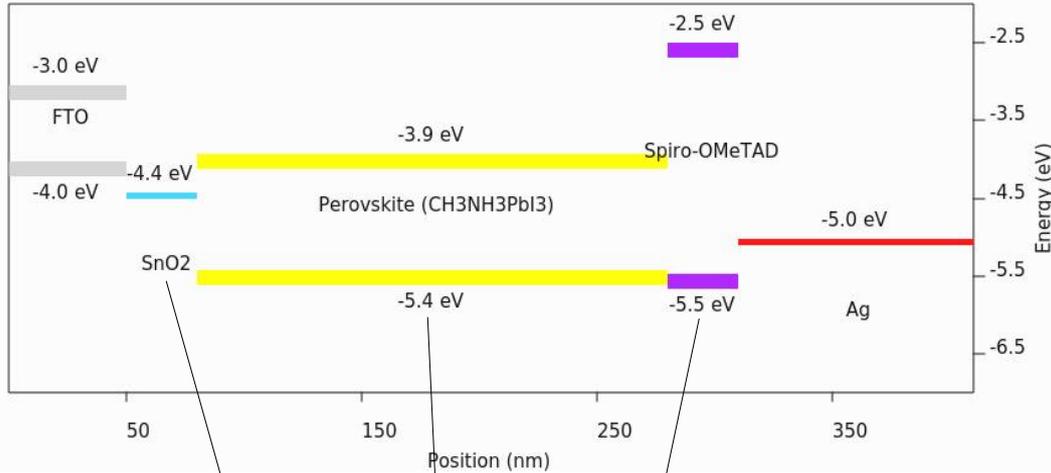
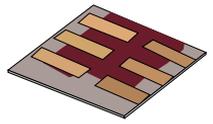
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Health warning:



- Because this talk is for a general audience (Chemistry, Geography, Social science, and finance PhD students), I'm avoiding the following terms:
 - Fermi level, Equilibrium, Recombination, Urbach tail slope etc..
- Thus the following explanation is very much a simplification to get us going.
- I will come back and cover it in detail in another talk.

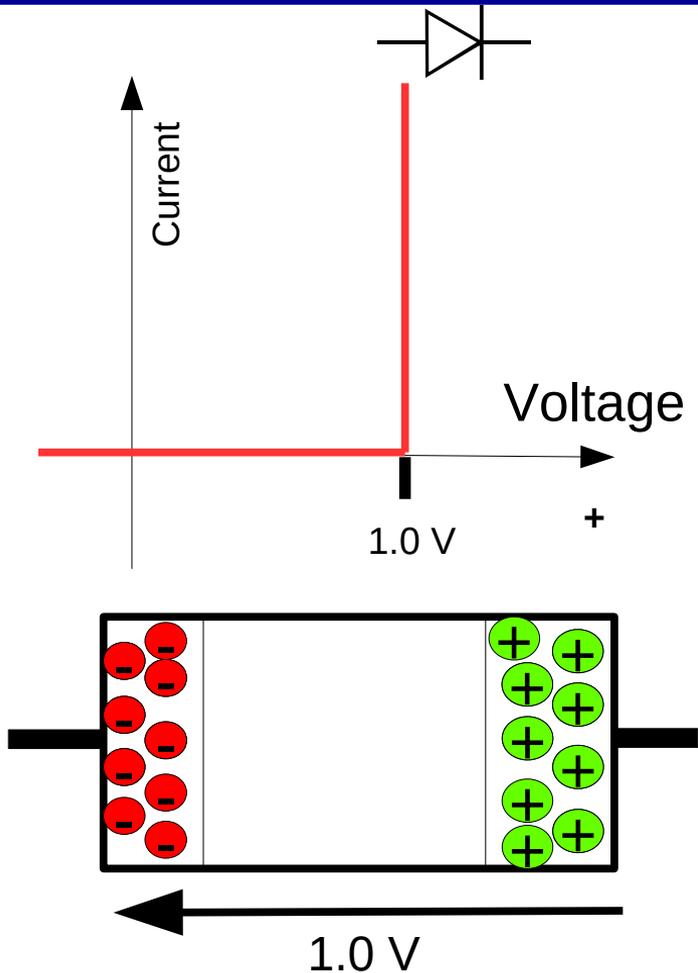
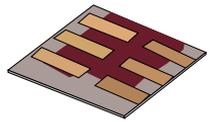
Understanding the turn on of a solar cell (diode) in the dark.



- This device has so called n-i-p structure.
 - The SnO_2 layer has a lot of excess electrons.
 - The Spiro-OmeTAD layer has a lot of excess holes.
- This charge just sits there and generates a potential voltage across the device.
- This is the same effect as you see when touching a Van de Graaff generator. Charge and Voltage/potential are linked by Gauss's law.

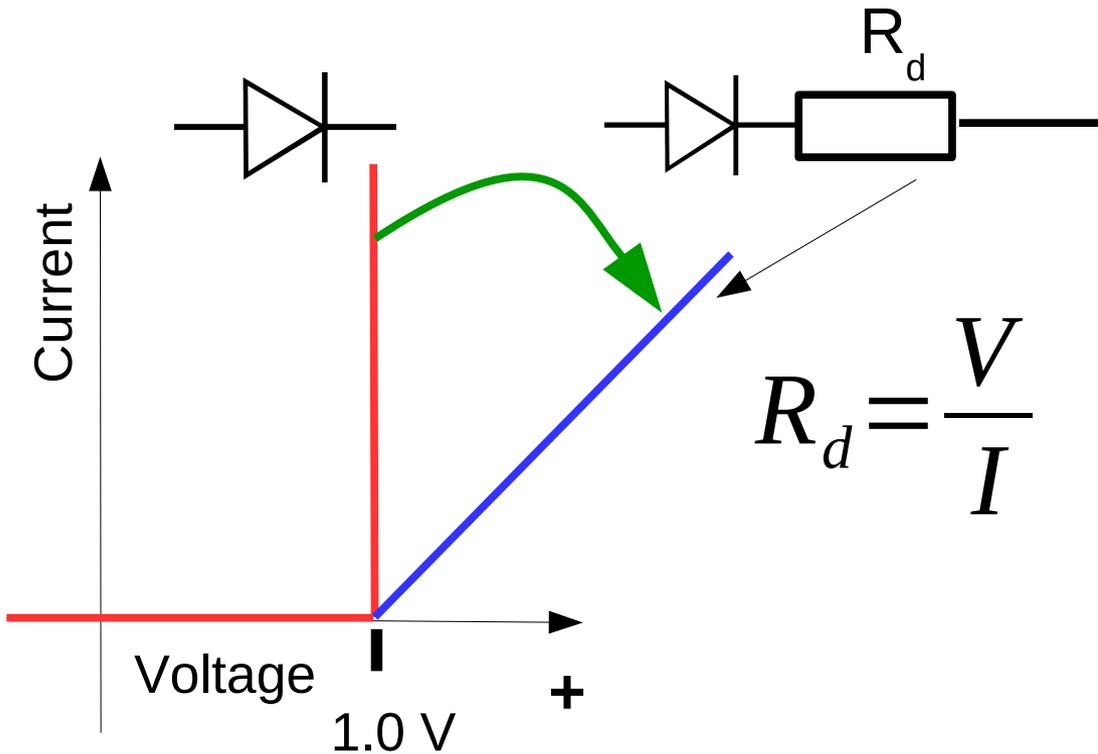
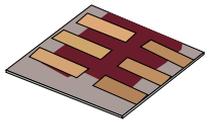


The current voltage curve of an idea solar cell (diode)



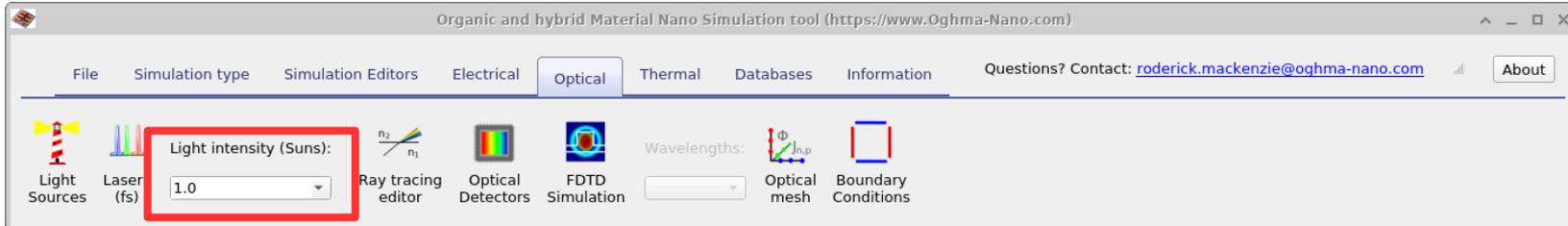
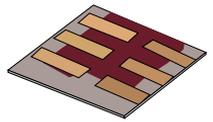
- This voltage is called the built in potential (V_b).
- This voltage must be overcome for the solar cell (diode) to turn on.
- Even in the dark this potential of about 1V is present over the diode.
- This results in a device which is more or less off below V_b and with a very rapid turn on after this point.

But our device has some resistance (everything does)



- This resistance makes the JV curve slope over*
- This is the general form of the dark voltage current curve of a solar cell*
- See previous health warning, this is an over simplification. I should really have 10 slides on recombination and the ideal diode equation. But this will do for now.

Task 2: Let's run a dark current voltage simulation

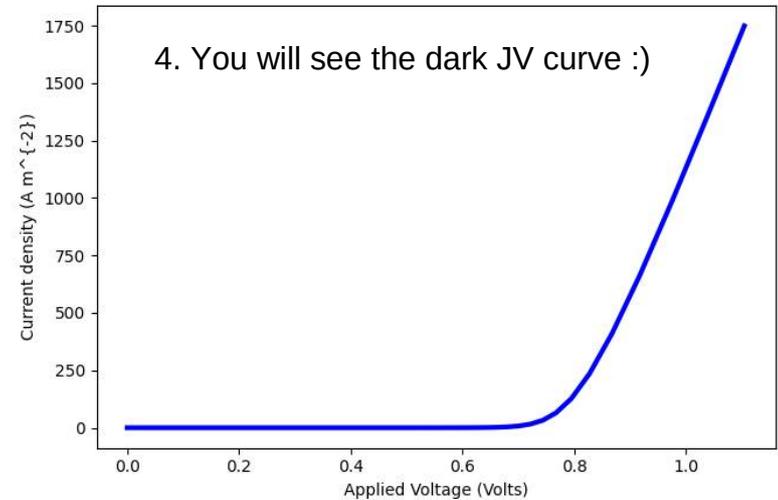


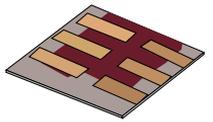
1. Set the light intensity to 0 Suns



2. Run the simulation

3. Double click on jv.dat





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•Fundamentals (cont)

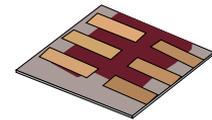
- The anatomy of a light current voltage curve**
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• Advanced topics

- Recombination
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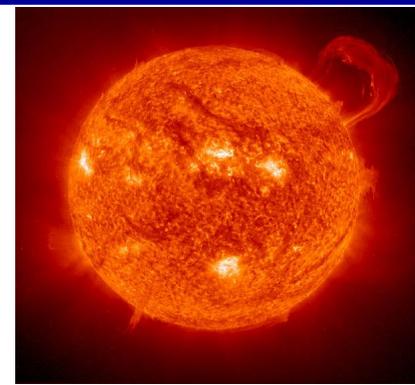
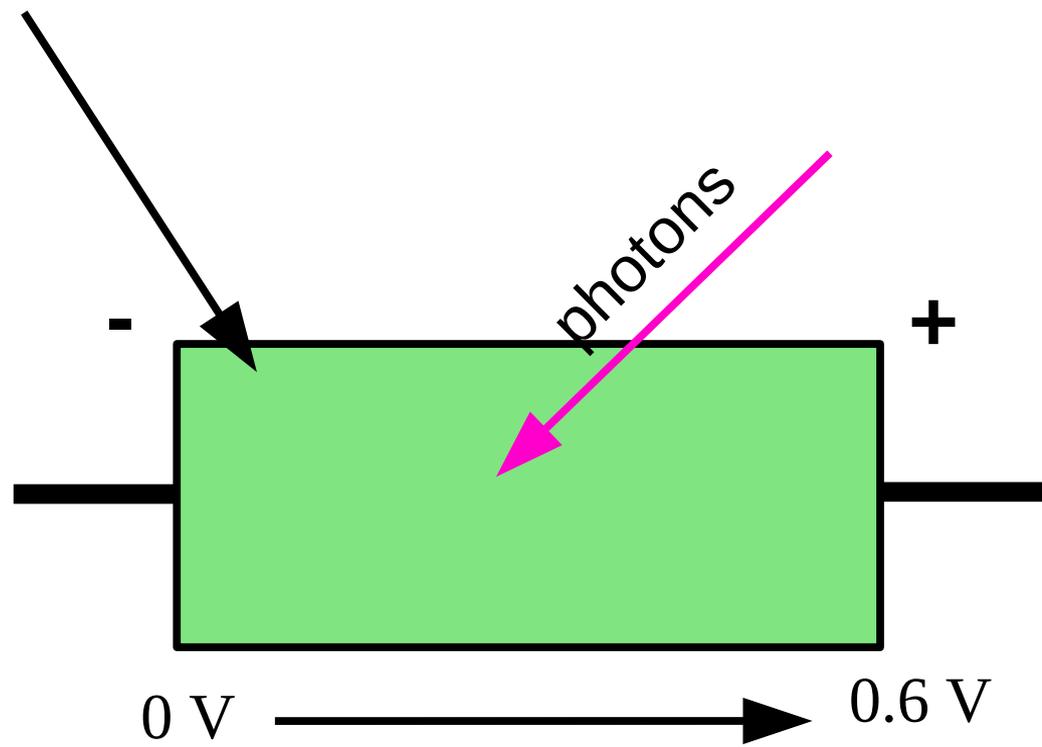
• Mobile ions

- Mobile ions
- Time domain perovskite simulation

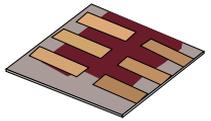


Now let's expose our device to light:

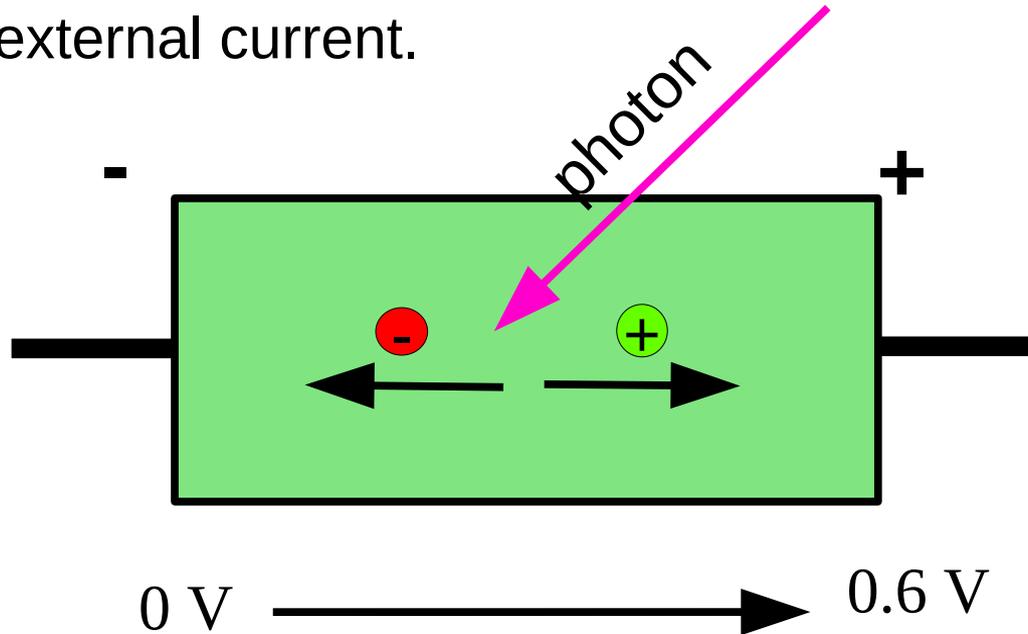
- Light adsorbing material (the perovskite)



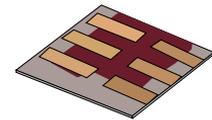
When a photon is adsorbed in a material.....



- An electron and a hole will be generated.
- And the field pulls them away from each other to the contacts, this generates external current.

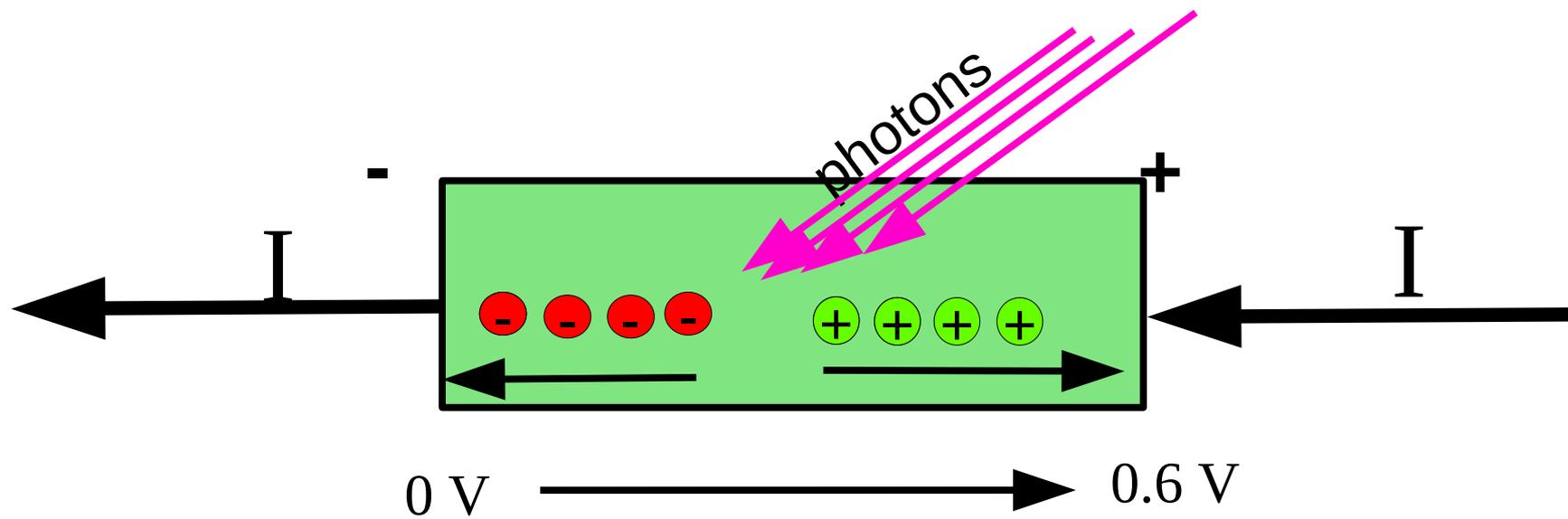


[I'm skipping the drift vs diffusion discussion]

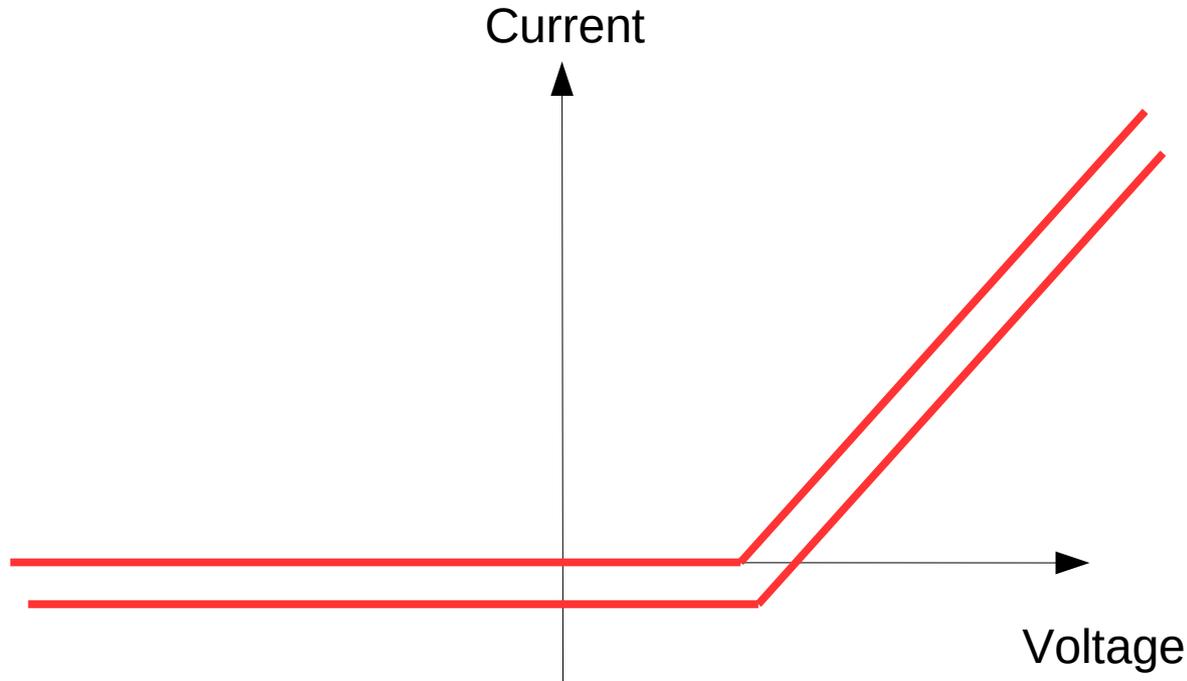
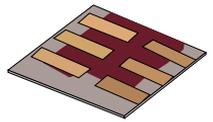


When a photon is adsorbed in a material.....

- If lots of photons hit the diode lots of positive and negative charges move to the contacts and we get current in the external circuit.

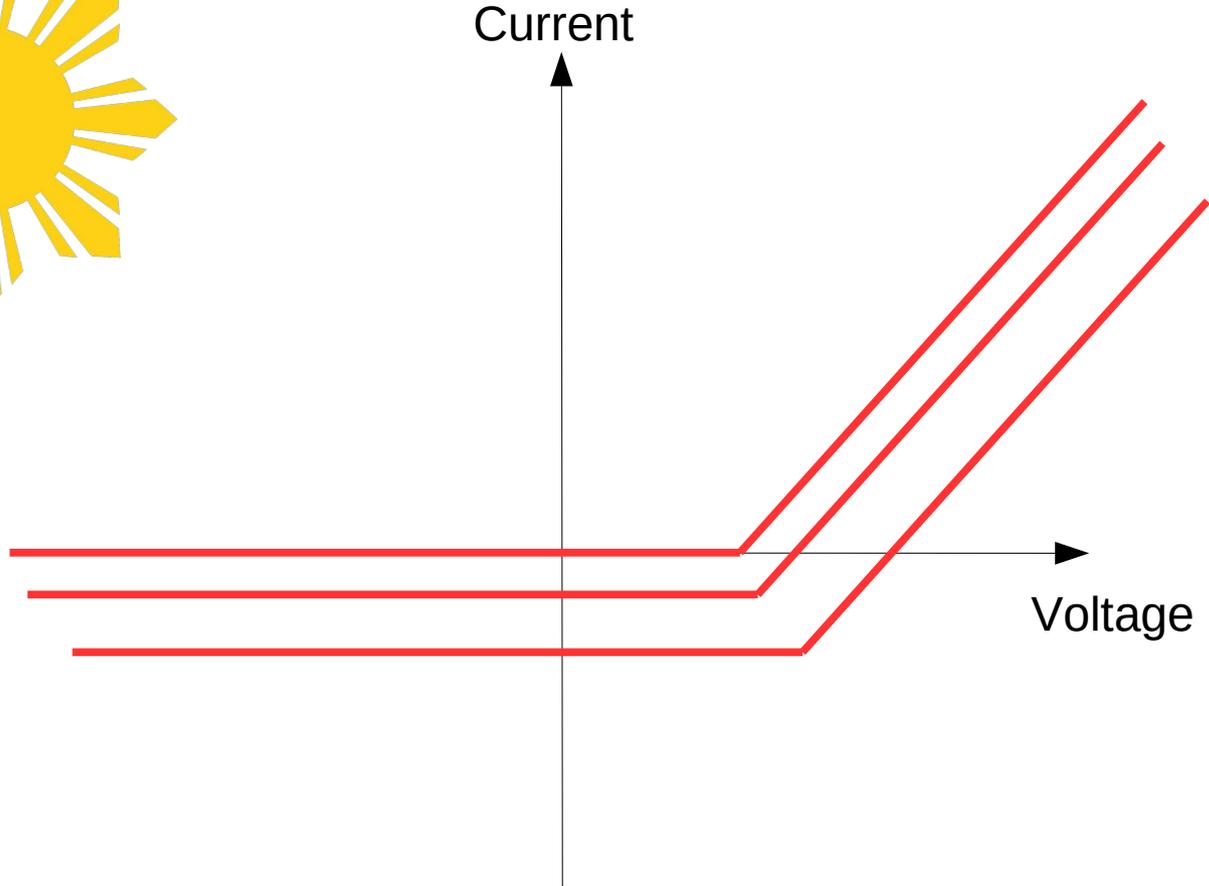
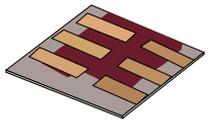


What do the JV curves look like in the light

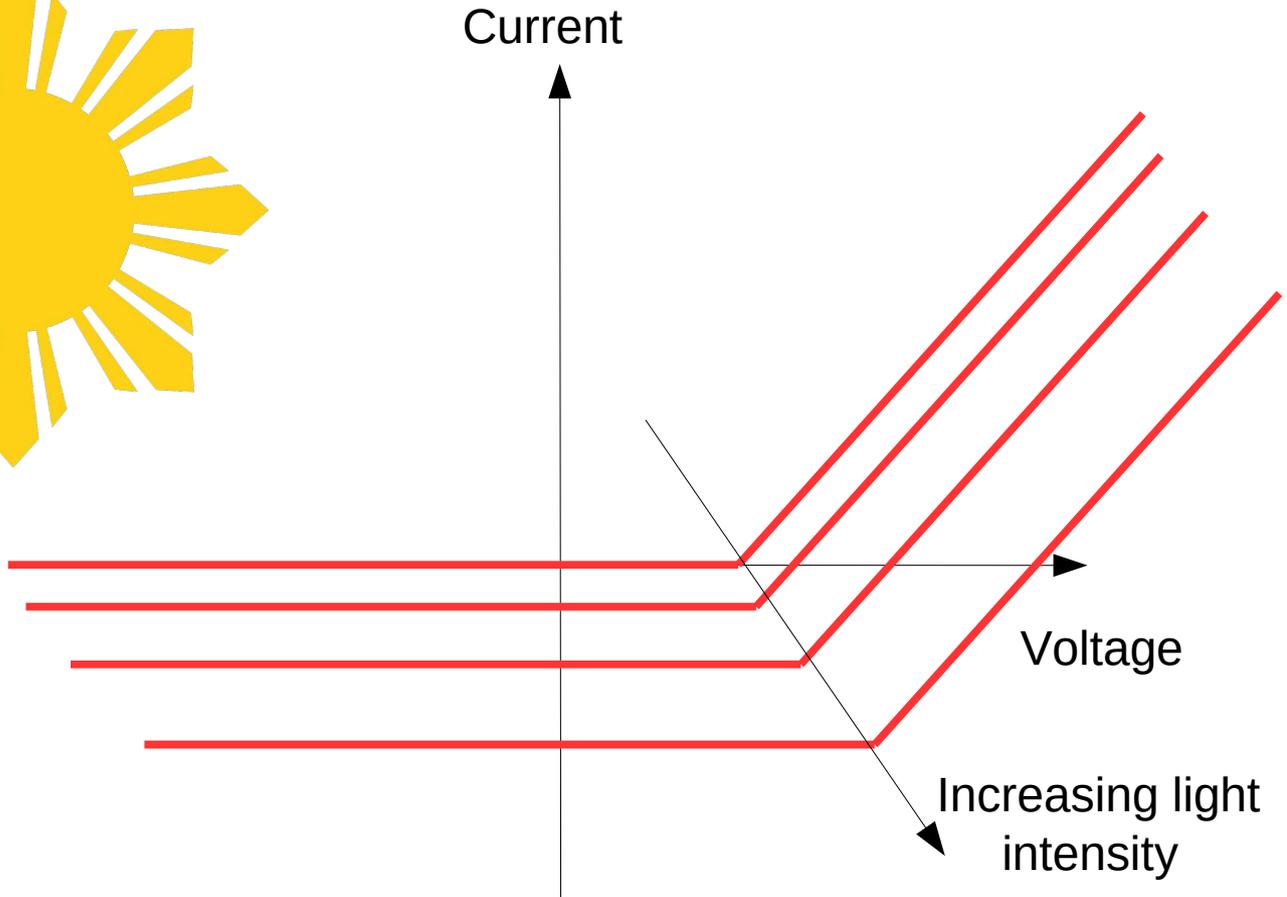
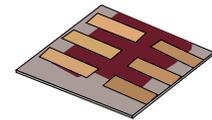


- Negative current means the current is coming out of the device rather than going into it.
- It's generating electricity.

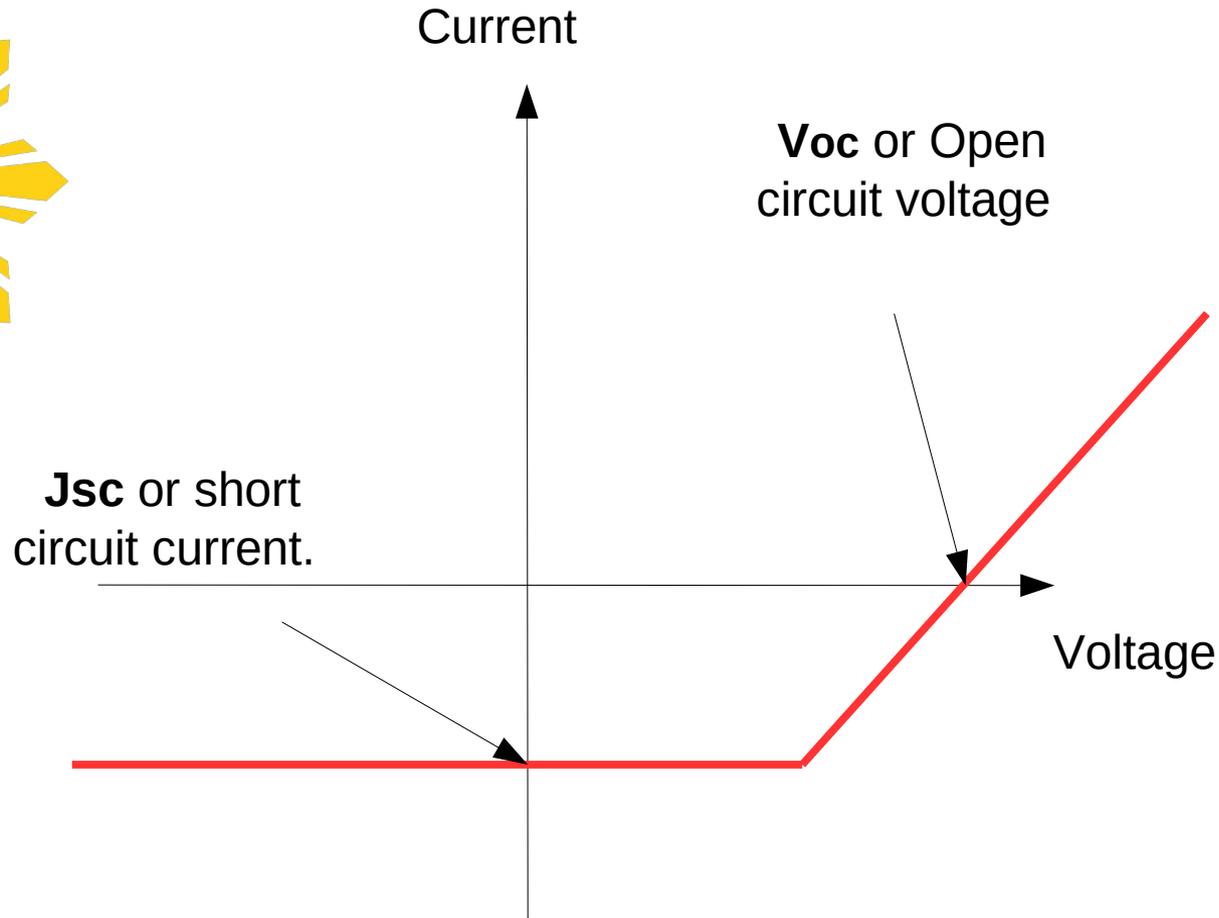
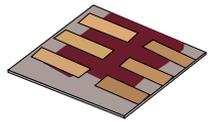
What do the JV curves look like in the light

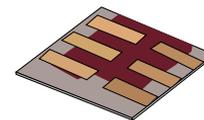


What do the JV curves look like in the light



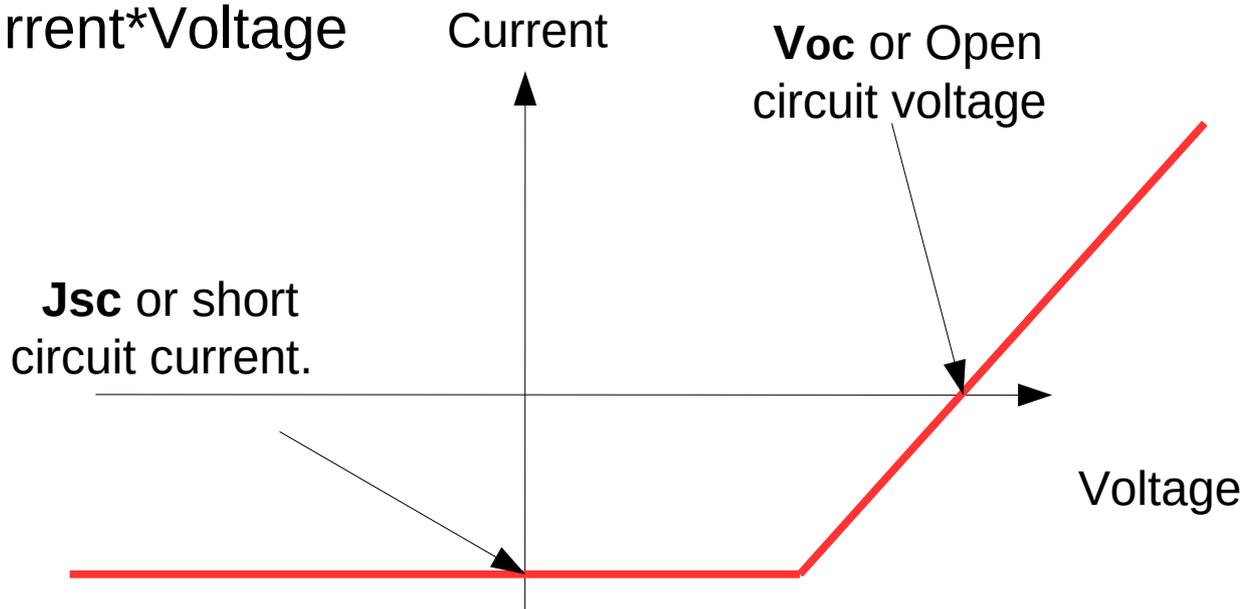
What do the JV curves look like in the light



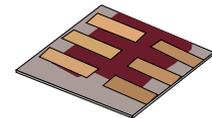


What do the JV curves look like in the light

Power=Current*Voltage

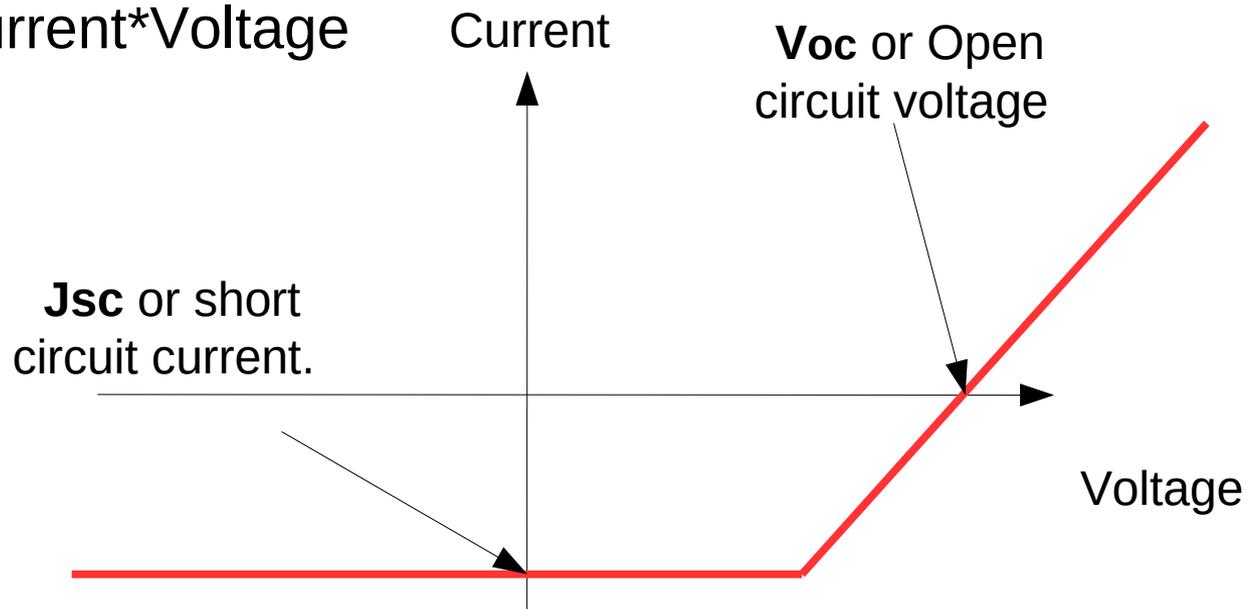


- How much power is produced at Voc?
- How much power is produced at Jsc?
- Where will maximum power be produced?



What do the JV curves look like in the light

Power=Current*Voltage



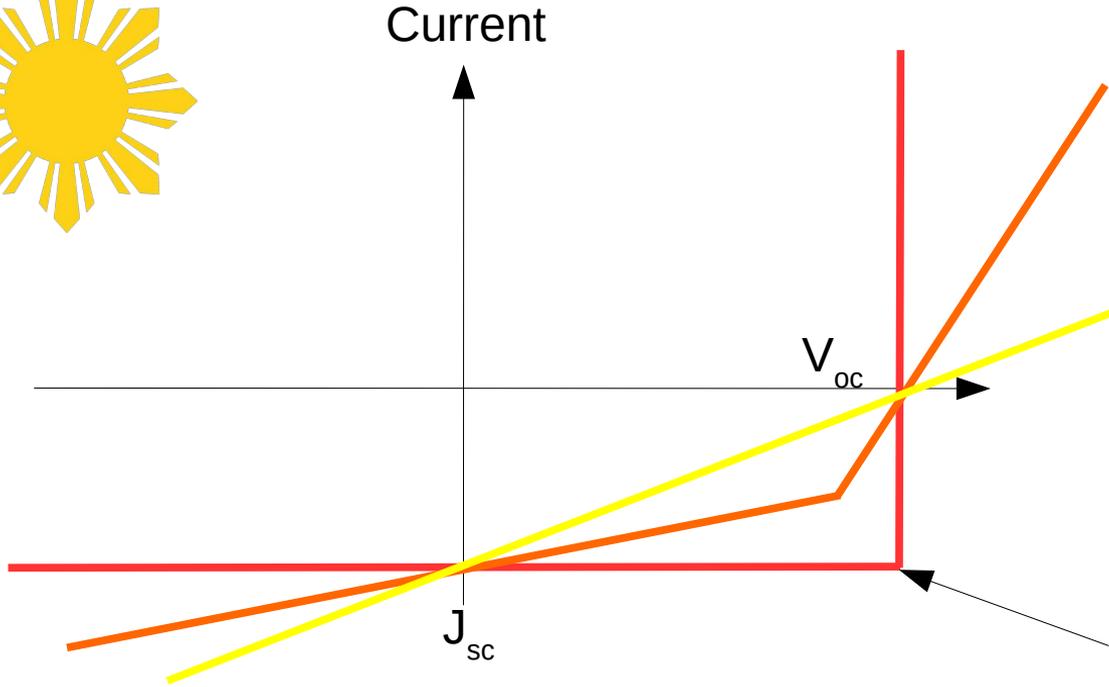
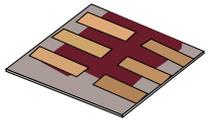
- How much power is produced at Voc?
- How much power is produced at Jsc?
- Where will maximum power be produced?

$$P=0*V_{oc}$$

$$P=J_{sc}*0$$

$$P=J*V \text{ (for } J, V \text{ @ max } P)$$

Fill factor (FF)

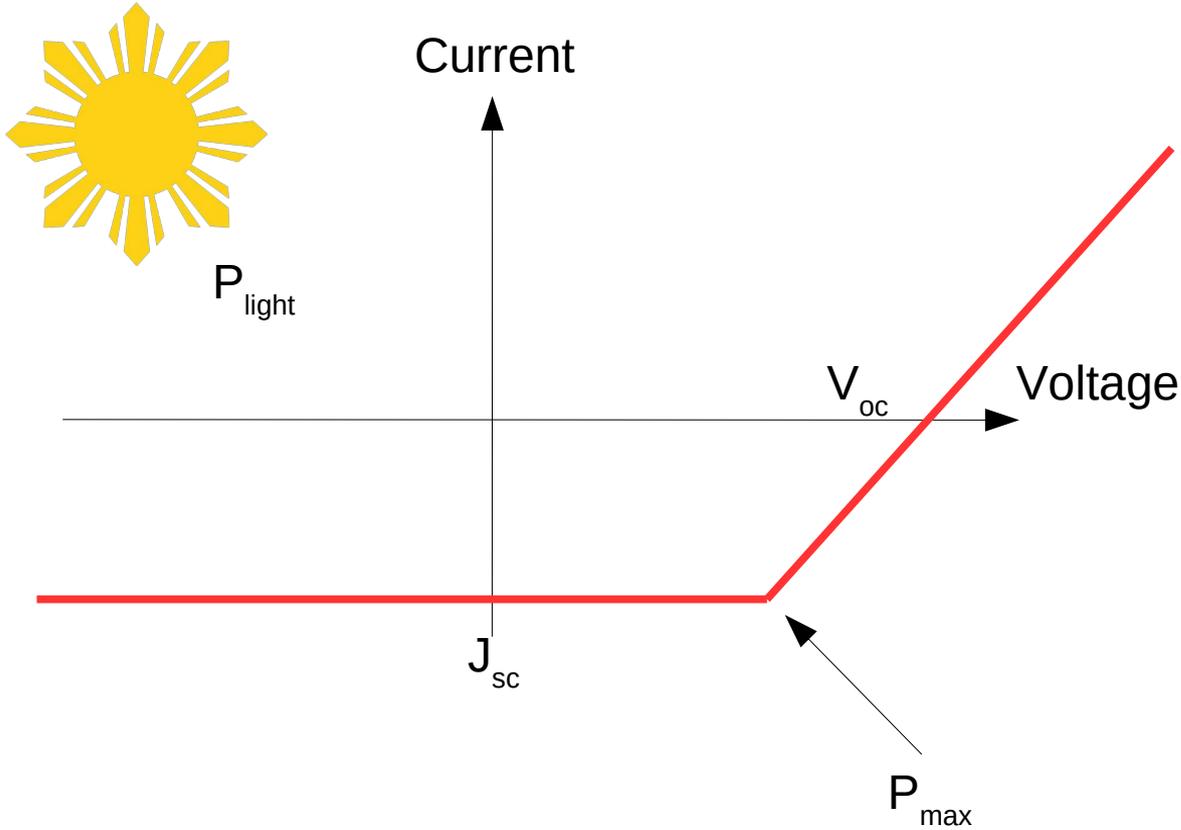
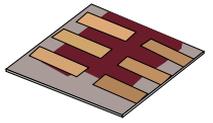


• Fill factor is a measure of how square the current voltage curve is.

• The more square the better and the higher P_{max} will be.

$$FF = \frac{V(@P_{max}) J(@P_{max})}{J_{sc} V_{oc}}$$

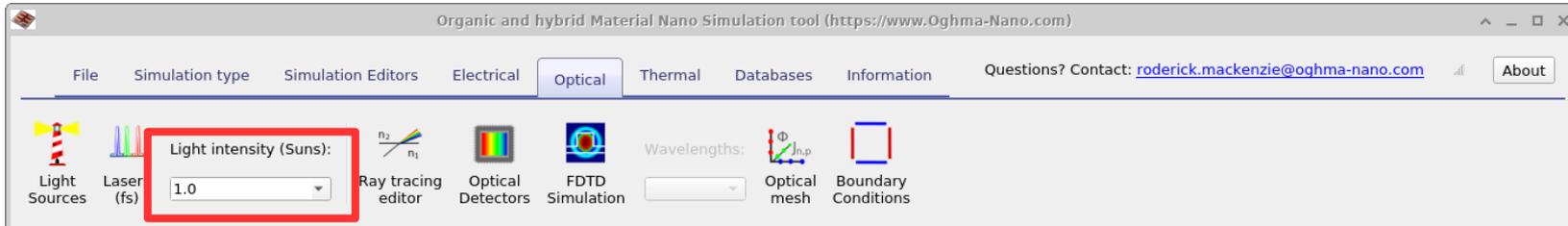
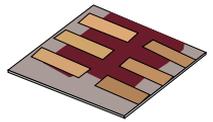
Power conversion efficiency (PCE)



- This is the efficiency of the cell for a silicon cell it is about 24%
- For an organic cell it's generally 16-20%
- For a perovskite cell it's about 20%.

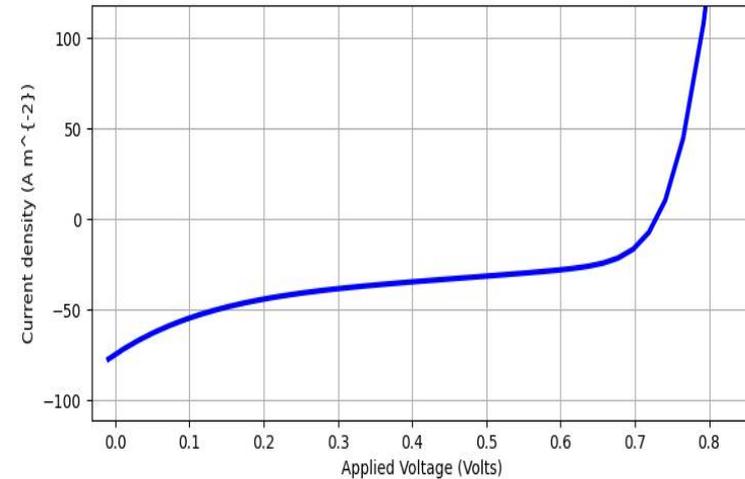
$$PCE = \frac{J(@ P_{max}) * V(@ P_{max})}{P_{light}}$$

Task 3: Simulating a light JV curve

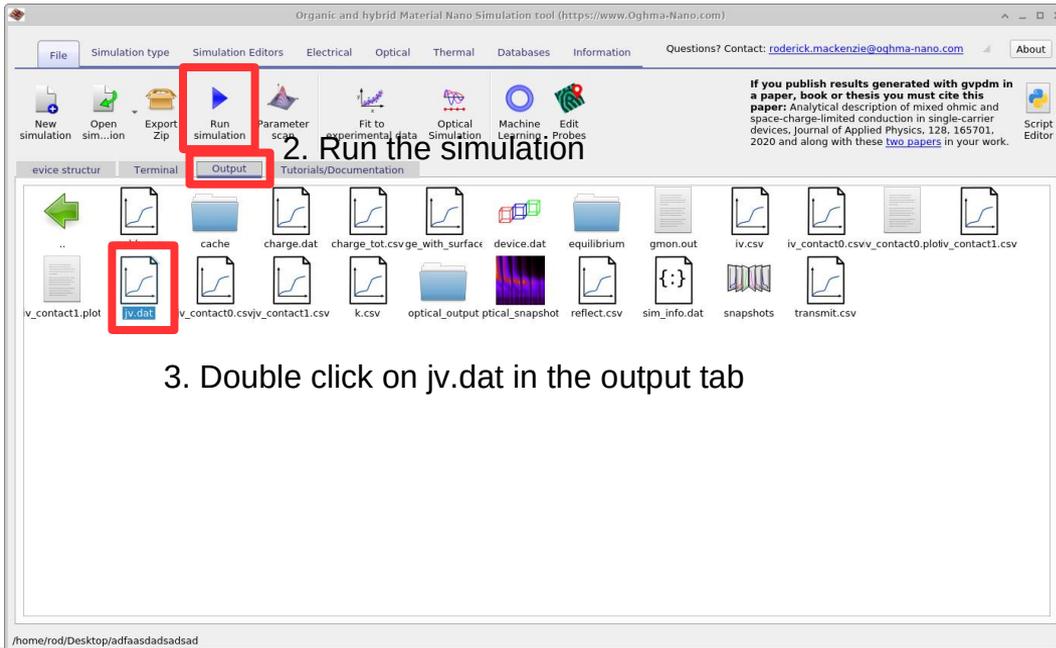


1. Set the light intensity to 1 Suns

4. You will see the light JV curve :)



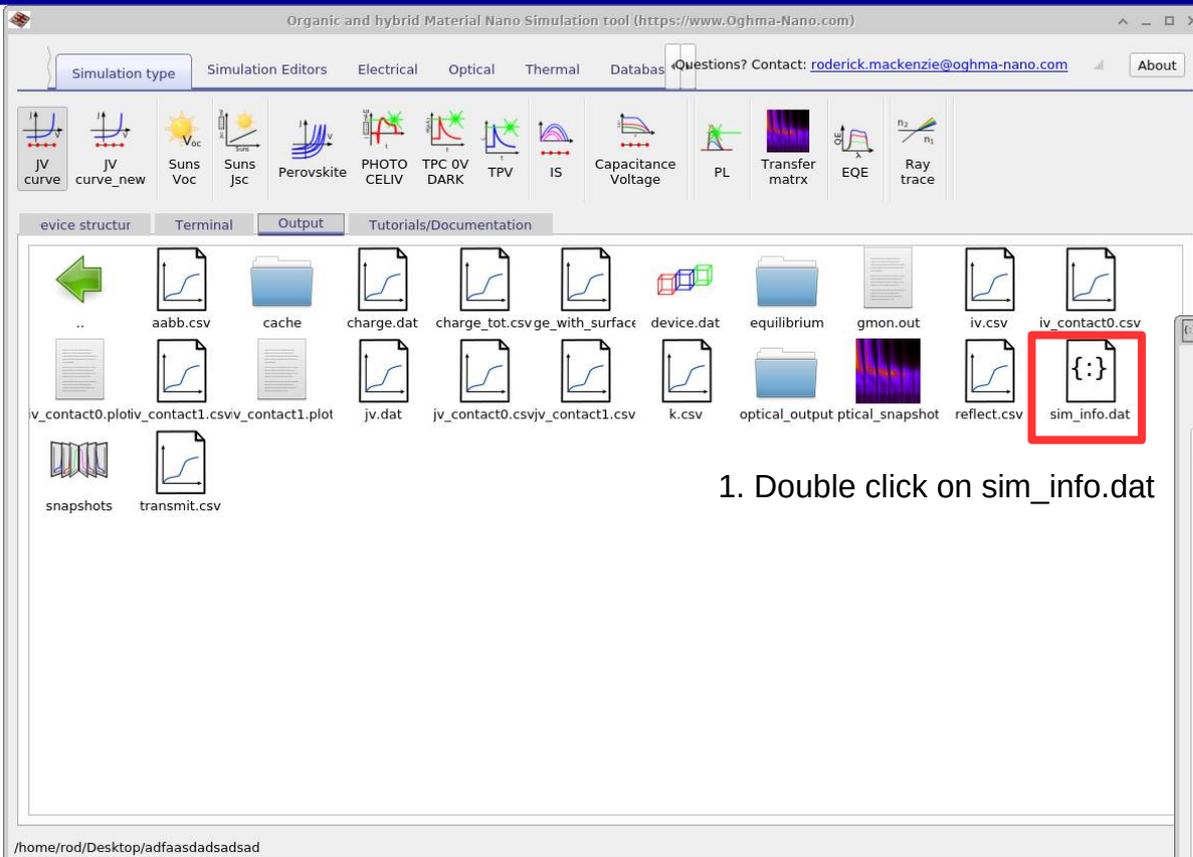
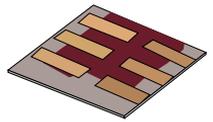
Press 'g' to show the grid, and use the zoom tool to make the curve look like this.



2. Run the simulation

3. Double click on jv.dat in the output tab

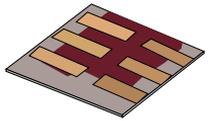
Task 4: Extracting values of PCE, FF, Voc, Jsc



2. See if you can find PCE, FF, Voc and Jsc in the sim_info.dat file

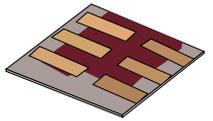
Information	Value	Unit
Edit	{:} json_file	Icon
Current density at max power	-2.800870e+01	Am ⁻²
Voltage at max power	5.967230e-01	V
Fill factor	0.307590	a.u.
Power conversion efficiency (PCE)	1.671344	Percent
Max power	16.713436	W m ⁻²
V _{oc}	0.728072	V
J _{sc}	-7.463084e+01	A m ⁻²
Recombination rate at Voc	6.147938e+27	m ⁻³ s ⁻¹
Average carrier density at P _{max}	4.157567e+22	m ⁻³
Trapped electrons at Voc	-6.410203e+11	m ⁻³
Trapped holes at Voc	-6.410203e+11	m ⁻³
Free electrons at Voc	1.987492e+22	m ⁻³
Free holes at Voc	2.223089e+23	m ⁻³

Task 5: V_{oc} , J_{sc} and FF of other solar cells

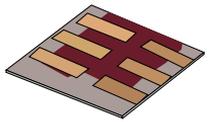


- What is the J_{sc} , V_{oc} and Fill Factor (FF) of this solar cell?
- How do these numbers compare to:
 - A typical Silicon solar cell?
 - A Organic Solar cell
 - A CIGS solar cell
- Use the internet to find these values

Task 6: Varying the light intensity



- Try varying the light intensity from 0.0 to 1.0 Suns in steps of 0.1 Suns.
- And see what happens to the JV curve.
- Try to import these files into excel (or some other plotting package) and plot a combined graph of all the curves. Hint: It might be easier to import iv.csv rather than jv.dat into excel.



•Introduction

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•New solar cell technologies

- Organic solar cells
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- Cadmium telluride solar cells
- Why Perovskites for solar?

•What is OghmaNano

- Making a new simulation

•Fundamentals

- Semiconductor fundamentals
- The anatomy of a dark current curve

•Fundamentals (cont)

- The anatomy of a light current voltage curve

•Parasitic components

- Optical materials
- Optical simulations

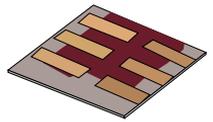
• Advanced topics

- Recombination
- Mobility
- The tau/mu product

• Mobile ions

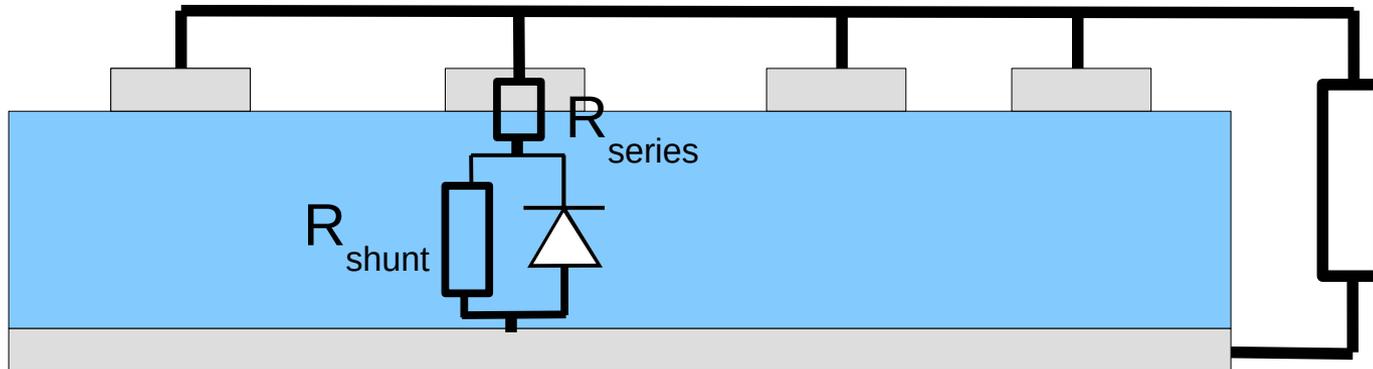
- Mobile ions
- Time domain perovskite simulation

Let's step back and think about our solar cell on a larger scale

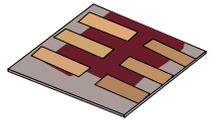


•So far we have considered a more or less perfect solar cell however a real one will have:

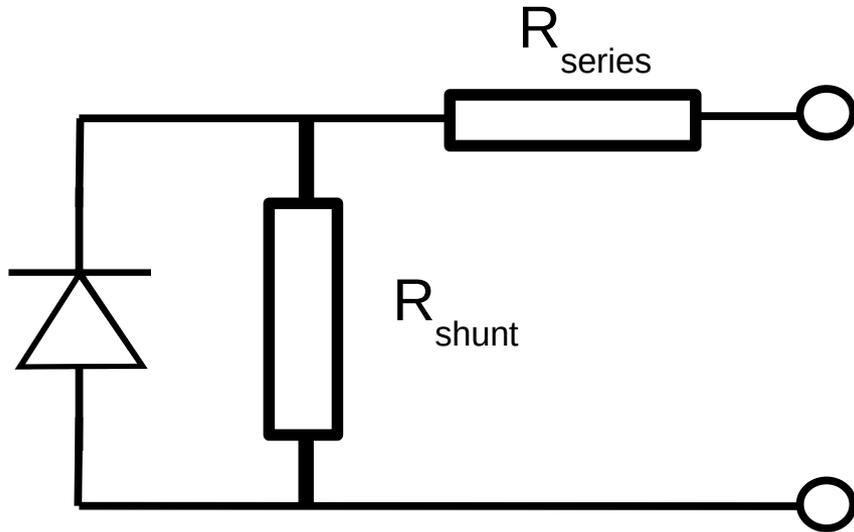
- Contacts
- And also some resistance associated with the semiconductor, caused by defects or impurities.



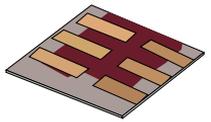
An equivalent circuit for a solar cell



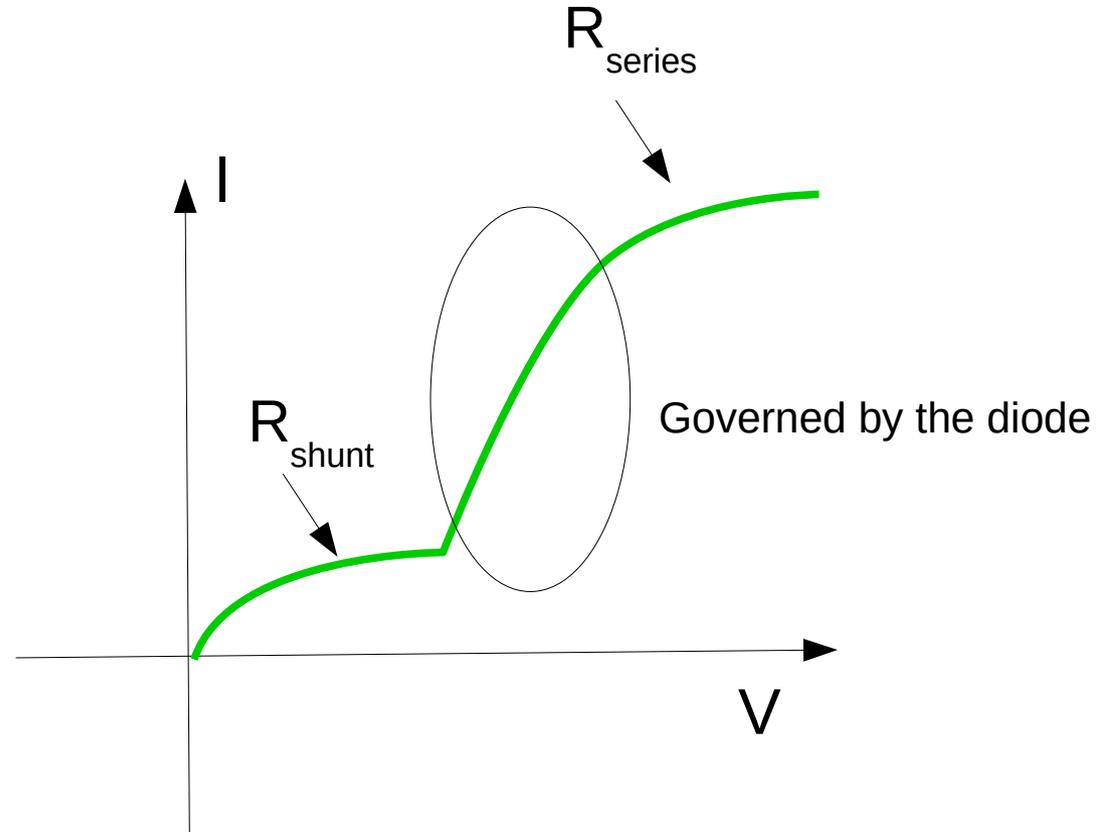
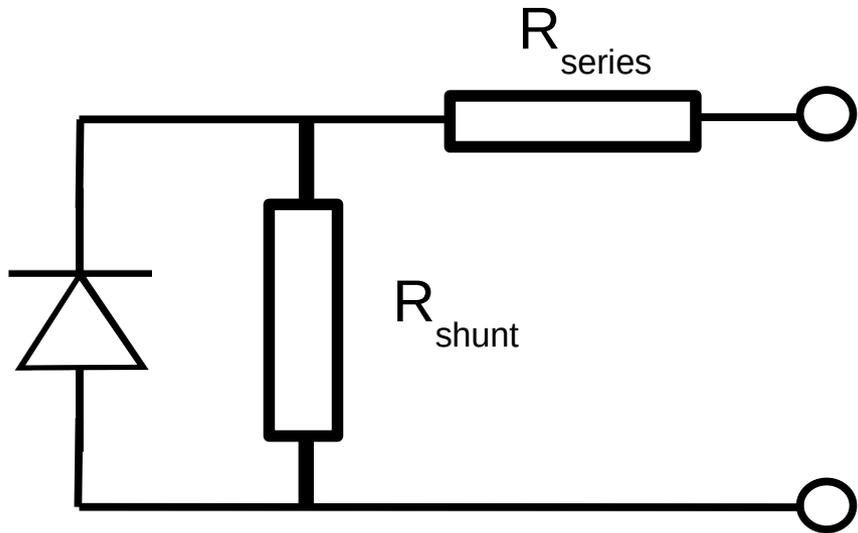
- Series resistance (1-10 Ohm)
- And shunt resistance (1 M Ohm)



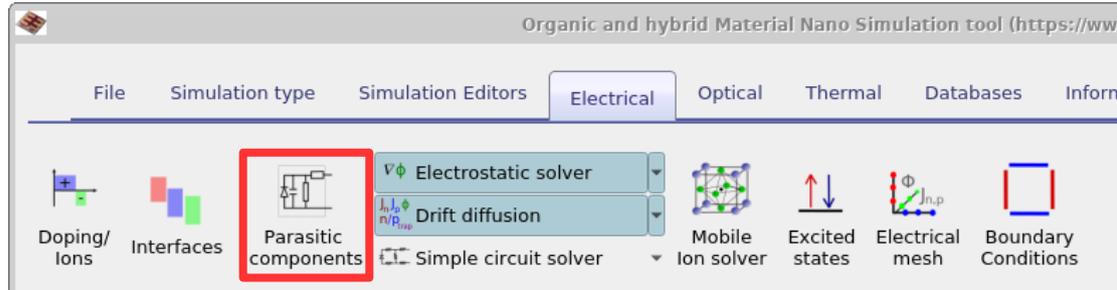
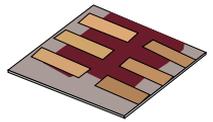
The resulting dark current voltage curve (on a log scale)



- Series resistance (1-10 Ohm)
- And shunt resistance (1 M Ohm)

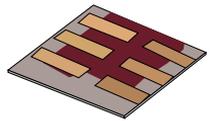


Task 7: Changing the values of R_{shunt} and R_{series}

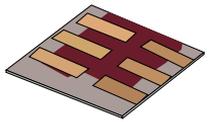


- Set the light intensity to 0 Suns.
- Then Run a simulation.
- Inspect the dark jv curve.
- Press 'l' to view the graph on a log scale.
- Then Open the parasitic resistance window and try reducing the shunt resistance to 10 Ohms m²
- What happens to the dark JV curve when plotted on a log scale?

Task 8: Changing the values of R_{shunt} and R_{series}



- Through experimentation try to put into words what affect the values of R_{shunt} and R_{series} have on the light JV curve.
- What happens to the solar cell efficiency as the shunt resistance is reduced? Plot a graph with shunt resistance on one axis, and device efficiency on the other (a minimum of four points) showing this effect. What is the reason for the trend on the graph?
- What values of series and shunt resistance, would produce the best possible solar cell? Enter these values into the device simulator and copy and paste the dark JV curve into your report.



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•Fundamentals (cont)

- The anatomy of a light current voltage curve
- Parasitic components
- Optical materials**
- Optical simulations

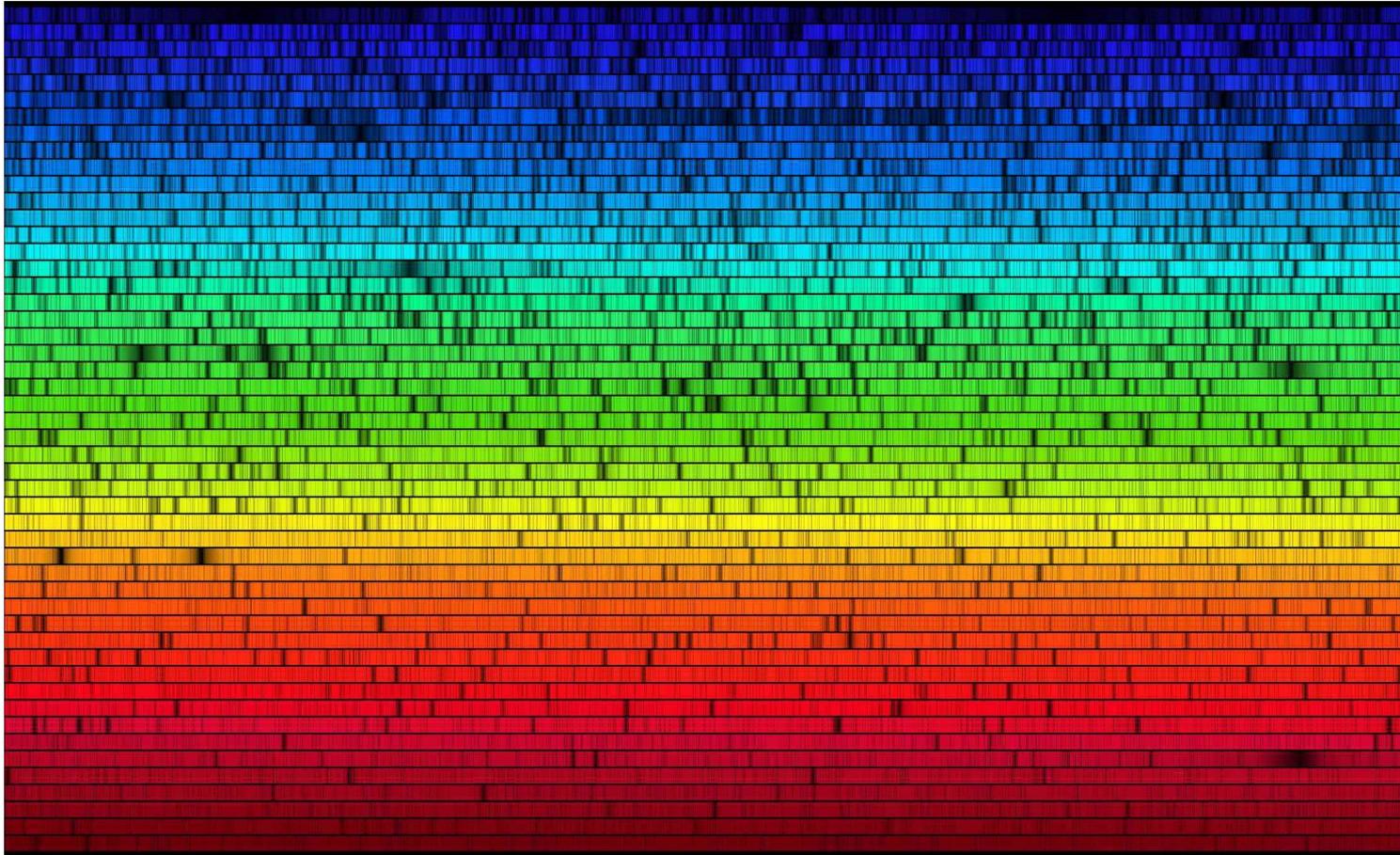
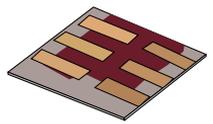
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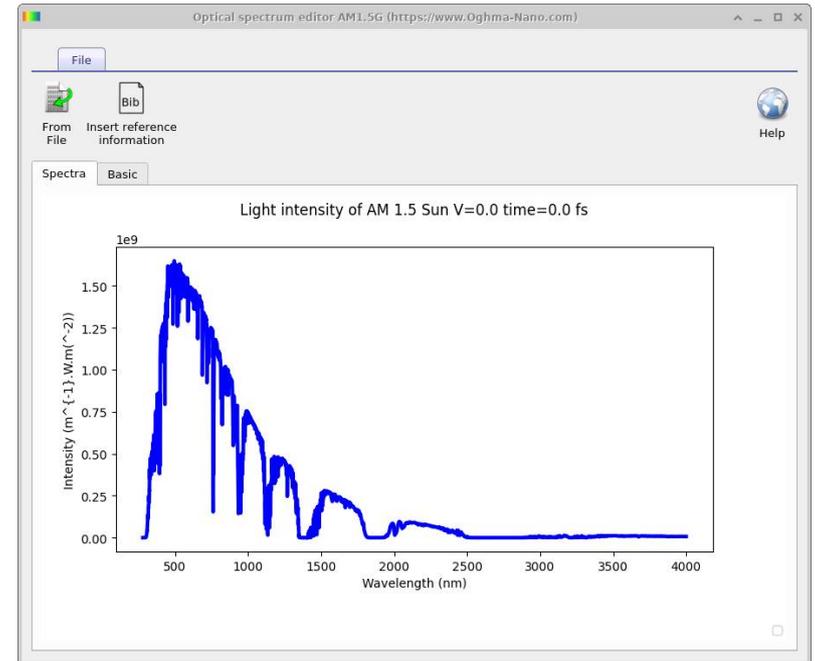
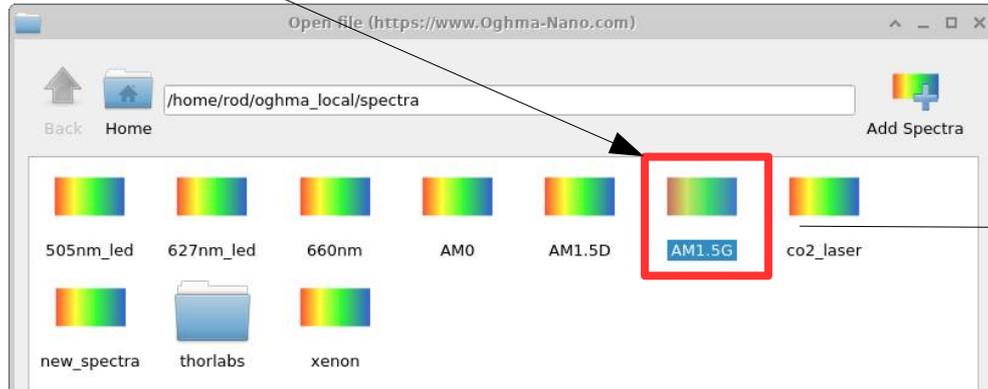
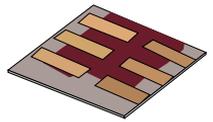
- Mobile ions
- Time domain perovskite simulation

Let's first look at what the sun's spectrum looks like before we consider material choices to absorb it's energy.

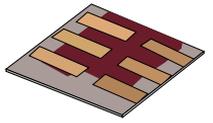


- That looks cool, I wonder which material will best absorb that light?

Let's plot that in a more conventional way.

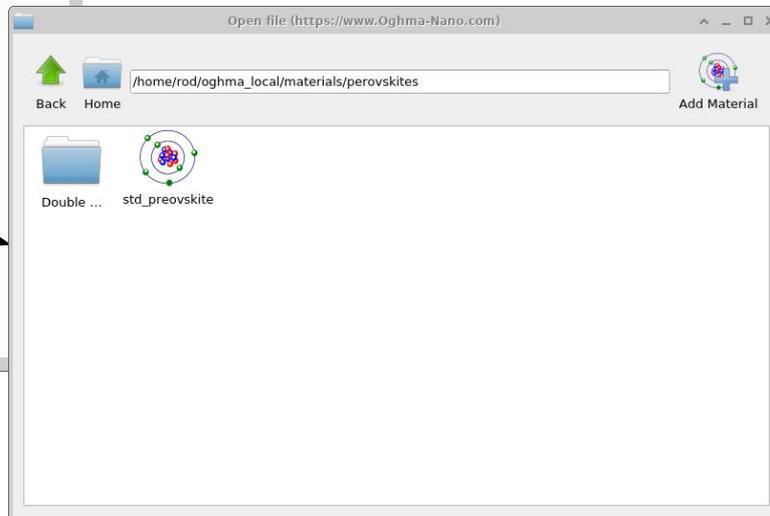
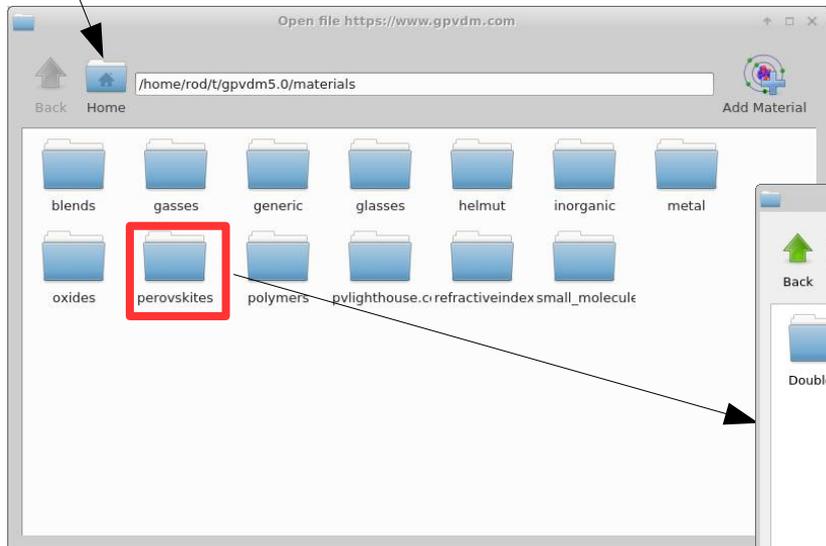
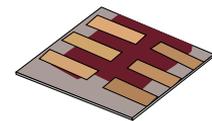


Task 9:

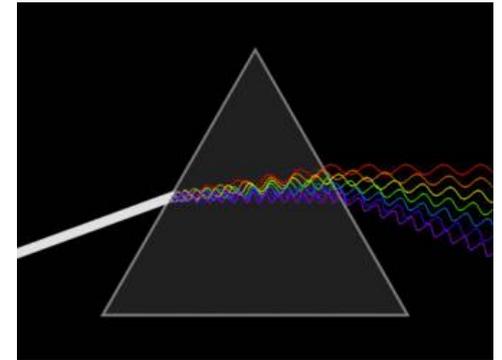
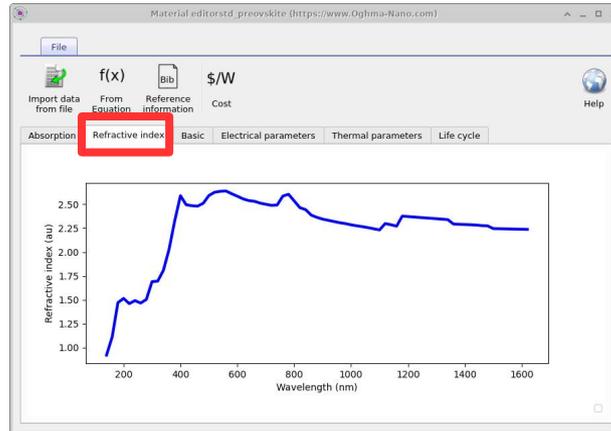
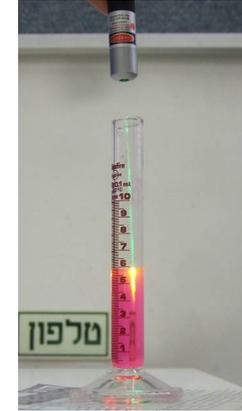
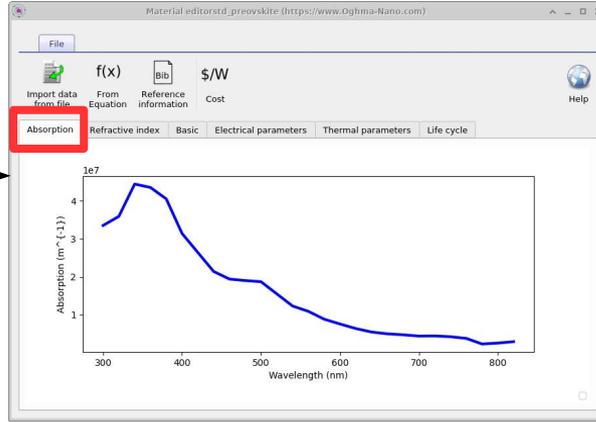
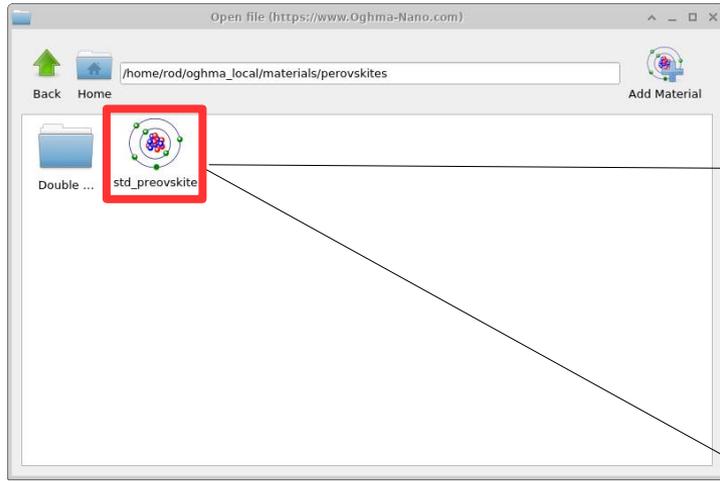
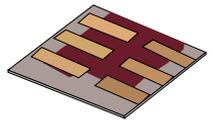


- Describe the main differences between the light which comes from the LED and the sun. Rather than referring to the various regions of the spectrum by their wavelengths, refer to them using English words, such as infrared, Ultra Violet, Red, and Green etc... you will find which wavelengths match to each color on the internet.
- If you were designing a material for a solar cell, what region of the spectrum would you most want to absorb?

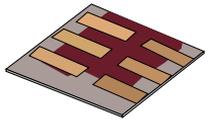
The materials from which solar cells are made.



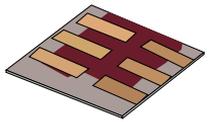
Have a look at the absorption and refractive index.



Task 10:



- What color of light does the the perovskite absorb best?
- Now have a look in the 'polymers' directory. Which polymer material do you think will absorb the suns light best? Give your reasoning for this.



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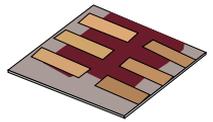
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- Mobility
- The tau/mu product

• Mobile ions

- Mobile ions
- Time domain perovskite simulation

Optical simulations: How does light interact with our device?



Organic and hybrid Material Nano Simulation tool (<https://www.Oghma-Nano.com>)

File Simulation type Simulation Editors Electrical Optical Thermal Questions? Contact: roderick.mackenzie@oghma-nano.com About

New simulation Open simulation Export Zip Run simulation Parameter scan Fit to experimental data **Optical Simulation** Machine Learning Edit Probes

If you publish results generated with OghmaNano in a paper, book or thesis you must cite this paper: Analytical description of mixed ohmic and space-charge-limited conduction in single-carrier devices, Journal of Applied Physics, 128, 165701, 2020 and along with these [two papers](#) in your work.

Script Editor

Device structure Terminal Output Tutorials/Documentation

Layer editor Contacts Electrical parameters Emission parameters Substrate xz-size xy yz xz

Optics

Run optical simulation Configure Transfer matrix Exponential profile Flat profile From file From QE spectra Constant value

Photon distribution absorbed Generation rate

Absorbed Photon density

Wavelength (μm)

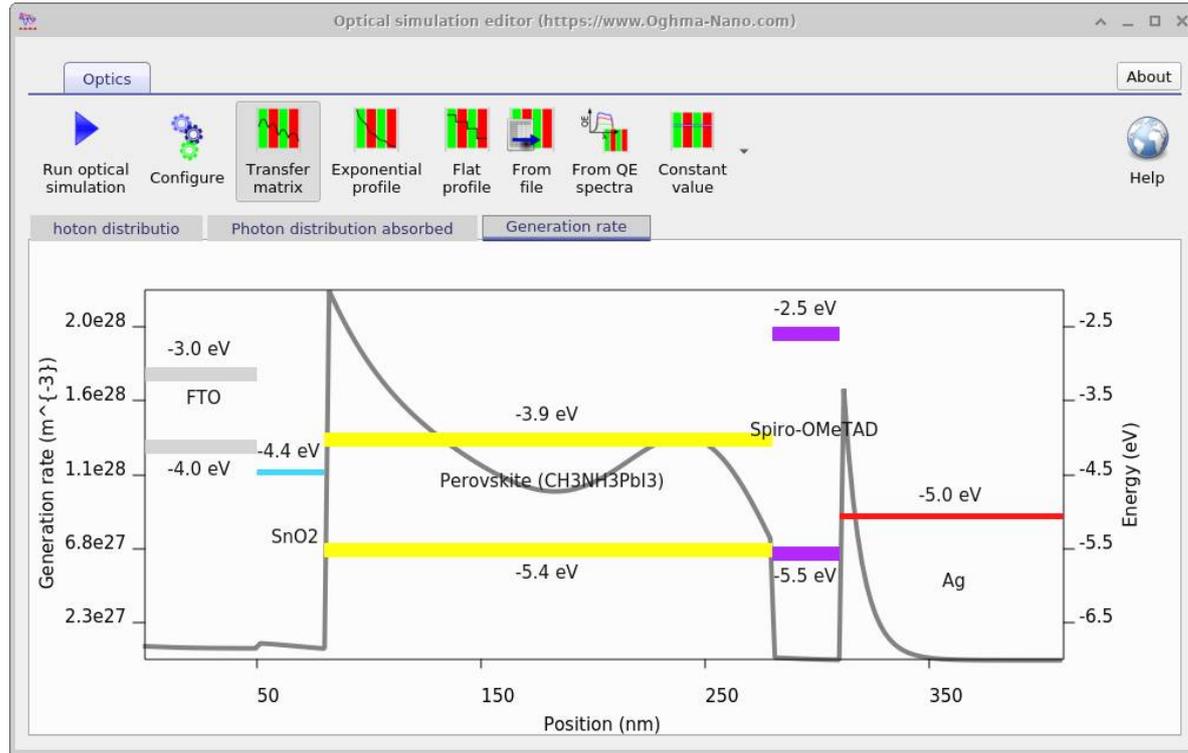
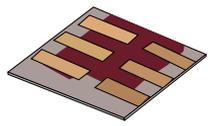
y-position (nm)

$1e34$

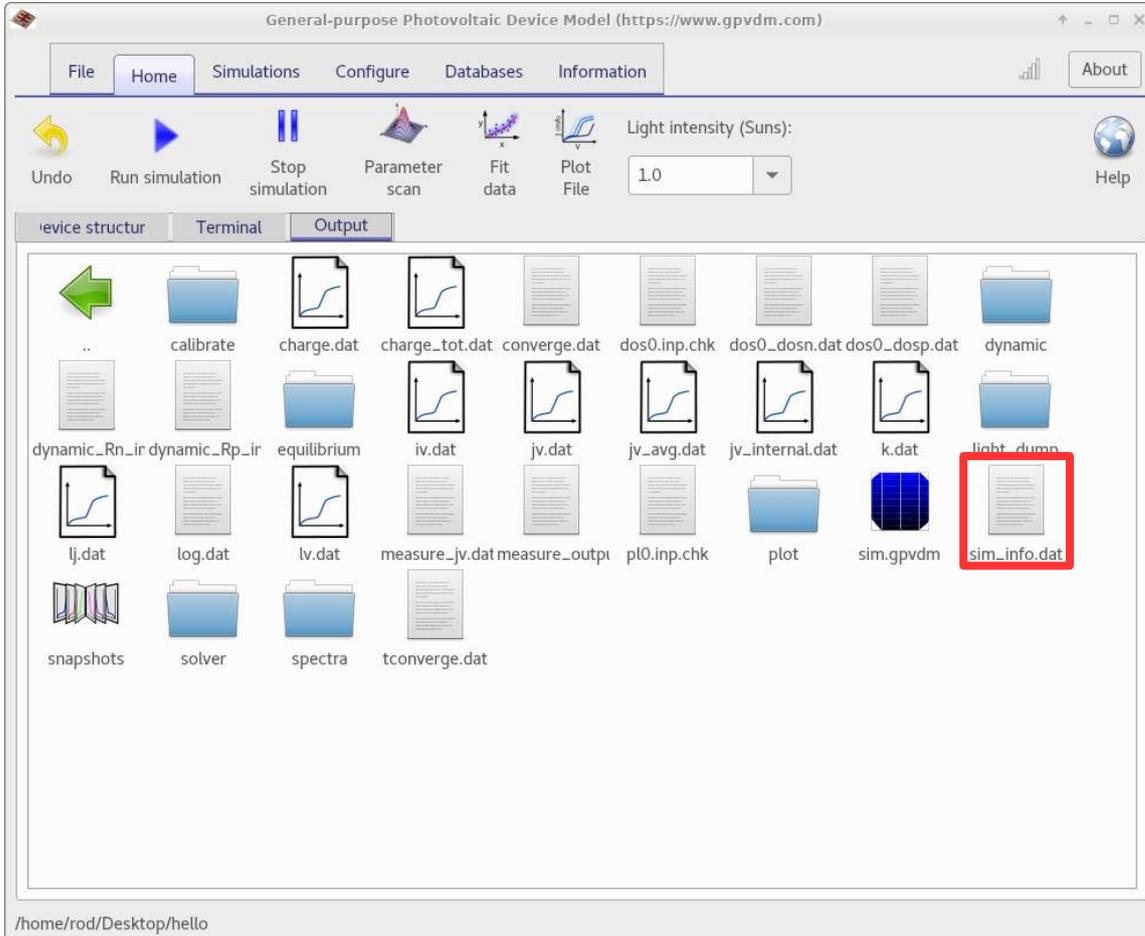
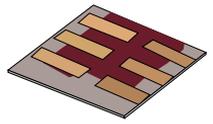
- Click “Run optical simulation” to run the simulation.

- You will get a plot of where light is absorbed within the device as a function of wavelength and

If you go to the “Generation rate” tab you will see a plot of total generation rate.

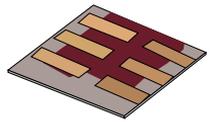


Let's look at sim_info.dat again, now we have run the optical simulation.

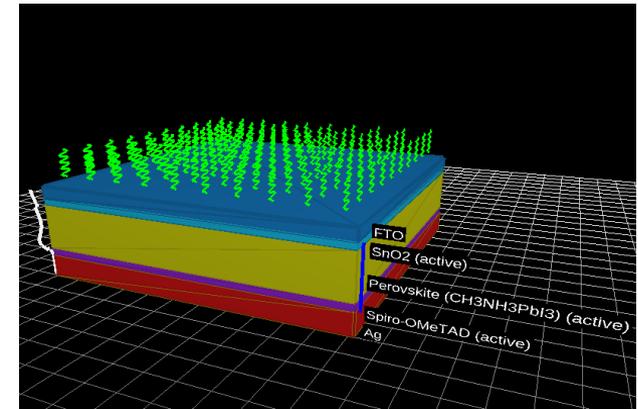


- Double click on it to open it.

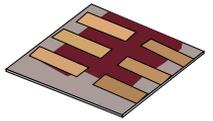
Photons absorbed in the active layer from sim_info.dat



- This will show you the maximum current that could be generated due to light absorption.

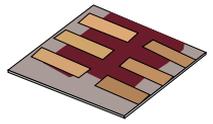


Task 11:



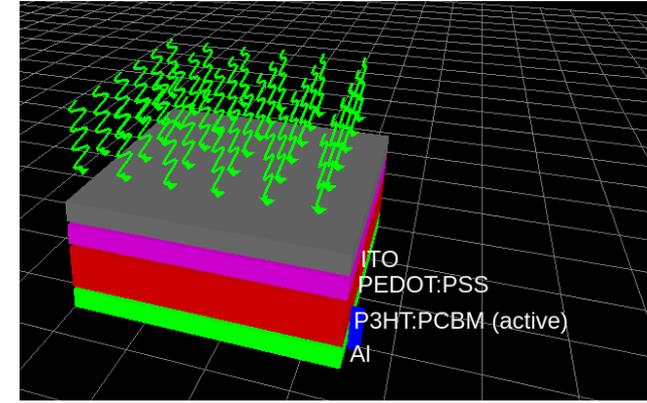
By running 5 or 6 with different active (perovskite) layer thicknesses, plot a graph of active layer thickness, v.s. the maximum current generated in the device. At what thickness do almost all photons get absorbed in the device? [Hint: I would run the simulations from 100nm to 800nm]

The layer editor used for changing the thicknesses of layers in a cell.

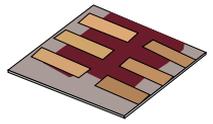


The screenshot shows the main application window with the Layer editor window open. The Layer editor window contains a table with the following data:

Layer name	Thicknes (m)	Optical material	Layer type	Solve optical problem	Solve therma problem	ID
FTO	5e-08	oxides/fto	contact	Yes	Yes	e...
SnO2	3e-08	oxides/SnO2	active layer	Yes	Yes	...
Perovskite ...	2e-07	perovskites/std_preovskite	active layer	Yes	Yes	...
Spiro...	3e-08	small_molecules/spiromeotad	active layer	Yes	Yes	...
Ag	1e-07	metal/ag	other	Yes	Yes	i...



You can change the thicknesses of the layers here..

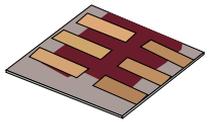


Layer editor (https://www.Oghma-Nano.com)

+ - ↓ ↑

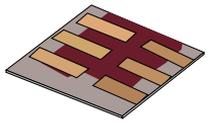
Layer name	Thicknes (m)	Optical material	Layer type	Solve optical problem	Solve therma problem	ID
FTO	5e-08	... oxides/fto	contact	Yes	Yes	e...
SnO2	3e-08	... oxides/SnO2	active layer	Yes	Yes	...
Perovskite ...	2e-07	... perovskites/std_preovskite	active layer	Yes	Yes	...
Spiro-...	3e-08	... small_molecules/spiromeotad	active layer	Yes	Yes	...
Ag	1e-07	... metal/ag	other	Yes	Yes	i...

- All values are in meters
- Think about how thick these layers are compared to the width of a human hair. (17 μm to 181 μm)



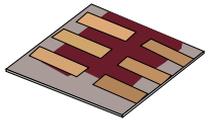
- Introduction
 - What is this lecture?
 - Why solar?
 - Why not silicon?
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- **Advanced topics**
 - **Recombination**
 - Mobility
 - The tau/mu product
- Mobile ions
 - Mobile ions
 - Time domain perovskite simulation

So is a thicker solar cell always better? Well think about this....

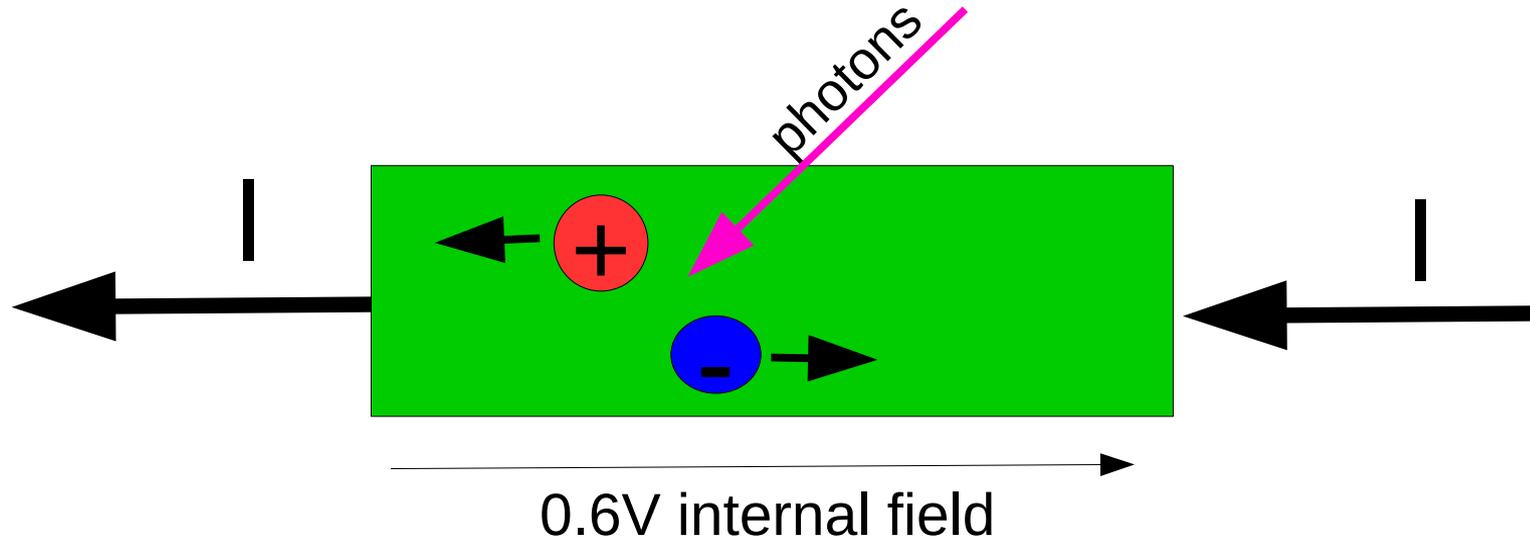


- Thicker means more material, so a more expensive device.
- It also means more energy (CO₂) has to be used to produce the devices as it's got more material in it.
- But more importantly....

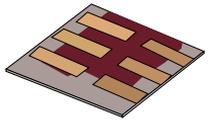
Recombination...



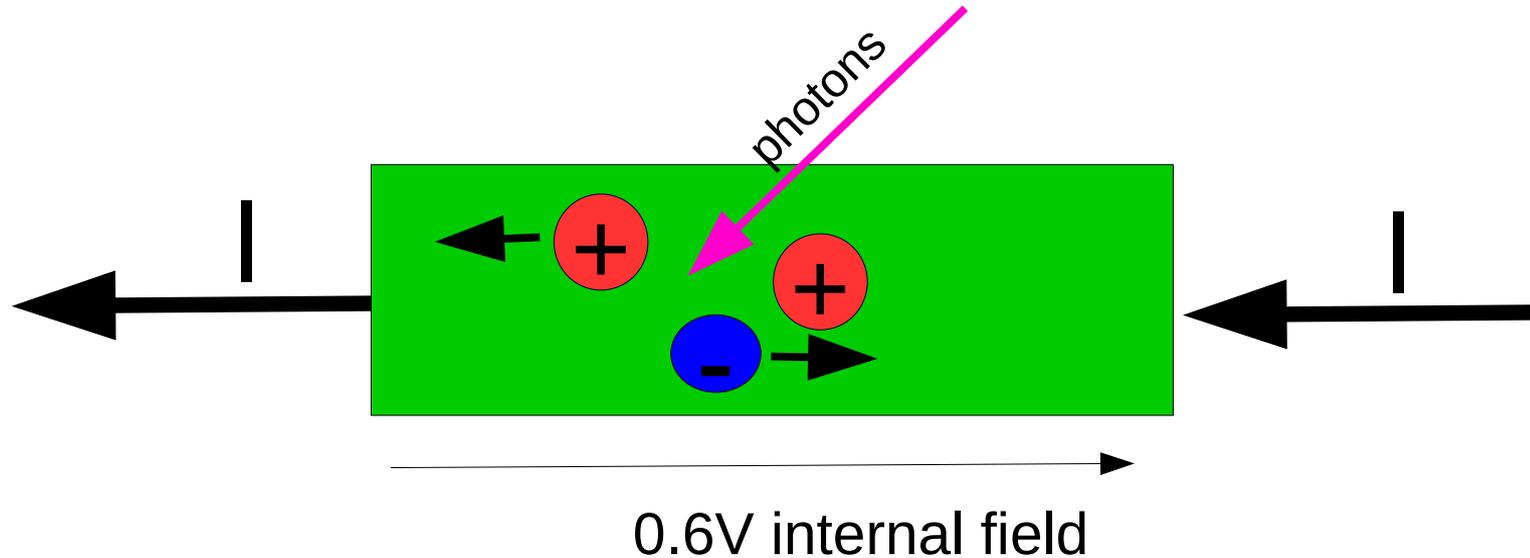
- Think about a photon generating a positive and negative charge in a solar cell.
- One charge gets dragged to one contact the other gets dragged to the other and you get external current.



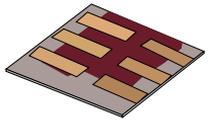
Recombination...



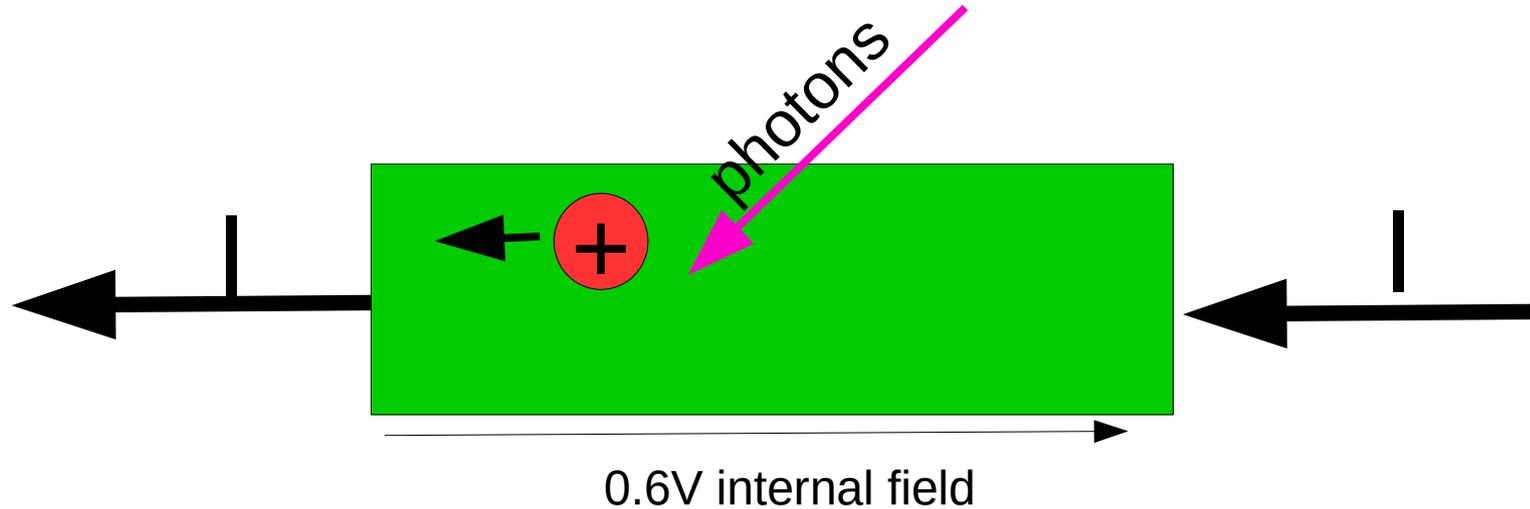
- But now imagine if one of these charge carriers meets a species of opposite charge on the way out...
- What will happen?



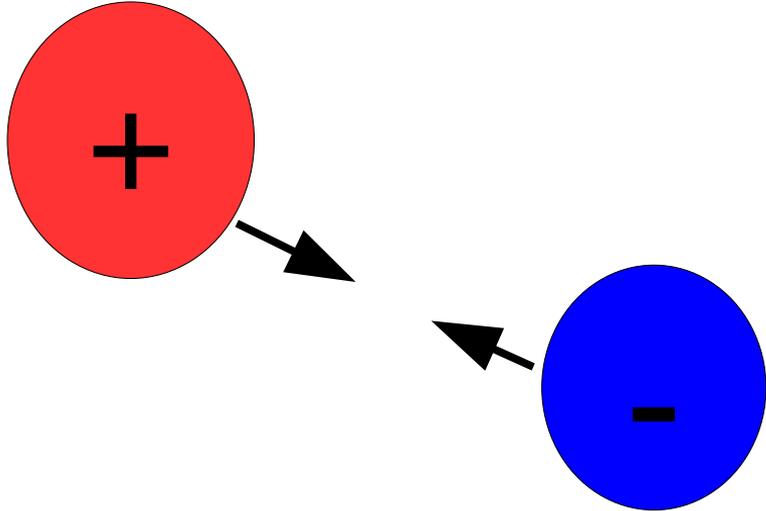
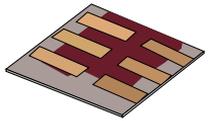
Recombination...



- Annihilation... so two charge carriers are lost..
- This seems bad. One way we can make this less likely to happen is to get the electrons/holes out of the device as quickly as possible so there is less chance of them bumping into a species of the opposite charge.



- So from a recombination stand point do we want a thick or thin device?

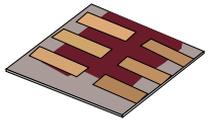


•The rate at which electrons/holes meet each other and get destroyed is given by this equation:

$$R(x) = k n(x) p(x)$$

- Where, k is a constant, n is the density of electrons and p is the density of holes.
- This type of recombination is called **bi-molecular recombination** because it involves two things. This is also sometimes referred to as Langevin recombination (but that is another story).

Task 12:

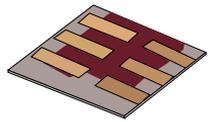


•We can define an average recombination time of a carrier using the formula:

$$\tau = \frac{n+p}{2R(x)}$$

- Try to find the “Recombination time constant” in the sim_info.dat file.
- In no more than two sentences describe what an electron and hole are.

Task 13:



Plot a new graph of active layer thickness v.s. device efficiency this time using a recombination constant k of 1×10^{-15} . By looking at your graph, what is the optimum device thickness?

- The recombination constant k can be set in the model here>

Electrical parameter editor (https://www.Oghma-Nano.com)

Enable Drift Diff. Enable Auger Dynamic SRH traps Equilibrium SRH traps Excitons Excited states

Configure Help

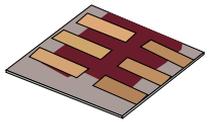
SnO2 Perovskite (CH3NH3PbI3) Spiro-OMeTAD

Free carriers

Electron mobility	0.024	Symmetric	$\text{m}^2\text{V}^{-1}\text{s}^{-1}$
Hole mobility	0.0025	Symmetric	$\text{m}^2\text{V}^{-1}\text{s}^{-1}$
Effective density of free electron states (@300K)	4.36e24		m^{-3}
Effective density of free hole states (@300K)	2.52e25		m^{-3}
n_{free} to p_{free} Recombination rate constant	1e-10		m^3s^{-1}
Free carrier statistics	Maxwell Boltzmann - analytic		type

Electrostatics

ξ	4.4	eV
E_g	3.6	eV
Relative permittivity	9.0	au



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- Fundamentals (cont)

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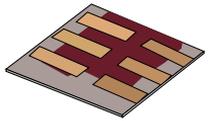
- **Advanced topics**

- Recombination
- **Mobility**
- The tau/mu product

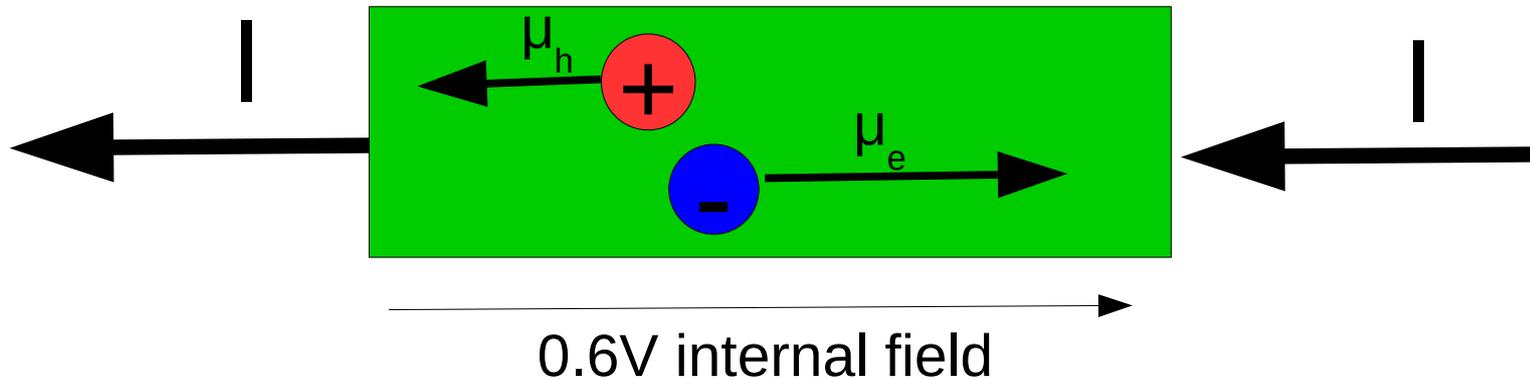
- Mobile ions

- Mobile ions
- Time domain perovskite simulation

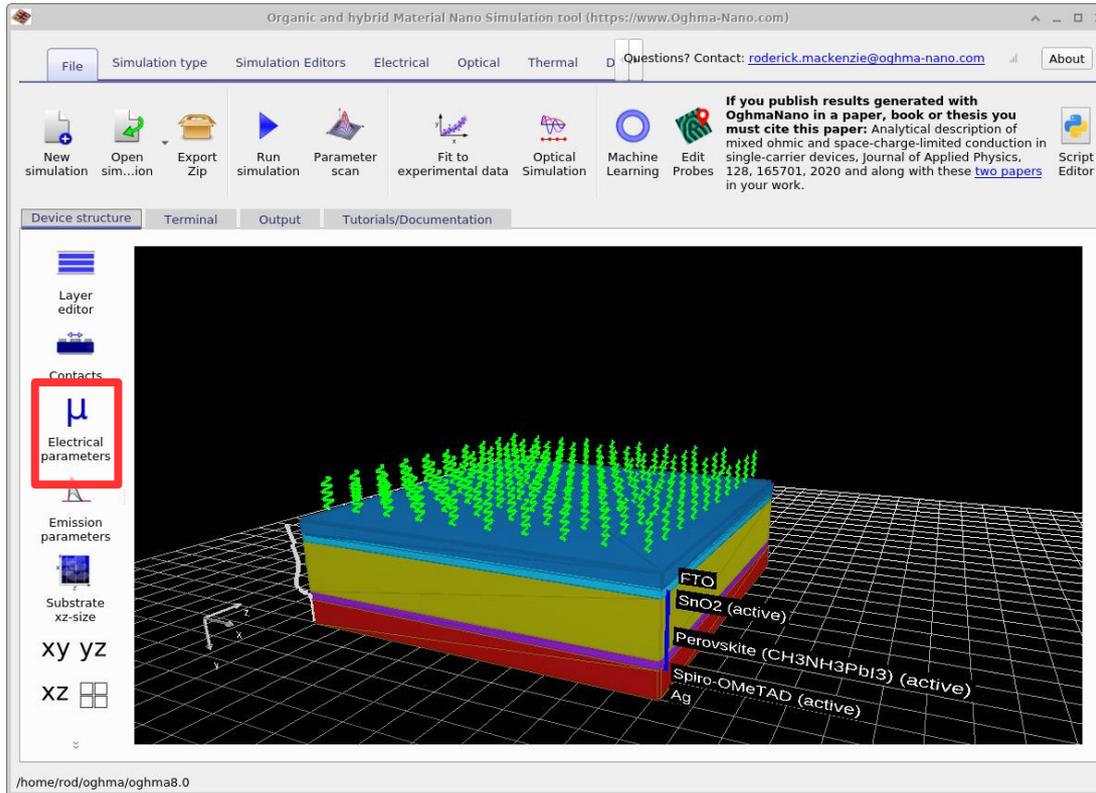
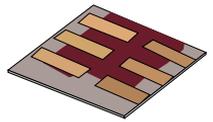
Mobility of charge carriers in solar cells.



- How fast electrons and holes can move in a solar cell is governed by a material property called **charge carrier mobility**.
- The higher the number the faster charge carriers move
- There are two values one for electrons μ_e and one for holes μ_h
- Generally having high values of mobility is considered good for solar cells.

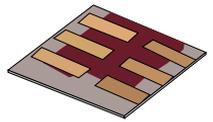


The electrical properties of the materials can be set here..



- Click on the Electrical parameter editor, under the device structure tab.

Setting the mobilities.



Electrical parameter editor (<https://www.Oghma-Nano.com>)

Enable Drift Diff. Enable Auger Dynamic SRH traps Equilibrium SRH traps Excitons Excited states Configure Help

SnO2 Perovskite (CH3NH3PbI3) Spiro-OMeTAD

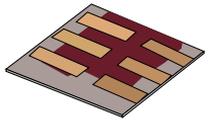
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Free carrier statistics	Maxwell Boltzmann - analytic		type

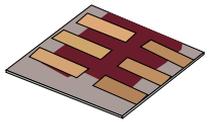
Electrostatics

χ_i	4.4	eV
E_g	3.6	eV
Relative permittivity	9.0	au

Task 14:



- What is the optimum active layer thickness with the lower mobility value? If you wanted a really efficient solar cell what values of mobility and recombination rate would you use?
- Have a play and see what mobility does to the dark and light JV curve. Try reducing it by one order of magnitude.
- What does this do the PCE value, Voc, FF and Jsc?



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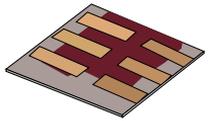
- **Advanced topics**

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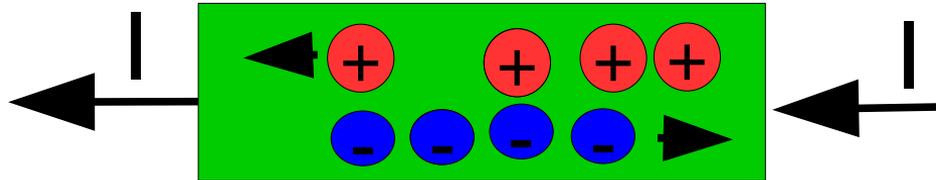
- Mobile ions

- Mobile ions
- Time domain perovskite simulation

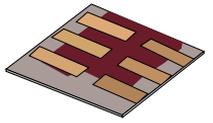
A solar cell goodness factor the $\mu\tau$ product



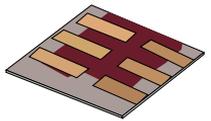
- **μ** is the electron/hole **mobility** and **τ** is the time it takes a charge carrier to recombine.
- If **τ** is very slow then it takes a long time for carriers to recombine so there is a good chance of photogenerated carriers getting out of the device to do useful work. (good)
- If **μ** is very high, carriers can escape the device very quickly so there is no time for them to recombine, again giving a good chance of photogenerated carriers escaping the device to do useful work. (good)
- Both of these quantities are high then the device will be good. :)
- We therefore talk about a **$\mu\tau$** product () of a cell, and when it is high the cell is good when it is low the cell is inefficient.



Task 15:



- You can find the recombination time constant in the `sim_info.dat` file after having performed a JV simulation. By averaging the electron and hole mobilities calculate the $\mu\tau$ product for this device.



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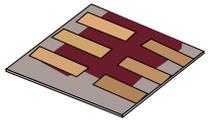
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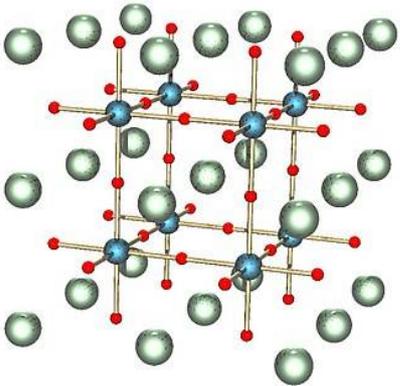
Mobile ions



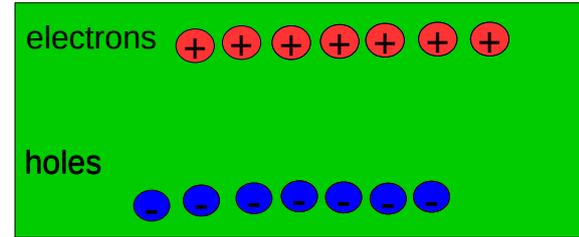
- Perovskites are special because not only do they have electrons and holes in them but they also have mobile ions.

- These ions do not contribute to current but just swish around in the cell.

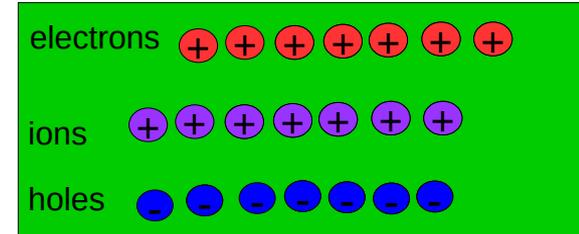
- These ions can cause hysteresis in the current voltage characteristics.



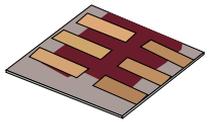
- Normal solar cells



- Normal solar cells

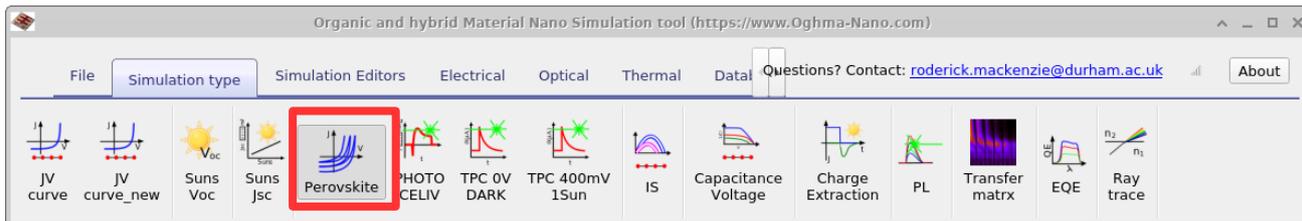
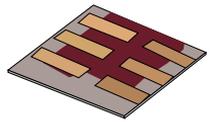


Outline

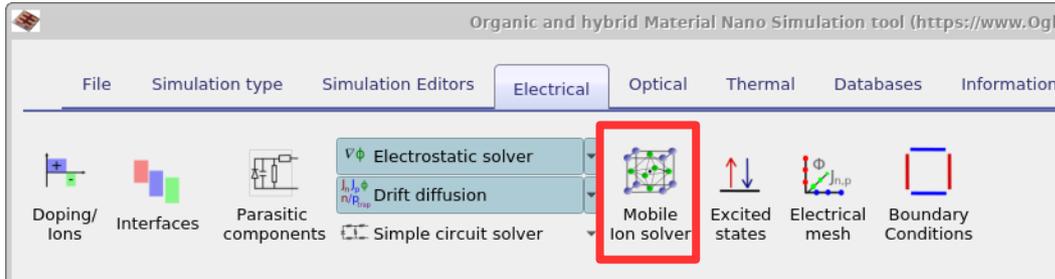


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Turning on mobile ions

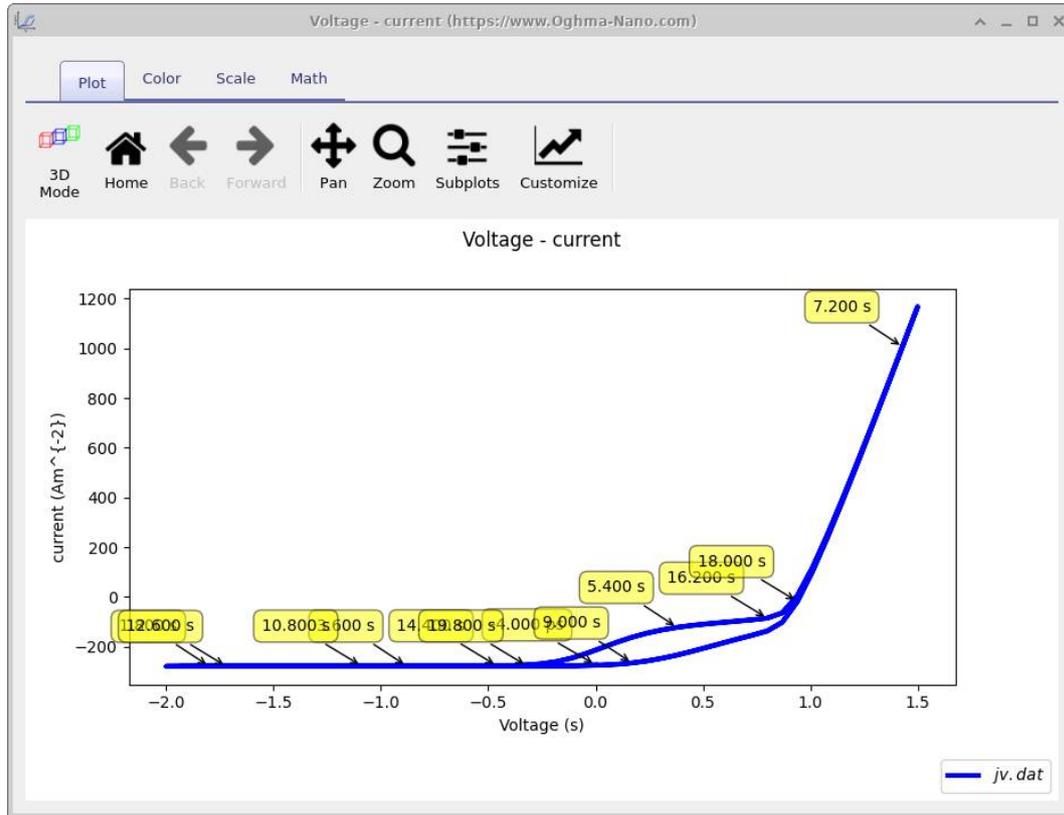
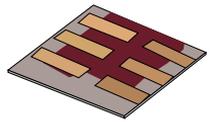


- Change the simulation mode from the steady state JV curve to “Perovskite” this selects time domain voltage sweeps rather than assuming steady state.



- Then enable the mobile ion solver by depressing the “Mobile ion solver button.”

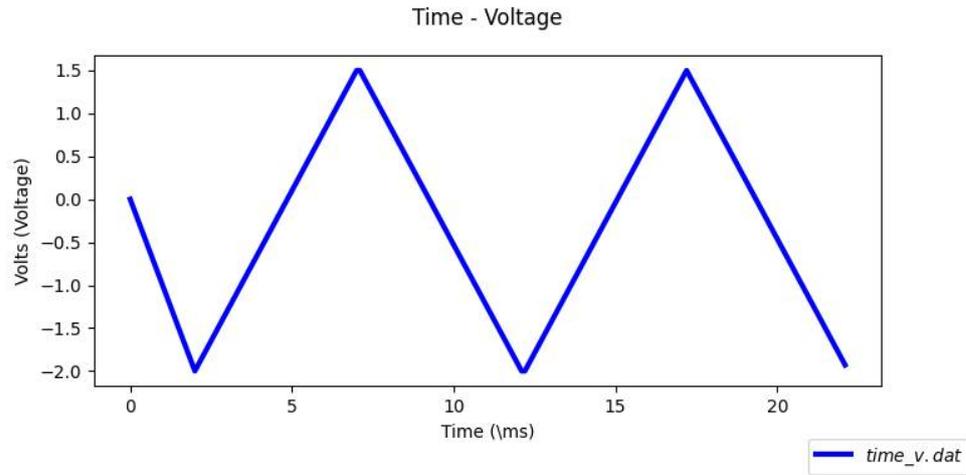
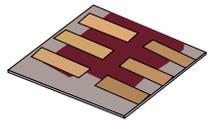
Running the simulation...



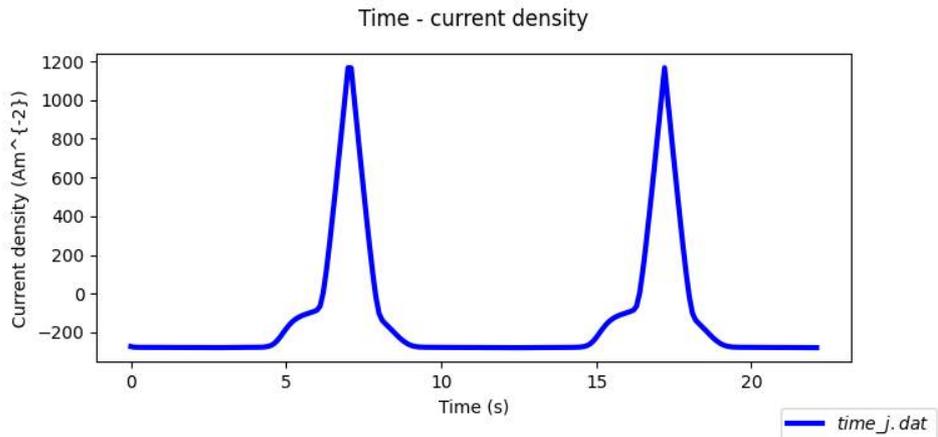
- Run the simulation (blue play button) then open the file ***jv.dat***
- Notice it's a jv curve but it changes as a function of time*
- Plot time_v.dat and time_j.dat***, these plot voltage and current against time.

pulse_v.dat, pulse_j.dat

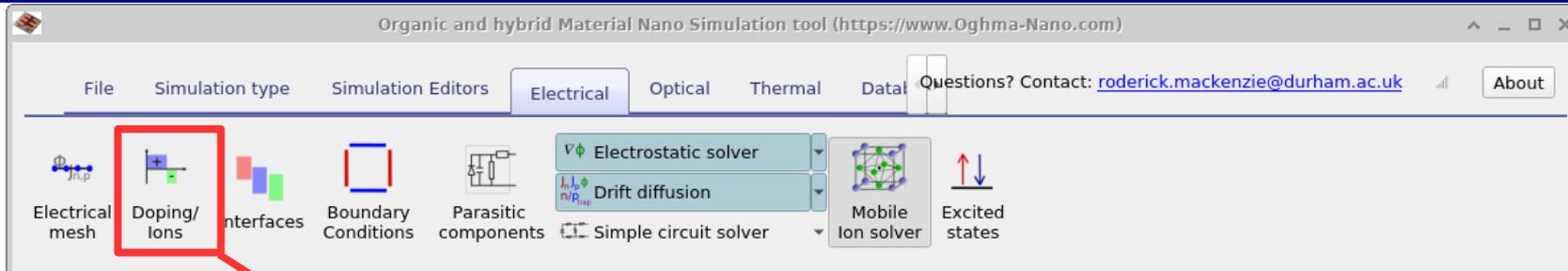
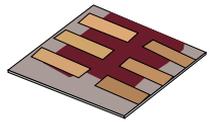
Current/voltage against time.....



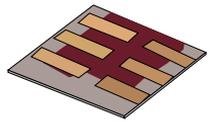
- Notice the saw wave of the time domain JV experiment and the resulting current transient.



You can edit the density of ions using the ion/doping editor.



Editing time domain simulations



General-purpose Photovoltaic Device Model (https://www.gpvdm.com)

File Home **Simulations** Configure Databases Information

Time domain simulation editor. Steady state simulation editor

Simulation mode: **Time domain** (selected)

Time domain experiment window (https://www.gpvdm.com)

Experiment Laser Simulation

time mesh Circuit Configure

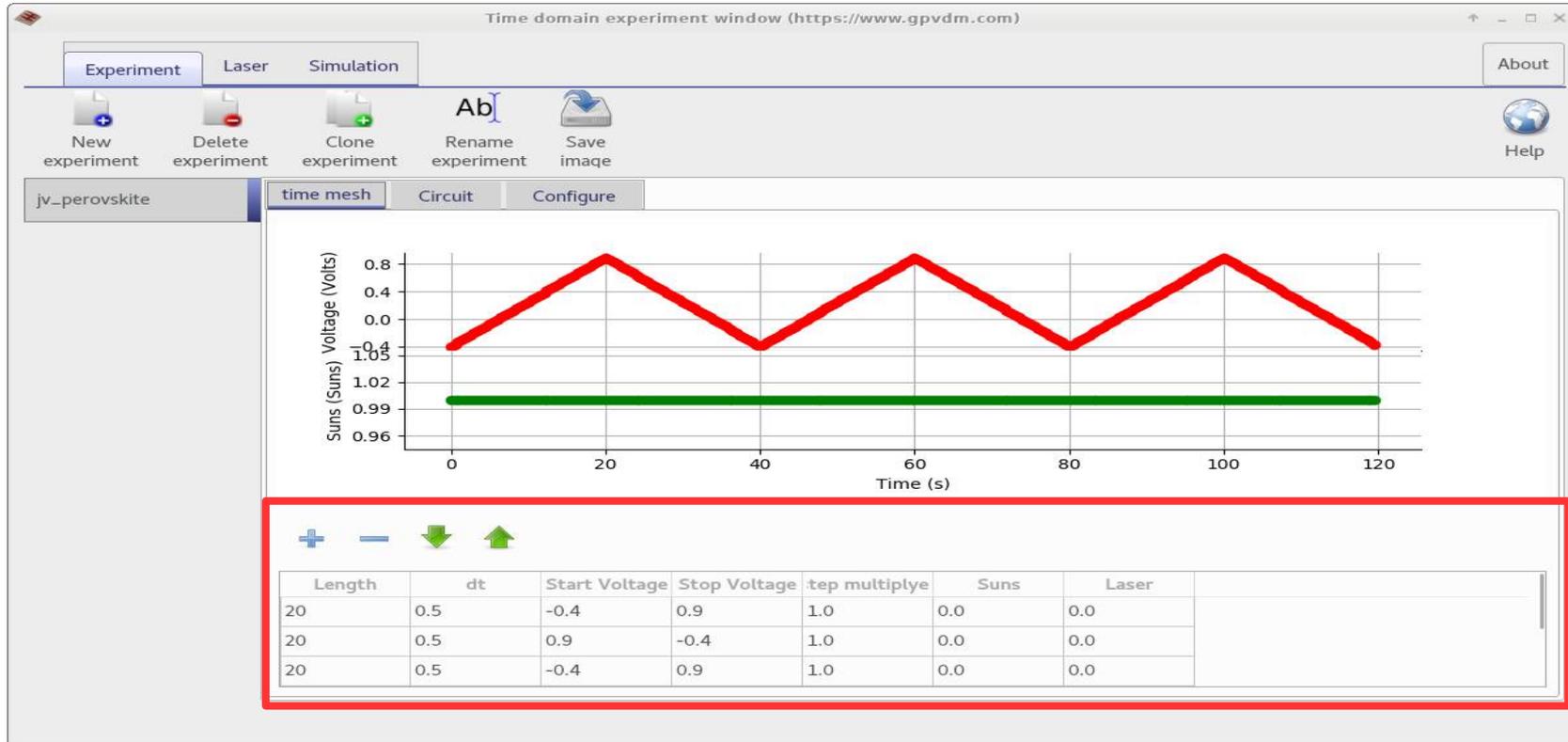
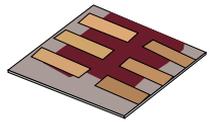
Suns (Suns) Voltage (Volts)

Time (s)

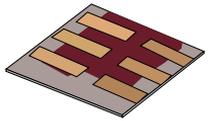
Length	dt	Start Voltage	Stop Voltage	tep multiplie	Suns	Laser
20	0.5	-0.4	0.9	1.0	0.0	0.0
20	0.5	0.9	-0.4	1.0	0.0	0.0
20	0.5	-0.4	0.9	1.0	0.0	0.0

- We can edit time domain simulations using the ***Time domain simulation editor tool***

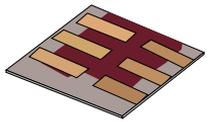
Edit the applied voltage/light intensity



Task 16:



- Try changing the duration of the voltage sweeps, to half the value it is currently set to. What does this do to the JV curves.



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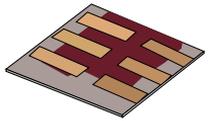
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Thanks



Thanks to Jesús Capistrán (Instituto de Energías Renovables, UNAM) for useful feedback!