

Supporting information

for

Optimization of absorption bands of dye-sensitized and perovskite tandem solar cells based on loss-in- potential values.

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Program description

The code of the program (in C) is attached as separate file (*code.c*). The code can be compiled to executable file by most compilers under Windows or Linux (for example Dev C++ for Windows which can be downloaded at <http://www.bloodshed.net/dev/devcpp.html>). Upon launching the user has 4 options:

1. Generate IPCE
2. Optimize cell
3. Simulate cell
4. Exit

1. Generating IPCE

When this option is chosen, the program first asks for the number of spectra to be generated (1-10). They will be saved in separate files from *ipce1.txt* to *ipce10.txt*. After entering the number of spectra, program asks for the shape and parameters of each spectrum. Square shaped spectrum needs 3 parameters: height between 0 and 1, beginning of the interval and its end in nm (between 300 and 2500). They should all be given in one line, separated by spaces. Note that for the absorption onset optimization the end of the interval should be longer than the expected absorption onset (for general cases the interval can be from 300 to 2500 nm, see the exemplary attached file *ipce1.txt*). Gaussian shaped spectrum needs 4 parameters. When 'Cancel' is chosen, the spectrum with the current number is not modified. First 3 of them are the same as in square shape, maximum amplitude and two wavelengths between which the amplitude is preserved. The last parameter is the decay half-width σ , which determines shape of the slopes according to the formula (6). When the desired number of curves is generated, program returns to main menu.

2. Cell optimization

After choosing this mode, program first asks for the number of junctions (sub-cells) that constitute entire simulated device. Then it asks for V_{loss} on each junction of the system, FF is fixed at a reasonable value of 0.73. Finally it asks for the mode of operation, full or decaying currents. In multi-junction devices, when the 'full current' mode is chosen only the sub-cells matching the current of the first sub-cell will contribute to the final efficiency, the rest is dismissed. In 'decaying current' mode all the sub-cells with non-zero currents will contribute to the result and the lowest of these currents will be picked as I_{sc} . For the simulation of single cell 'full current' mode is chosen automatically. IPCE for the n^{th} sub-cell is taken from *ipcen.txt* file. Simulations works as follows. The program is calculating the current of the first

cell by integration according to formula (2) beginning in 300nm and with the step of 0.5nm. After each step, rest of the sub-cells have their currents integrated until the point they reach the current of the sub-cell over them (n^{th} sub-cell tries to match the current of $(n-1)^{\text{th}}$ sub-cell) or their currents rises no more. The light absorbed by the cells over the n^{th} is taken into account. Wavelength onsets corresponding to each sub-cell are stored and used to calculate voltage of each part according to formula (3), which leads to calculating V_{oc} as in (5). I_{sc} is picked according to the chosen mode and efficiency is calculated according to formula (1) with P_{in} fixed at 100mWcm^{-2} . Results after each step are written to the file *output.txt*. Its header has number of junctions and V_{loss} of each junction. Underneath there are results of each calculation step: onsets for all the subcells, number of “useful” junctions according to the chosen current mode, I_{sc} , number of the sub-cell with the lowest current, V_{oc} and efficiency. Dismissed sub-cells have their onset wavelength set as 0. When the current of the first sub-cell rises no more, simulation ends and program closes itself (to prevent accidental overwriting *output.txt*).

3. Simulating cell

This part simulates actual (tandem) cell with the given parameters. It asks for the number of sub-cells, V_{loss} for each subcell and FF. It also asks for the cutoff factor CF. It is a parameter with the values between 0 and 1. It gives information where to take the onset for calculating V_{oc} – for each sub-cell it will be taken at the wavelength, where the amplitude is equal to the maximum amplitude multiplied by CF. IPCE curves are taken in the same manner as in optimize cell section. Then the program calculates current for each sub-cell, taking into account the light absorbed by the sub-cells above. The amount of light that goes through the sub-cell at a given wavelength is given by formula (S1).

$$Light(\lambda) = \left(1 - \frac{IPCE(\lambda)}{IPCE_{max}}\right) \quad (S1)$$

The cutoff wavelength, current and voltage (including loss) of each sub-cell is written out. Then the lowest current is chosen as I_{sc} , V_{oc} and efficiency are calculated and also written out and the program returns to main menu.

In both optimize cell and simulate cell operation modes user IPCE spectra can be used, provided they maintain the structure:

$IPCE_{max}$

300[Tab]IPCE(300)

300.5[Tab]IPCE(300.5)

...

2500[Tab]IPCE(2500)

User can also provide his own sunlight spectrum by substituting the file *AM15ext.txt*. It has the format in which the first column represents wavelength and the second one – photon flux multiplied by elementary charge. By default, the file attached uses ASTM G173-03 reference spectra.

4. Exit

Self explanatory.

Figure

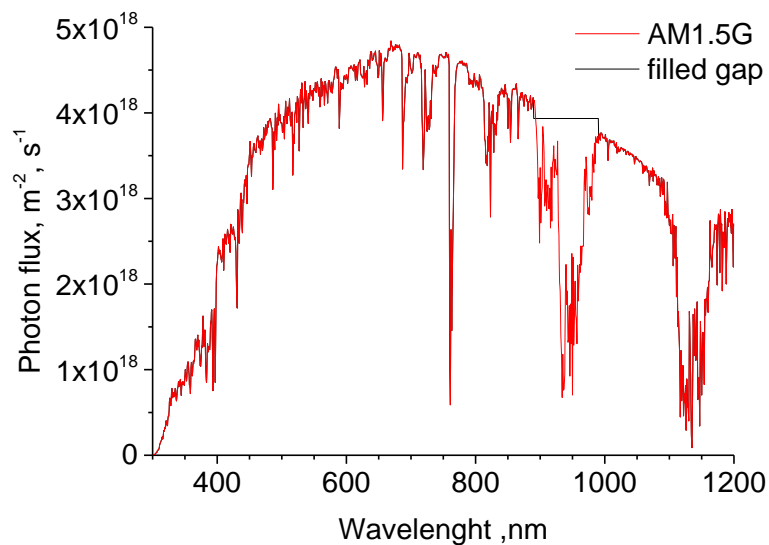


Figure S1. Photon flux for AM1.5G reference sunlight spectrum used in all calculations and the modified spectrum with filled gap in 890-990 nm range due to water vapor absorption for control calculations.