Standardized Method to Report Perovskite Solar Cell V_{OC} Losses

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Overview of MATLAB Script and Functionality

SCRIPT_Vocrad_EQE_fit_Urbachtail_NRVocLoss_QLED.m

This script determines the maximum achievable open circuit voltage, V_{oc}^{rad} (i.e. the V_{OC} in the radiative limit), of your solar cell from the real optical response of the device by evaluating your external quantum efficiency (EQE) data. In addition, it calculates the non-radiative voltage losses (ΔV_{oc}^{NR}) and the corresponding external luminescence quantum efficiency (Q_e^{LED}) with the input of the measured V_{OC}.

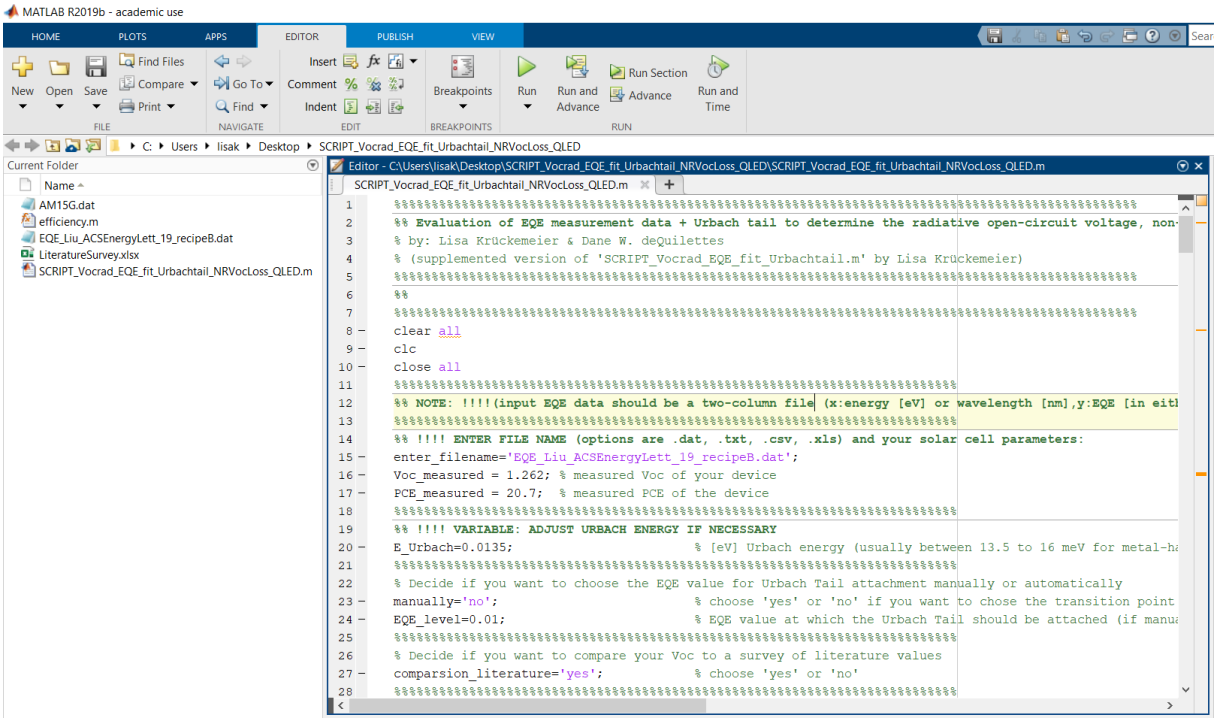


Figure. Screenshot of the main MATLAB script used to calculate V_{oc}^{rad}, ΔV_{oc}^{NR}, and Q_e^{LED}.

Checklist for MATLAB Scripts and Data Sets

In order to use this MATLAB script, you will need the following scripts and data files, which need to be contained in the same file directory.

(1) Main MATLAB script: **SCRIPT_Vocrad_EQE_fit_Urbachtail_NRVocLoss_QLED.m**

(2) Additional MATLAB function:

i. The MATLAB function **efficiency.m** calculates the efficiency and characteristic parameters of a solar cell under AM1.5g illumination

(3) Data set files:

i. **AM15G.dat** is the AM1.5 global solar irradiance spectrum which is used as illumination source for the solar cell
(first column: *energy* in eV, second column: *photon flux* in $s^{-1}cm^{-2}(eV)^{-1}$)

AM15G.dat - Editor

Datei Bearbeiten Format Ansicht Hilfe

```
3.1000000e-001  1.8447284e+017
3.1102990e-001  1.9059377e+017
3.1205980e-001  1.9250159e+017
3.1308970e-001  1.9561783e+017
3.1411960e-001  1.8944021e+017
3.1514950e-001  1.8103615e+017
3.1617940e-001  1.6930022e+017
3.1720930e-001  1.7663120e+017
3.1823920e-001  1.8275202e+017
3.1926910e-001  1.5973040e+017
3.2029900e-001  1.6945956e+017
3.2132890e-001  1.8889248e+017
3.2235880e-001  2.0325833e+017
3.2338870e-001  1.8143897e+017
3.2441860e-001  2.1734996e+017
3.2544850e-001  1.8516166e+017
```

ii. The EQE dataset of the perovskite solar cell for which you want to determine the maximum achievable V_{OC}. **The EQE data (second column) of your solar cell can be in absolute values or percentage-% with respect to energy (eV) or wavelength (nm), which will be in the first column**. The **data format options** are **.dat, .txt, .csv, .xls**. The dataset will be converted to energy in eV and EQE in absolute values. In this example: **EQE_Liu_ACSEnergyLett_19_recipeB.dat**

*EQE_Liu_ACSEnergyLett_19_recipeB.dat - Editor

Datei Bearbeiten Format Ansicht Hilfe

```
4.13333333333333        0.040481675
4                       0.108612
3.875                   0.2376965
3.75757575757576        0.36020825
3.64705882352941        0.4609545
3.54285714285714        0.5603
3.44444444444445        0.5699975
3.35135135135135        0.56795025
3.26315789473684        0.531854
3.17948717948718        0.57506175
3.1                     0.60372325
3.02439024390244        0.67570025
2.95238095238095        0.75112525
2.88372093023256        0.80349175
2.81818181818182        0.830106
2.75555555555556        0.84012675
2.69565217391304        0.817607
2.63829787234043        0.832261
2.58333333333333        0.833554
2.53061224489796        0.828813
```

energy in eV EQE in absolute values

iii. **LiteratureSurvey.xlsx** contains a selection of pioneering perovskite device work that is used to generate a plot to reference and compare your device non-radiative voltage loss and external luminescence quantum efficiency on the same thermodynamic scale (irrespective of band gap and composition).

Procedure

(1) Before you run the script you need to **enter the filename of the EQE dataset** which you want to analyse. Also **enter the measured open-circuit voltage V_{oc} (V) and the power conversion efficiency PCE (%)** of your device.

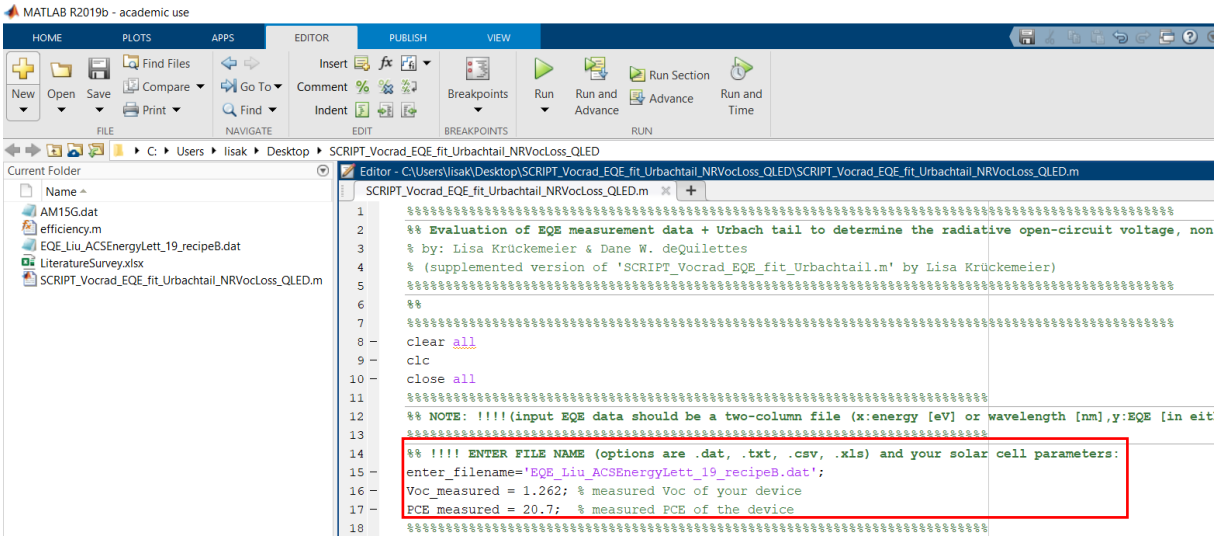
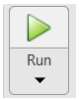


Figure. Screenshot of script showing where data and values should be input (red box).

(2) Run the Script.



A figure window pops up showing the EQE data over energy on a semi-logarithmic scale. Here you will need to select the energy region across the absorption onset (red square below) over which an Urbach tail will be fit.

(3) Zoom in.

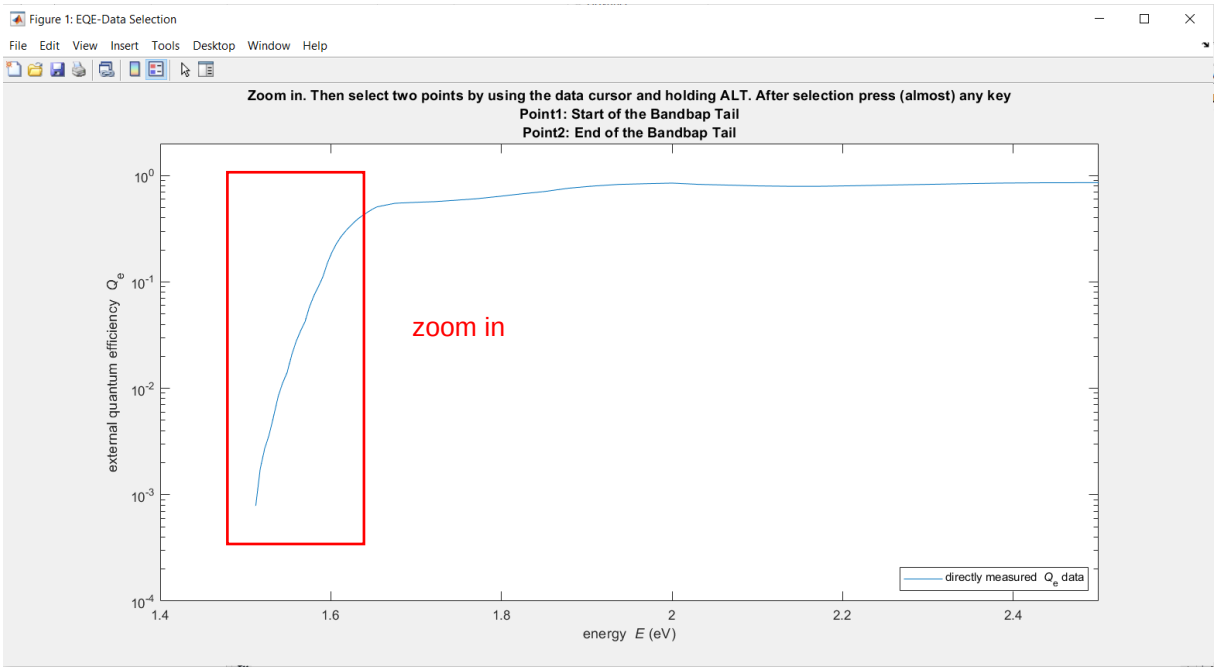


Figure. Measured device raw EQE data as a function of energy (eV).

Pick two data points with your mouse by holding ALT or SHIFT.

i. First select a data point at the lower enegy end of the bandgap tail.
ii. Next, select a second data point at the start of the bandgap tail (higher energy).

iii. Then press enter or (almost) any other key to continue.

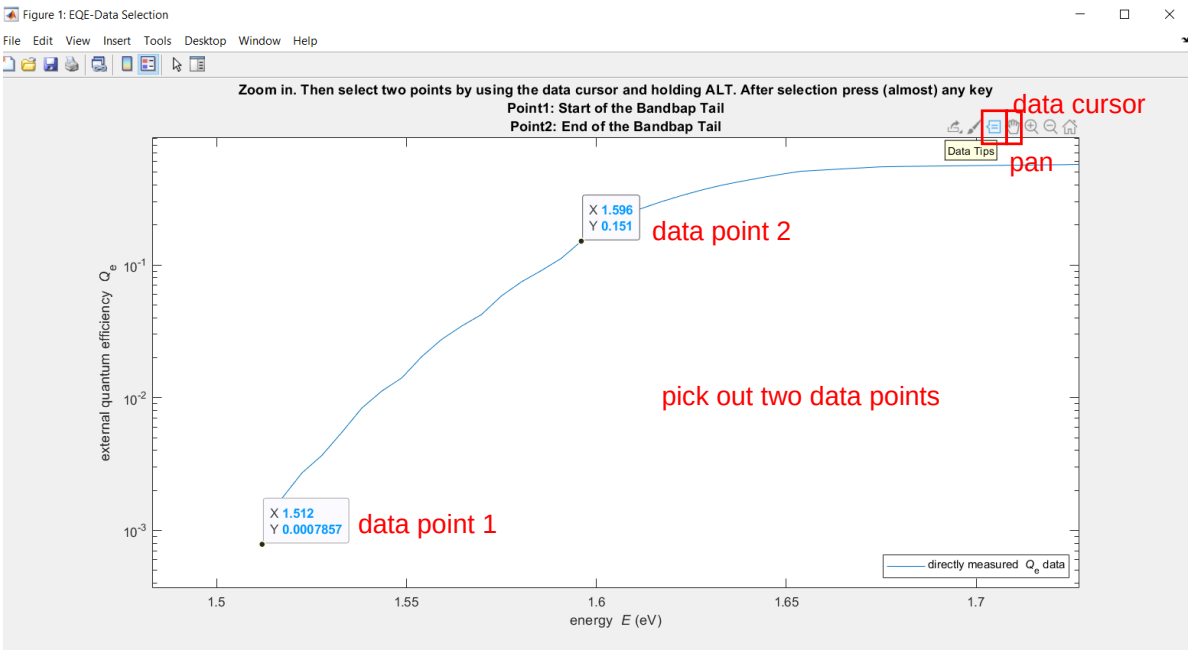


Figure. Zoomed in window of the measured EQE data versus energy (eV) and an example of selecting data points over which to fit the Urbach tail.

When the MATLAB script is finished running, five more figures will appear, the workspace fills with variables and important results are saved as respective .dat files and .mat files.

The quality of the Urbach tail fit can be evaluated by checking:

1) That the **slope** of the tail matches your experimental data. If it does not match, you can **adjust it manually by changing the Urbach tail energy (E_Urbach)** (eV) in the script.

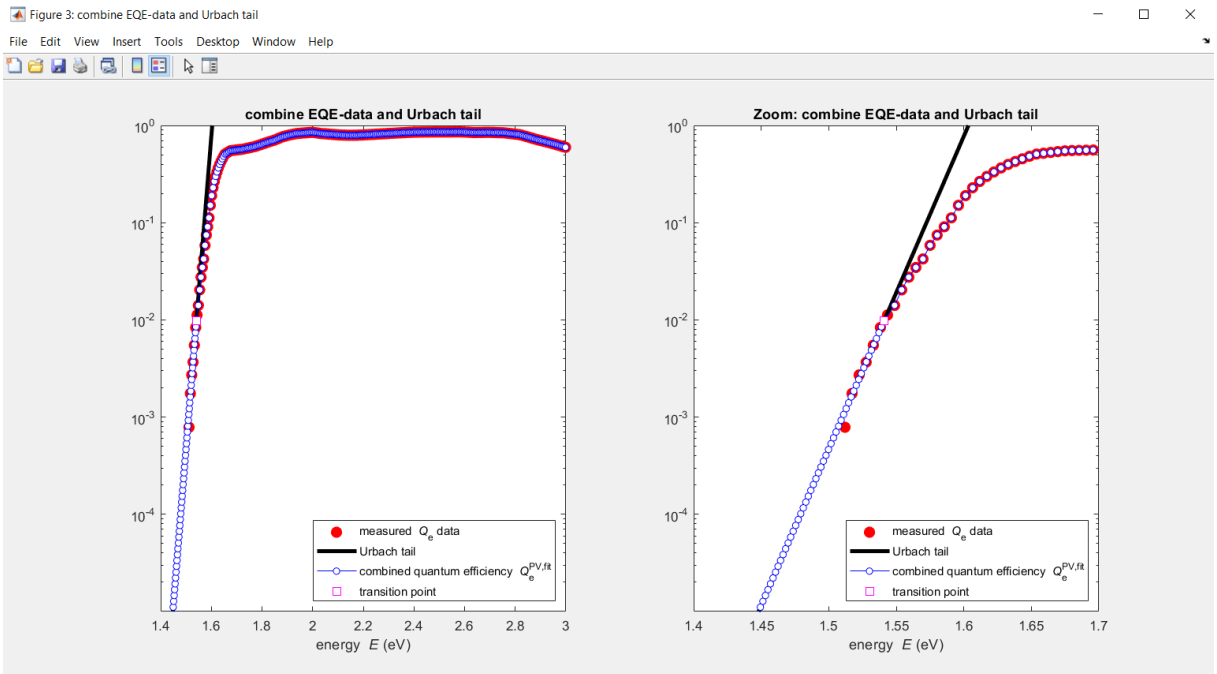


Figure. Combined quantum efficiency data of the measured EQE (red circles) and an Urbach tail fit (black line and blue circles). The coordinates where data has been extrapolated and stitched is marked as the transition point (pink square).

2) The shape of the predicted electroluminescence spectrum. For traditional metal halide perovskites, the spectrum should appear symmetric about the mean emission energy. **The Urbach tail can be manually adjusted so that the EL spectrum looks like you would expect. Typical Urbach energies range from 13-17 meV.**

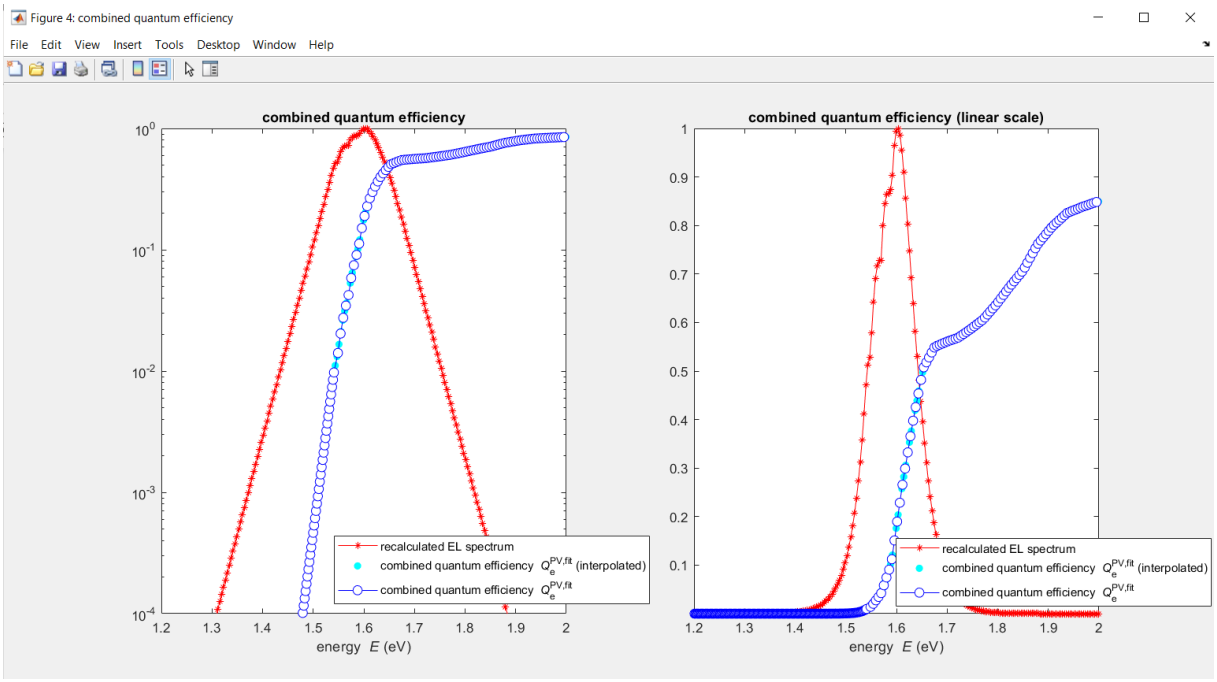


Figure. Combined external quantum efficiency $Q_{\mathrm{e}}^{\mathrm{PV,fit}}\left(E\right)$ (blue) and the corresponding electroluminescence (EL) spectrum (red) calculated from the opto-electronic reciprocity theorem.

Results

Graphical representations of the calculated results are presented in the final two figures. Using the full extrapolated EQE spectrum, the maximum theoretical V_{OC} ($V_{\mathrm{oc}}^{\mathrm{rad}}$) is calculated and reported in the bar graph shown below. This is compared to your measured device V_{OC} and used to calculate the non-radiative voltage loss $\Delta V_{\mathrm{oc}}^{\mathrm{NR}}$ (i.e. $V_{\mathrm{oc}}^{\mathrm{rad}} - V_{\mathrm{OC}}$). This value can be compared to any other perovskite devices independent of composition and bandgap energy.

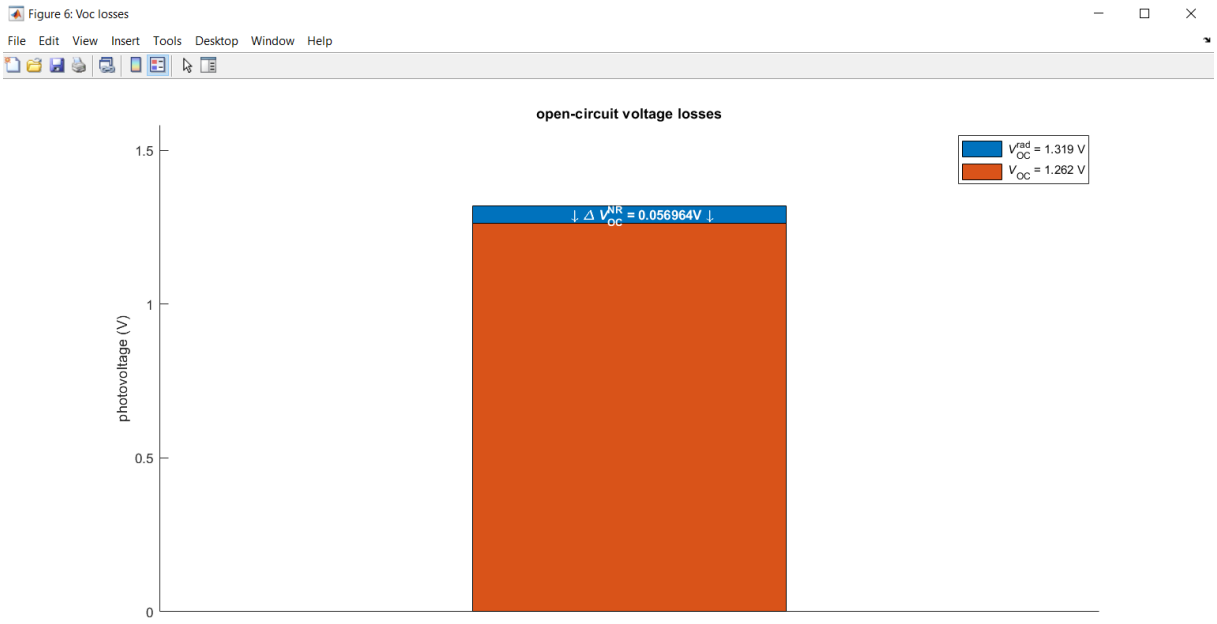


Figure. Bar chart of your device V_{OC}, $V_{\mathrm{oc}}^{\mathrm{rad}}$, and $\Delta V_{\mathrm{oc}}^{\mathrm{NR}}$.

The final plot shows $\Delta V_{\mathrm{oc}}^{\mathrm{NR}}$ as well as the external luminescence quantum efficiency ($Q_{\mathrm{e}}^{\mathrm{LED}}$), compared to a selection of pioneering perovskite device papers from literature.** This allows you to directly **compare your device voltage and implied external luminescence efficiency to the best in the field**. If you do not want to script to perform this comparsion, set comparsion_literature='no'.

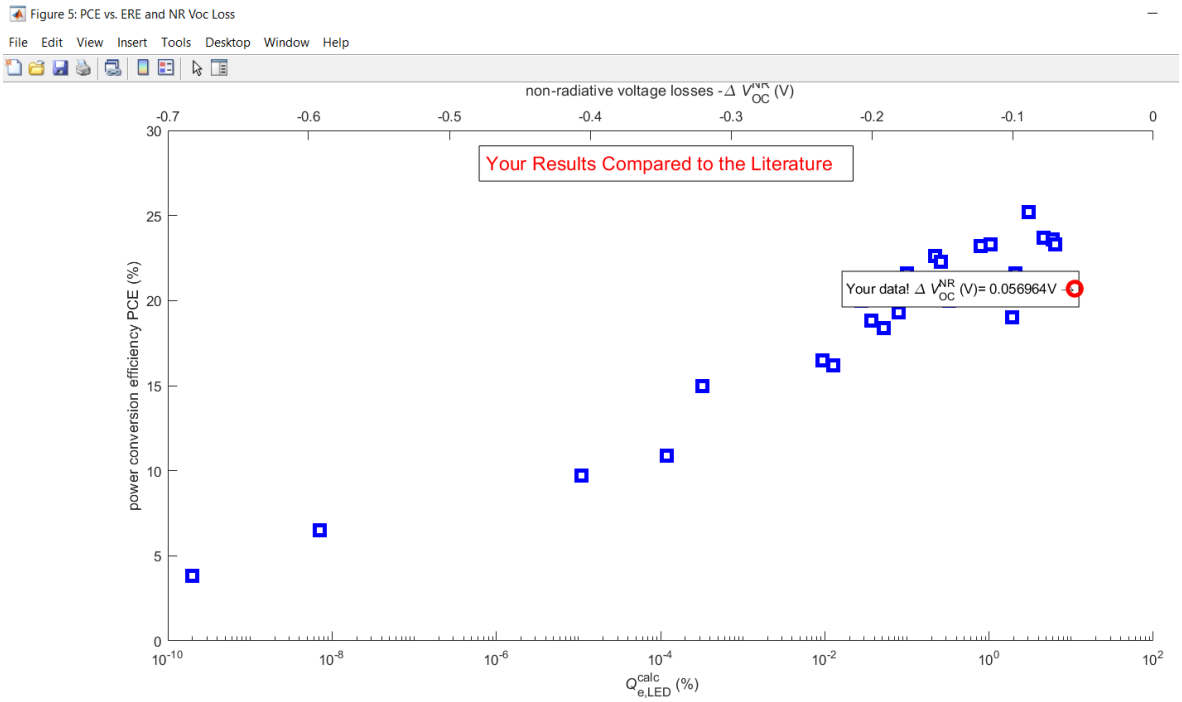


Figure. Power conversion efficiency (PCE) versus $Q_{\mathrm{e}}^{\mathrm{LED}}$ and $\Delta V_{\mathrm{oc}}^{\mathrm{NR}}$ of a selection of pioneering perovskite device work along with your data overlaid in red.

** Email danedeq@mit.edu if there is low voltage loss device data that you believe should be included in LiteratureSurvey.xls.

Access to Saved Data and Results

To acess the calculated values in the radiative limit, open the variable RESULTS_rad_limit or variable Voc_rad (V). The variable NR_Voc_loss states you non-radiative voltages losses (V), and Q_e_LED the external luminescence quantum efficiency (%), which is often referred to as the external radiative efficiency or LED quantum efficiency.

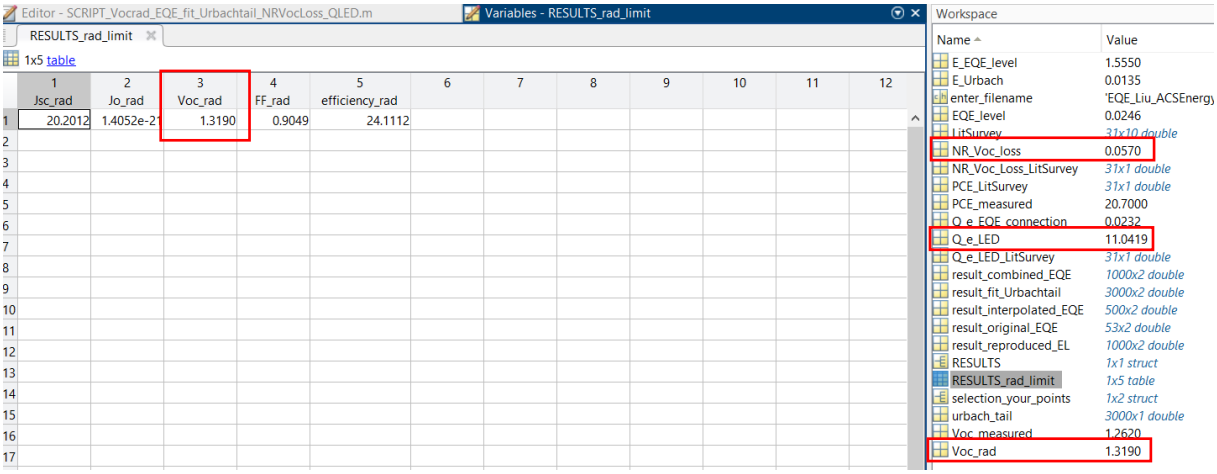


Figure. Screenshot of the RESULTS_rad_limit table showing the calculated V_{oc}^{rad}.

Troubleshooting

- The script can also be tested with the exemplary dataset (EQE_Liu_ACSEnergyLett_19_recipeB.dat) to test whether your EQE code is importing correctly.

- If the combined quantum efficiency data does not look correct, you can change the transition point (EQE_level) manually. The point should be somewhere where your measured EQE has a high signal-to-noise ratio. You can switch manually to ‘yes‘, otherwise the transition point will be picked automatically.

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%% !!!! VARIABLE: ADJUST URBACH ENERGY IF NECESSARY
E_Urbach=0.0135;                        % [eV] Urbach energy (usually between 13.5 to 16 meV for
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% Decide if you want to choose the EQE value for Urbach Tail attachment manually or automatically
manually='no';                          % choose 'yes' or 'no' if you want to chose the transitic
EQE_level=0.01;                         % EQE value at which the Urbach Tail should be attached
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

- Data is interpolated to get more data points in the energy range at the bandgap tail. Experimental datasets often have only a few points in this range and the calculation is more precise with higher energy resolution. If you don’t want to use this interpolation, uncomment lines 98-101.

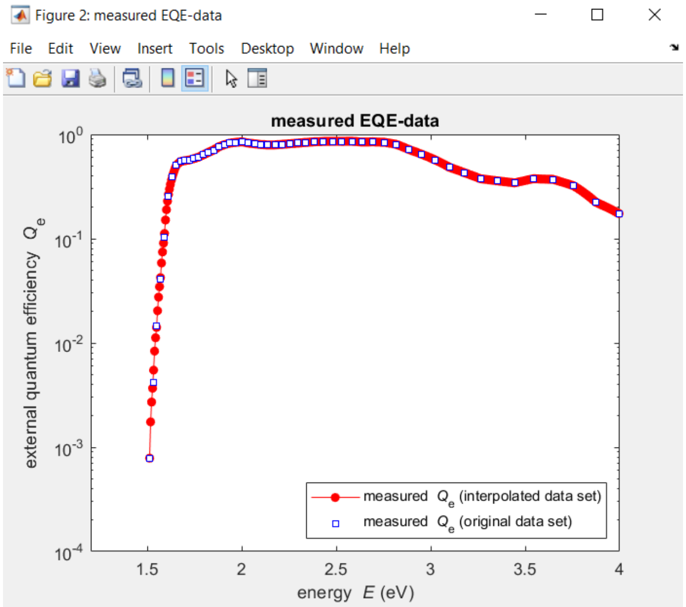


Figure. Measured EQE data (blue) versus energy and an interpolated version of the data set (red).

```
97      %% INTERPOLATION of the EQE data
98 -    E_EQE_int=linspace(E_EQE_original(1),E_EQE_original(end),500)';          % [eV],energy axis wi
99
100 -   EQE=interp1(E_EQE_original,EQE_original,E_EQE_int); %interpolation to the energy axis with small
101 -   E_EQE=E_EQE_int;
102     %}
103     %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
104     %{
105         %OR
106         %if an interpolation is not necessary
107         E_EQE=E_EQE_original;
108         EQE=EQE_original;
109     %}
110     %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```