GetMiu V1.00

Data processing software for Hyperspectral Imager powered by MATLAB R2017a

Features:

- Quasi fermi-level splitting (QFLS) mapping
- Urbach energy (Eu) mapping
- Voc prediction

Running environment

- Screen resolution: >1920*1080

Dr. Mingcong Wang 21th. July. 2020

Outline

Running procedures

Step 1: Copy the files below to a new folder

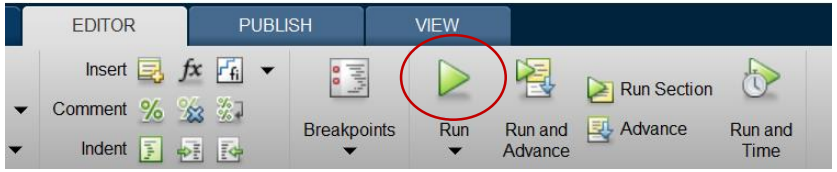
GetMiu.fig

GetMiu.m abs.dat

S49_surf_532 nm_325mW_1_10sec(cal).h5

Step 2: open **GetMiu.m** with MATLAB, then you can see the raw codes in the Editor window (right figure→)

Step 3: Press **F5** or click the '**Run**' button located in the menu bar to run the codes



Editor - GetMiu.m

fitdiff.m | len.m | Dalpha.m | TAload.m | TAs.m | GetMiu.m

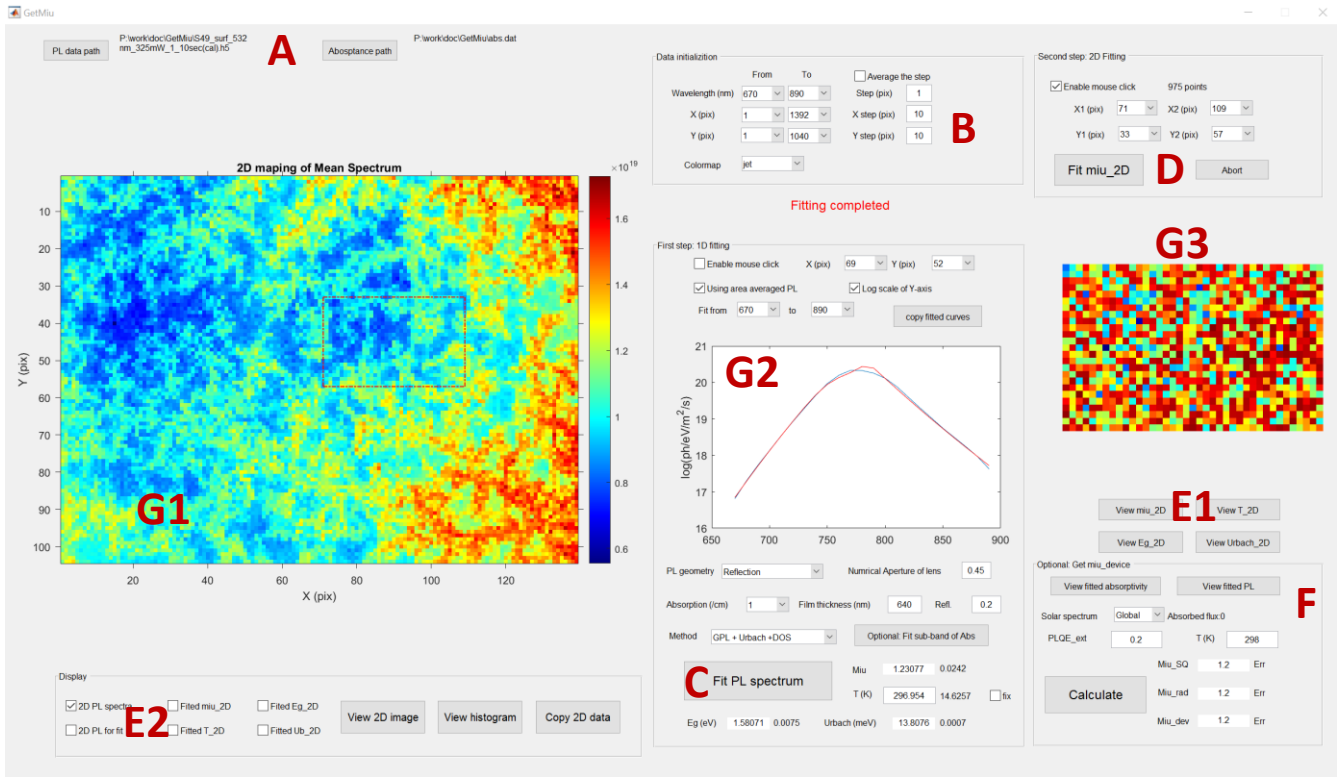
```
function varargout = GetMiu(varargin)
% GETMIU MATLAB code for GetMiu.fig
%      GETMIU, by itself, creates a new GETMIU or raises the existing
%      singleton*.
%
%      H = GETMIU returns the handle to a new GETMIU or the handle to
%      the existing singleton*.
%
%      GETMIU('CALLBACK',hObject,eventData,handles,...) calls the local
%      function named CALLBACK in GETMIU.M with the given input arguments.
%
%      GETMIU('Property','Value',...) creates a new GETMIU or raises the
%      existing singleton*.  Starting from the left, property value pairs are
%      applied to the GUI before GetMiu_OpeningFcn gets called.  An
%      unrecognized property name or invalid value makes property application
%      stop.  All inputs are passed to GetMiu_OpeningFcn via varargin.
%
%      *See GUI Options on GUIDE's Tools menu.  Choose "GUI allows only one
%      instance to run (singleton)".
%
% See also: GUIDE, GUIDATA, GUIHANDLES

% Edit the above text to modify the response to help GetMiu

% Last Modified by GUIDE v2.5 06-May-2020 11:33:50

% Begin initialization code - DO NOT EDIT
gui_Singleton = 1;
gui_State = struct('gui_Name',       mfilename, ...
                   'gui_Singleton',  gui_Singleton, ...
                   'gui_OpeningFcn', @GetMiu_OpeningFcn, ...
                   'gui_OutputFcn',  @GetMiu_OutputFcn, ...
                   'gui_LayoutFcn',  [] , ...
                   'gui_Callback',   []);
if nargin && ischar(varargin{1})
    gui_State.gui_Callback = str2func(varargin{1});
end
```

Overview of the interface



A: Read the PL-file and absorptance data

B: Select the 2D PL data (Displayed in G1)

C: Curve fit for Single point PL (Displayed in G2)

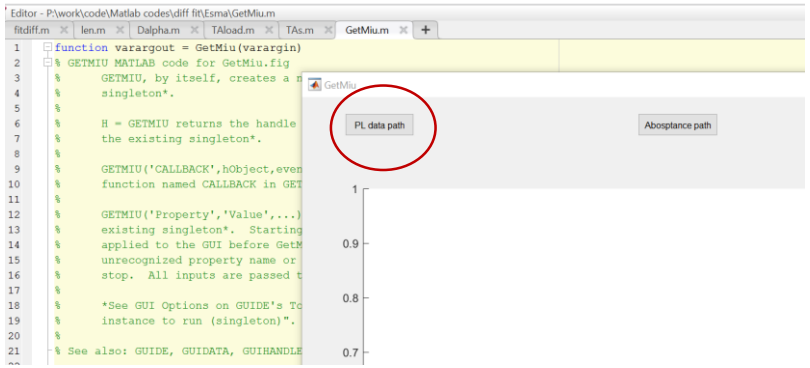
D: Curve fit for 2D area PL (Displayed in G3)

E1: View the fitted result

E2: View, analyze and copy the fitted result

F: Voc prediction (the value of PLQE is needed)

Data load



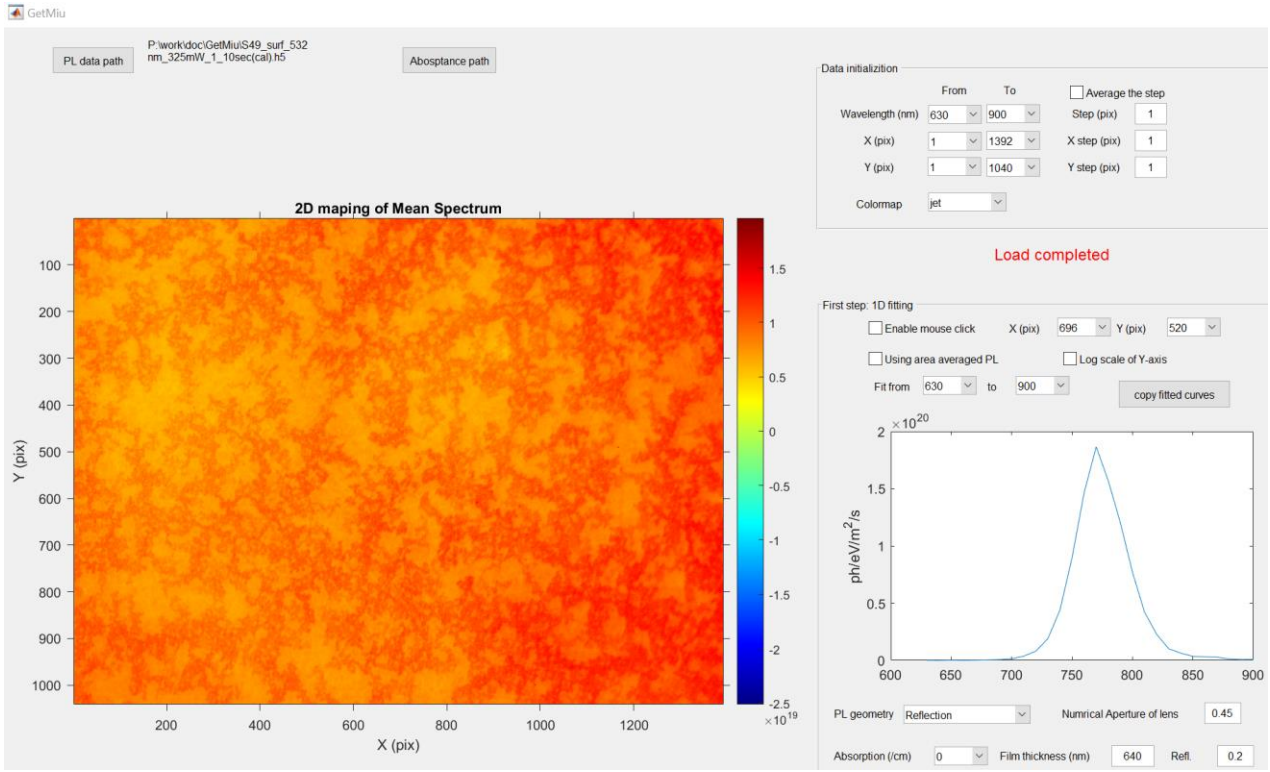
Load the PL file:

Step 1: Click 'PL data path' to select PL file (top figure)

Step 2: Choose the *.h5 file below and wait for the process to be completed (~10 seconds)

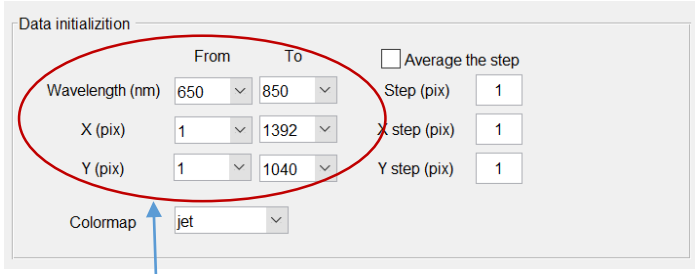
S49_surf_532 nm_325mW_1_10sec(cal).h5

Step 3: Now you can see the 2D mapping and the center point of the PL data (right figure→)



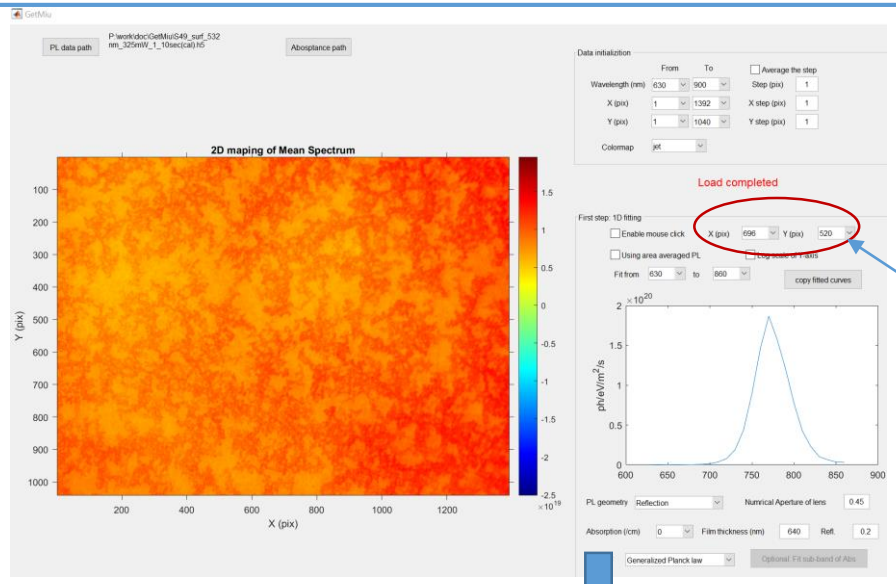
Data selection

- For each dimension (wavelength, x-axis and y-axis), you can reset data range and data step

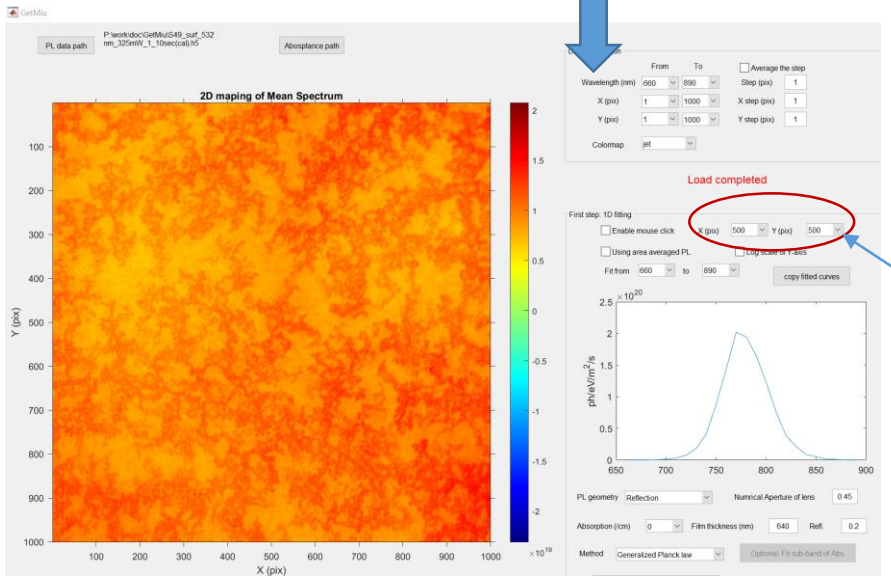


- Edit **range** here

→Function: initialize the raw data



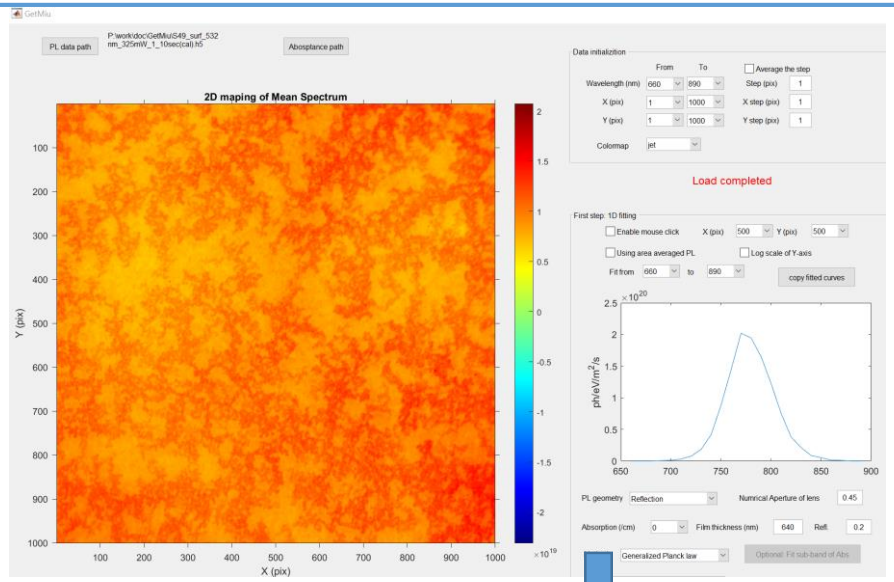
- Default setting
- Center point located at X=696, Y=520

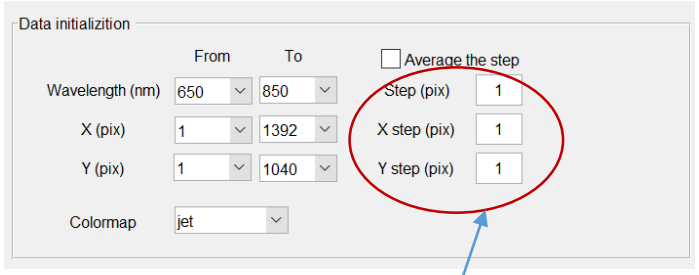


- Set wavelength: 660-590
- Set X: 1-1000
- Set Y: 1-1000
- Center point changes to X=500, Y=500

Data selection

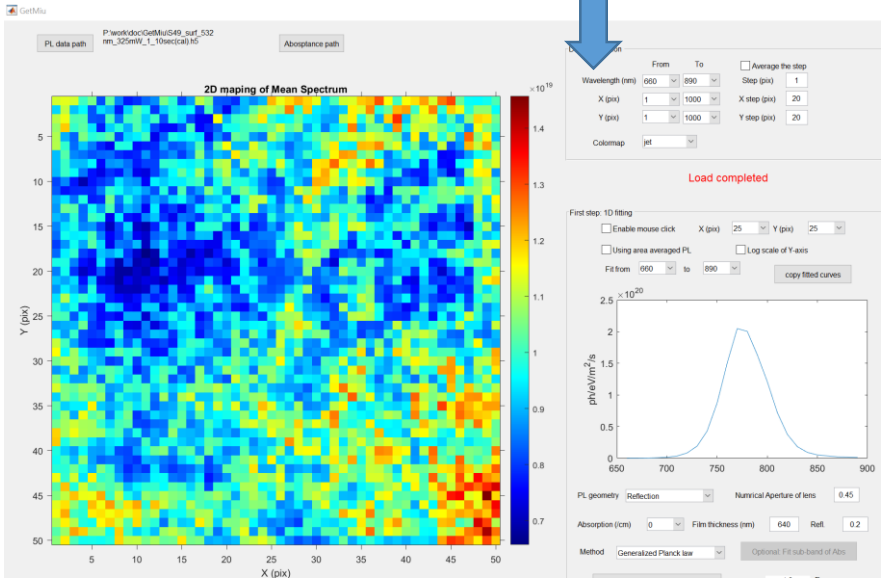
- For each dimension (wavelength, x-axis and y-axis), you can reset data range and data step





- Edit **data step** here

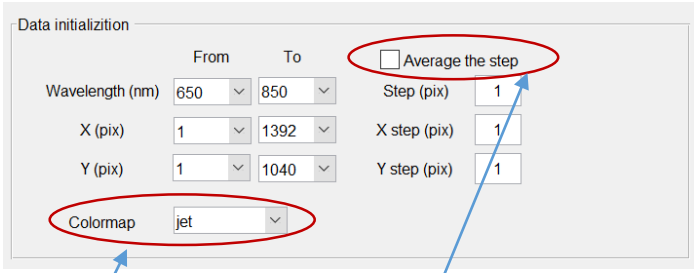
→Function: remove pixel overlap, reduce data size



- Set X-step: 20
- Set Y-step: 20

Data selection

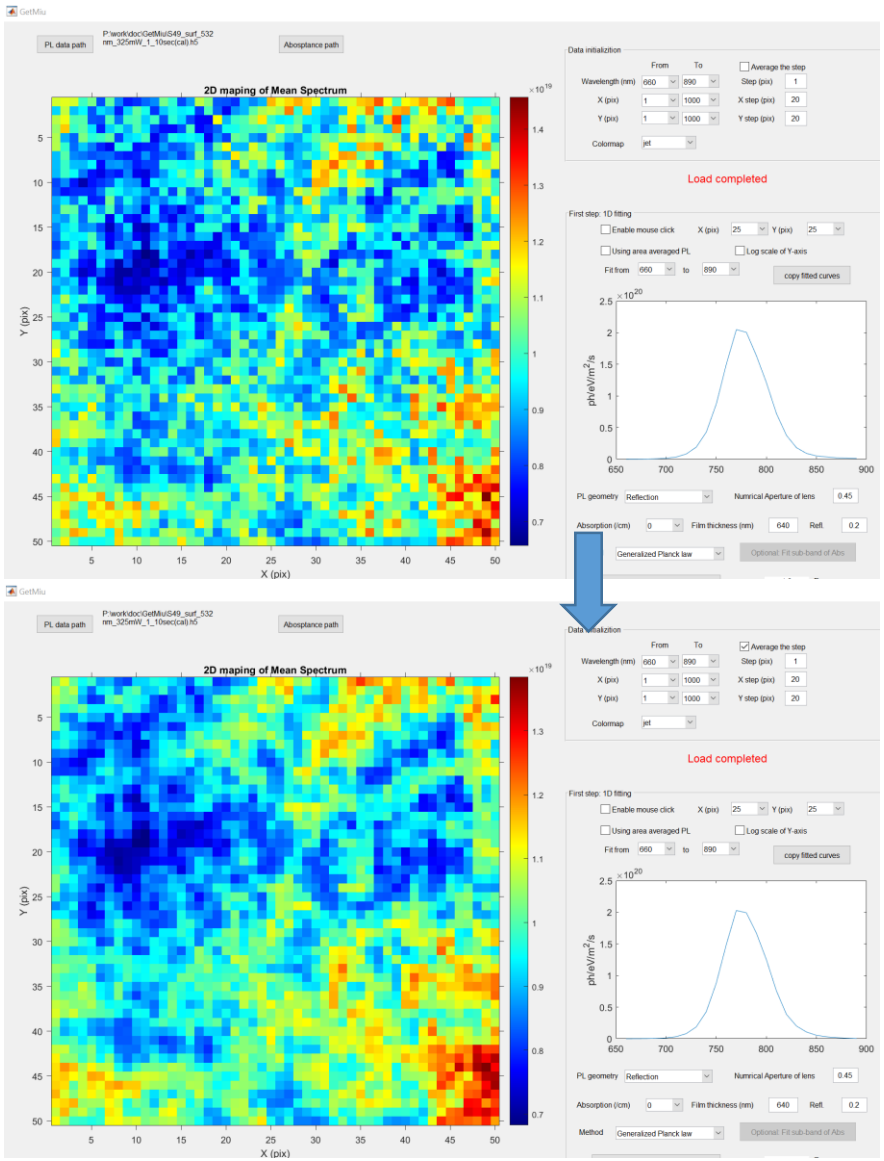
- For each dimension (wavelength, x-axis and y-axis), you can reset data range and data step



- Choose your favorite **colormap** here

- If the data steps have been reset, you can **average all the stepped data** as the new data

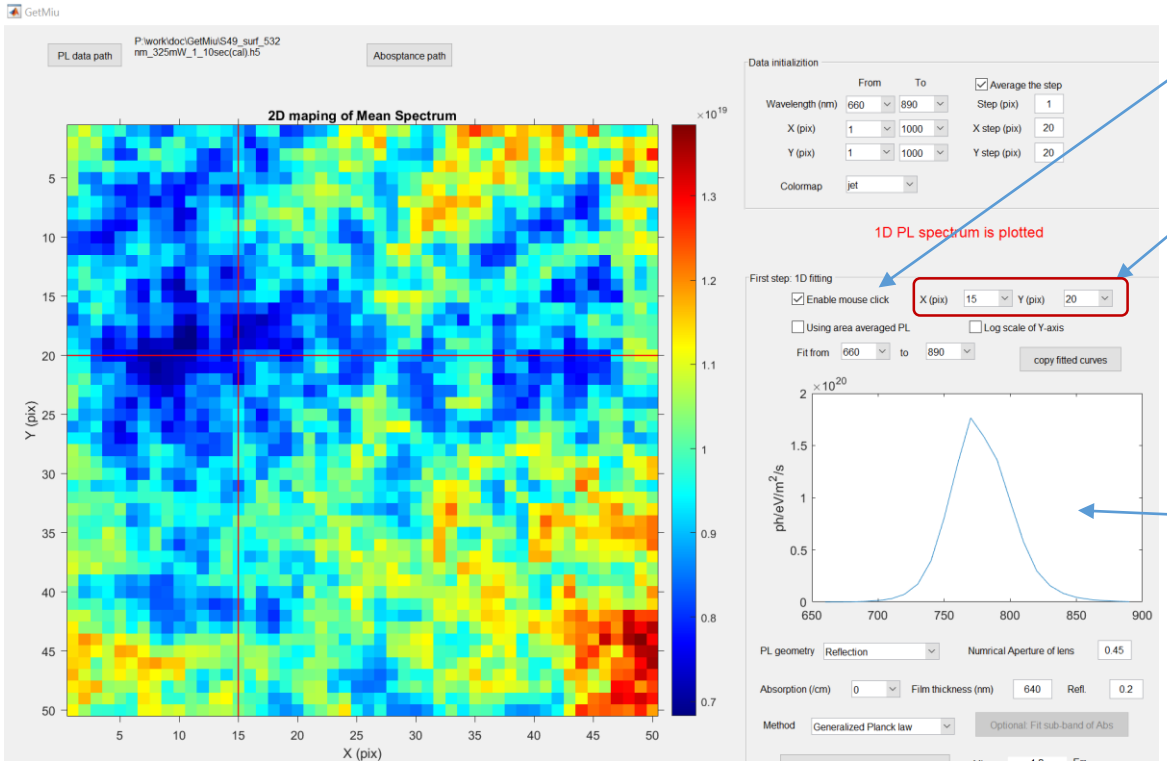
→Function: smooth the reduced data



- Tick 'Average the step'

PL curve fit -1D

- Select the **position** of the PL spectrum

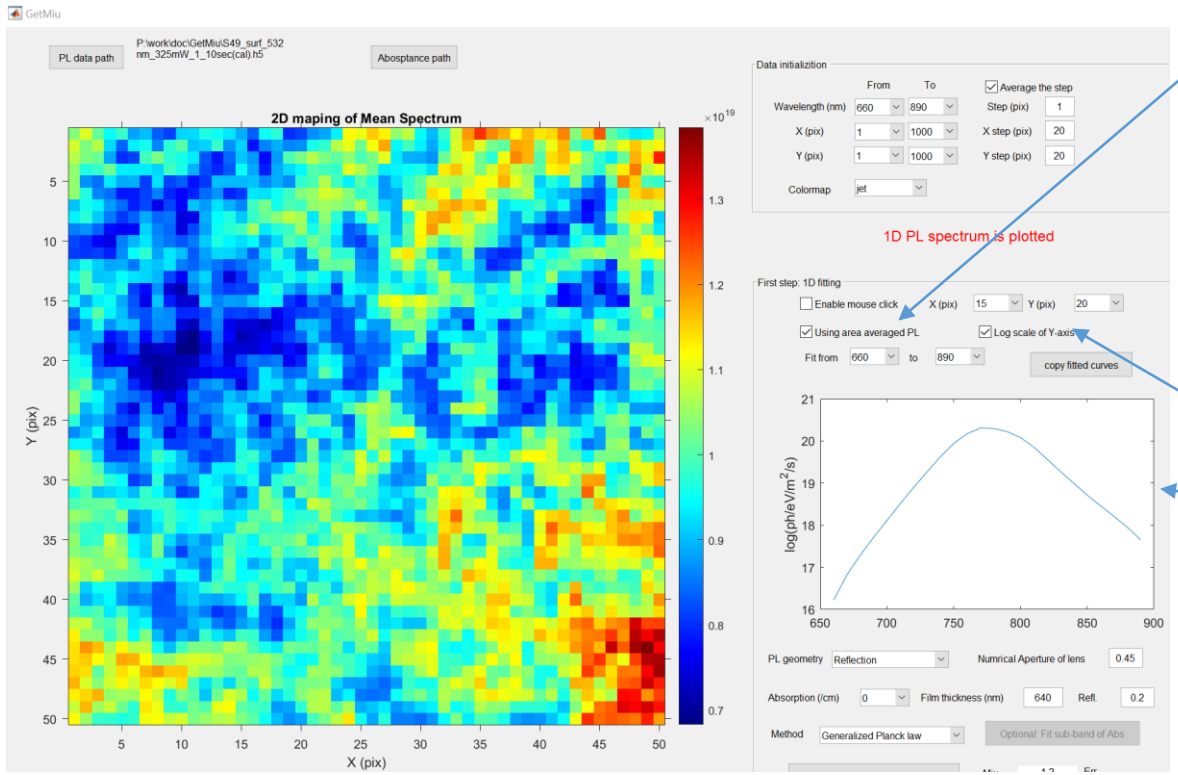


- Tick the checkbox then you can choose the position by mouse click
- An alternative way is selecting the X-axis and Y-axis

Preview of the PL spectrum

PL curve fit -1D

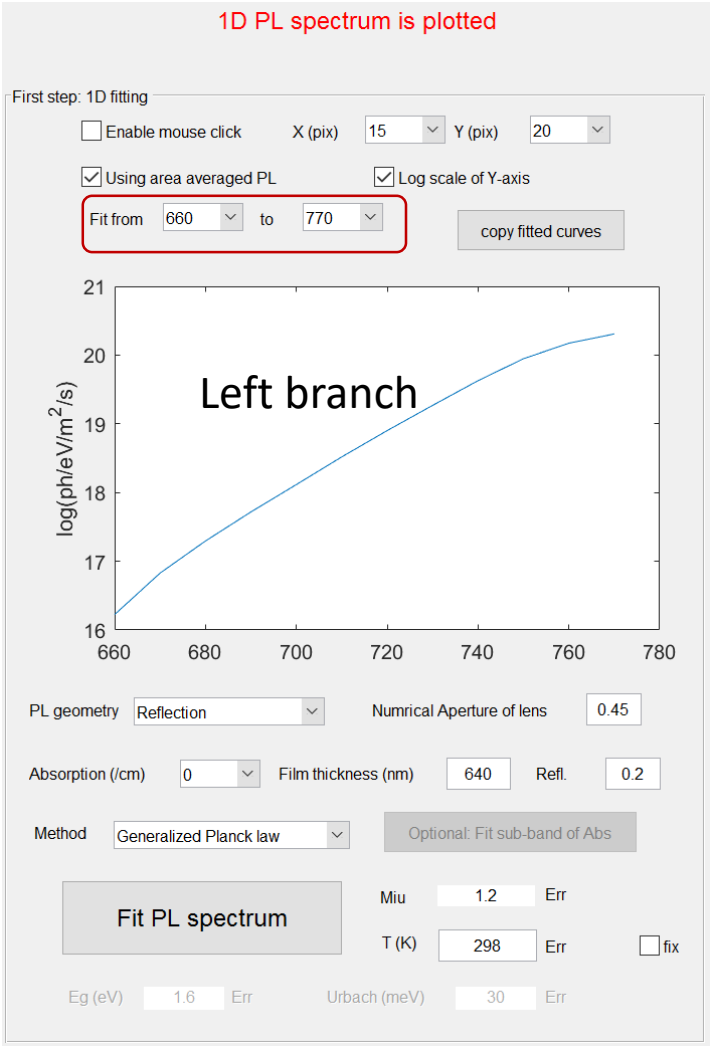
- Select the **position** of the PL spectrum

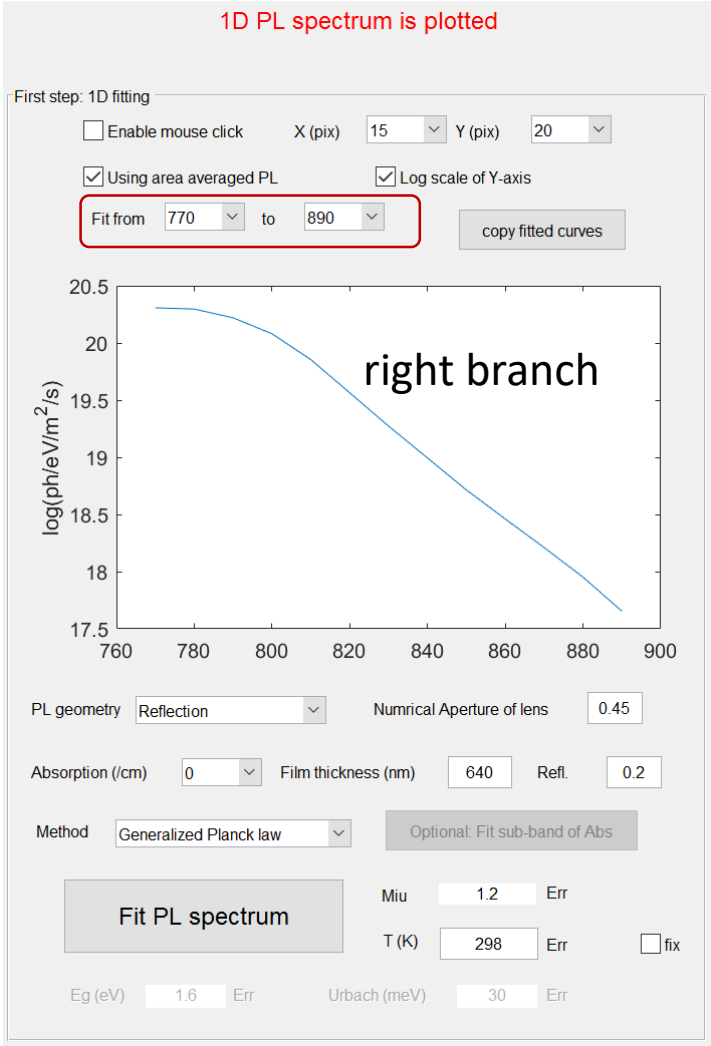


- When 'Using averaged PL' is ticked, the 1d PL spectrum is the averaged value of all the 2D PL spectra.
- Preview of the PL spectrum in log-scale

PL curve fit -1D

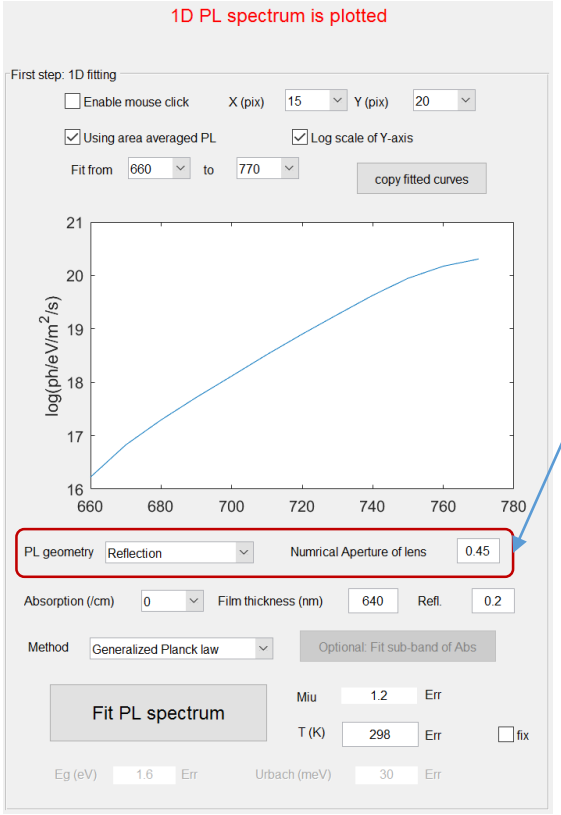
- Select the **wavelength** of the PL spectrum





PL curve fit -1D

- **Fit Options**

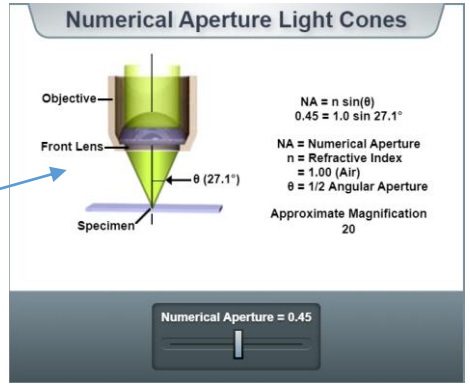


Absolute PL intensity calibration

PL geometry: **Reflection** (default) or **Integrating sphere**

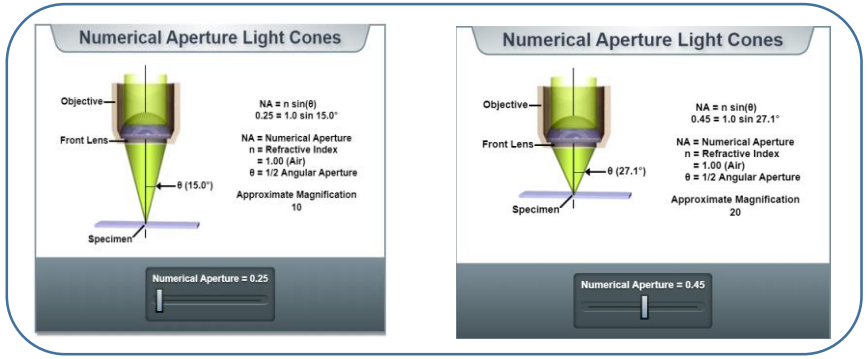
Reflection: CCD only collect a small solid angle of the PL photons from the top surface of the specimen

Collection cone

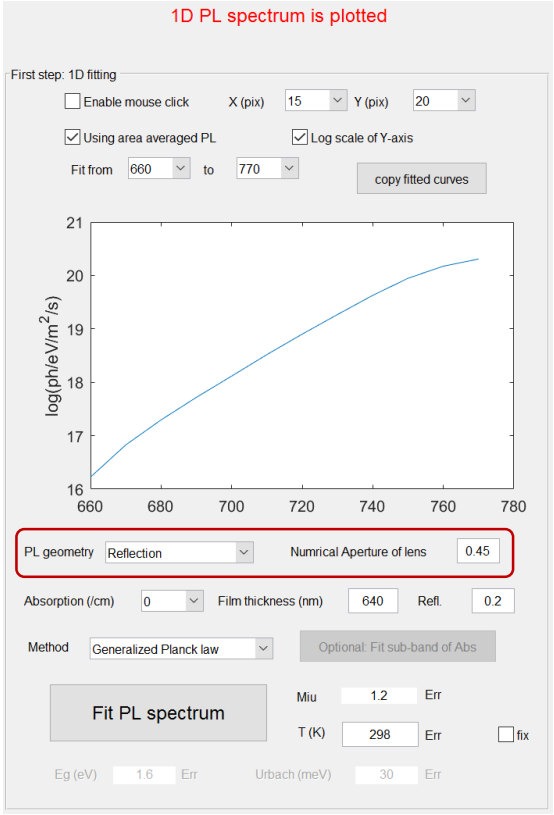


Integrating sphere: CCD collects all the PL photons by an integrating sphere (may not be the case of Hyperspectral imager)

PL curve fit -1D



- **Fit Options**



Numerical aperture of **objective lens**:
Objective lens: for PL detection (default value: 0.45, collection angle ~27.1°)

How does the code do the flux calibration?
Assuming photons obey Lambertian distribution:

Correction factor for objective lens:

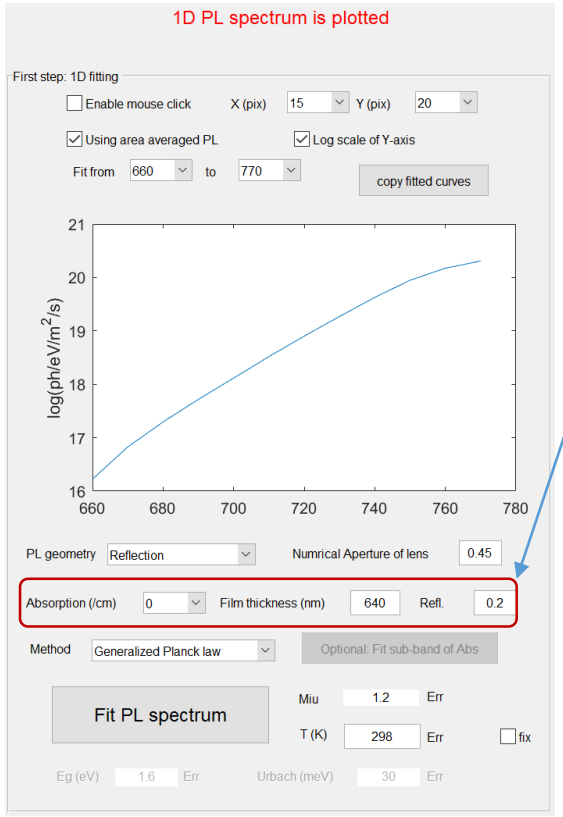
$$f_{lens} = 1 - cos^2\,\theta_{lens} \approx 0.2075$$

Calibrated PL Flux :

$$I_{PL} = I_{mesured}/f_{lens}$$

PL curve fit -1D

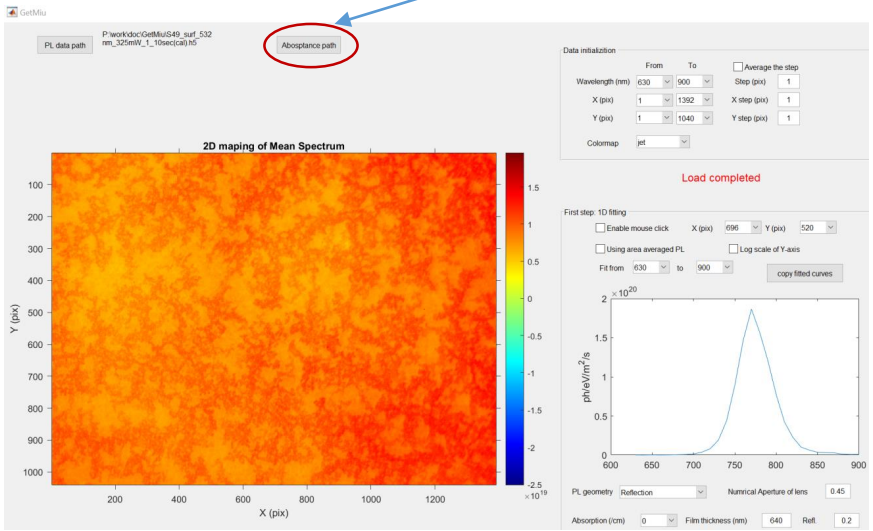
- **Fit Options**



Sample information

Select the absorption spectrum:

- Firstly you need to load the absorption file. Press this button to ope abs.dat
- For your own absorption files please format it in *.dat, *.txt or *.mat



abs.dat - Notepad

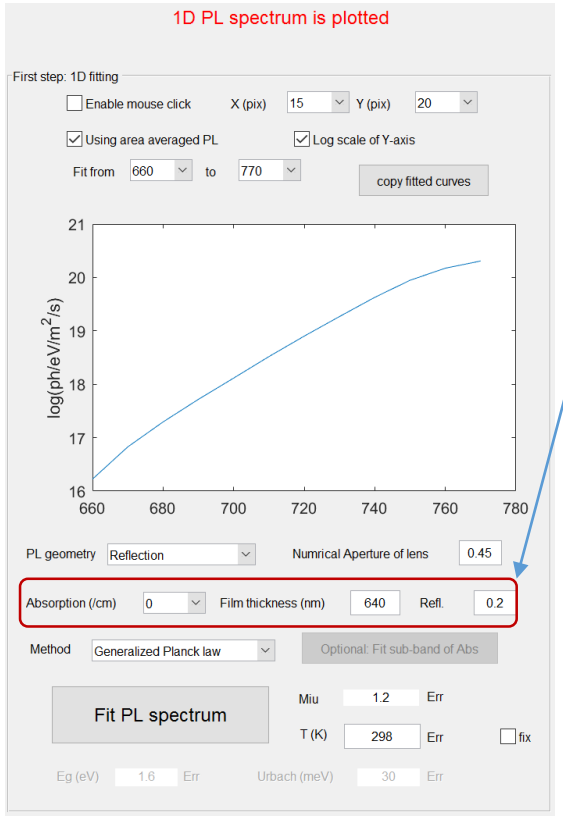
File Edit Format View Help

900	2487.564081
899	2498.342274
898	2514.05027
897	2521.917925
896	2531.765338
895	2544.588376
894	2552.491538
893	2562.383451
892	2574.272813
891	2585.189724
890	2592.146004
889	2601.100285
888	2607.076376

Wavelength value in cm^{-1}

PL curve fit -1D

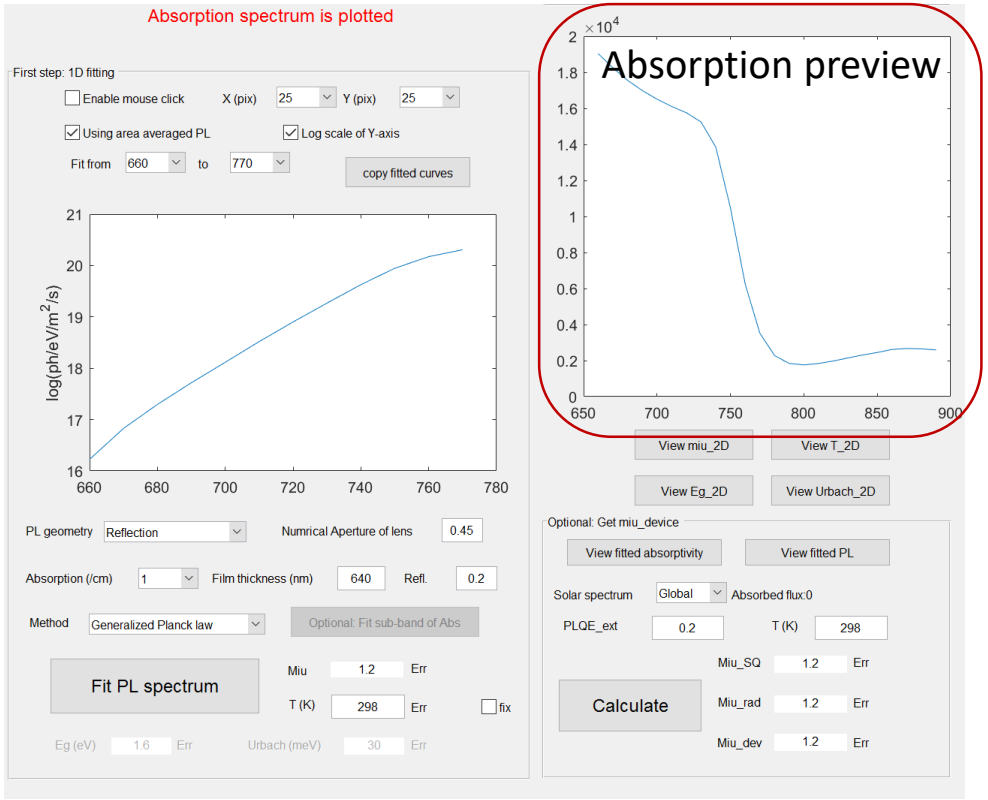
- **Fit Options**



Sample information

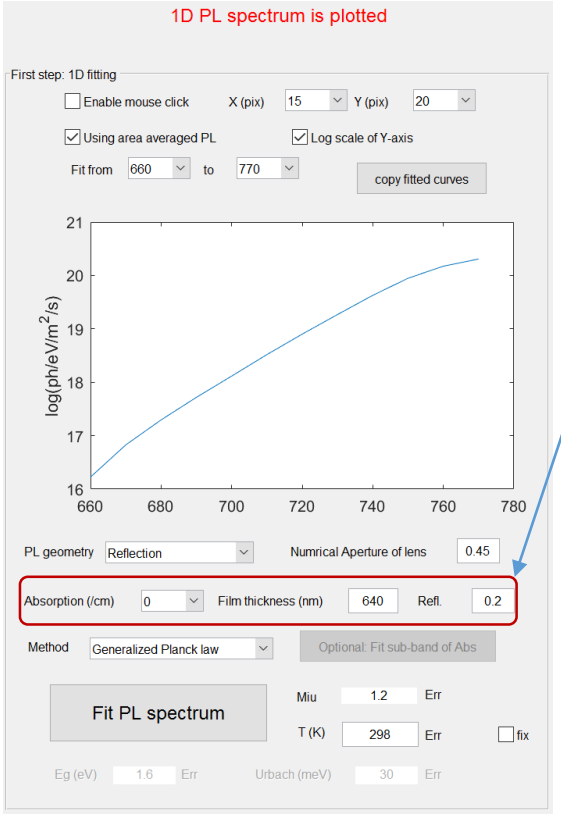
Select the absorption spectrum:

- Make sure the unit of absorption spectrum is cm^{-1}
- For a file with multi-columns, change the column number to switch the absorption spectra



PL curve fit -1D

- **Fit Options**



Sample information

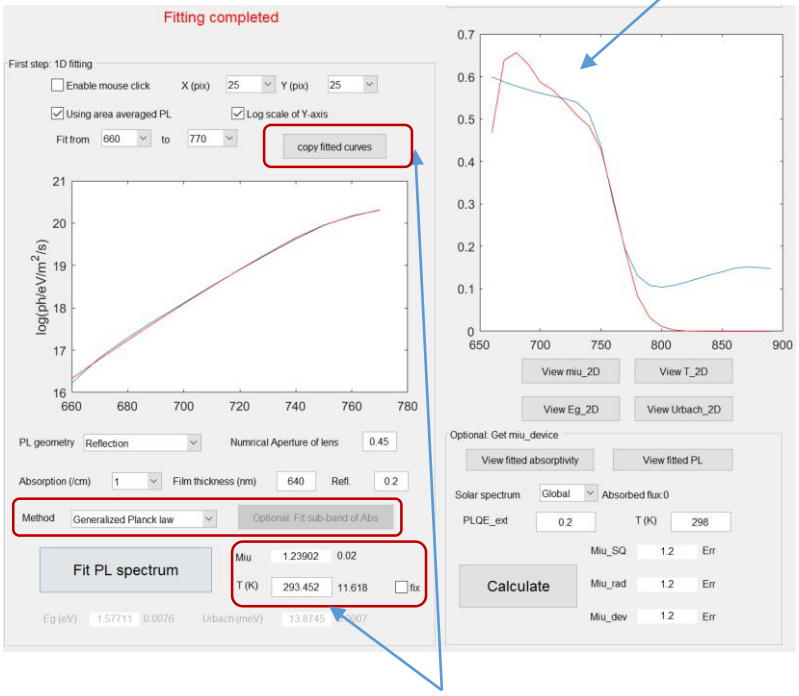
Input the film thickness (default value: 640 nm)

Input the reflectivity at film's surface (reflectivity for excitation source, default value: 20%)

PL curve fit -1D

Blue curve: absorptivity calculated from absorption coefficient
Red curve: absorptivity extracted from the PL spectrum with the help of fitted Miu and T

- **Fit Options**

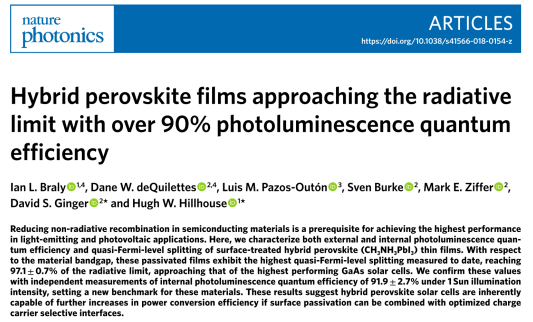


Fitted result: QFLS (Miu) and Temperature (T)
Optional: fitting with fixed temperature
Optional: copy fitted curves to clipboard

Generalized Planck law (GPL): only works for PL's left branch (high energy side)

$$I_{PL}(\varepsilon) = \left\{\frac{2\pi\varepsilon^2}{h^3c^2}\right\} \cdot \left\{\frac{1}{exp\left(\frac{\varepsilon-(E_F^{CB}-E_F^{VB})}{kT}\right)-1}\right\} \cdot \{a(\varepsilon, E_F^{CB}, E_F^{VB}, T)\}$$

Where h is Planck's constant ($4.136\text{x}10^{-15}$ $eV{\cdot}s$), c is the speed of light ($2.998\text{x}10^{8}$ m/s), k is the Boltzmann constant ($8.617\text{x}10^{-5}$ eV/K), ε is the photon energy in eV, $a(\varepsilon, E_F^{CB}, E_F^{VB}, T)$ is the occupation and temperature dependent spectral absorptivity, and I_{PL} is the spectral photoluminescence emission flux in units of $photons/(m^2{\cdot}s{\cdot}eV)$.


nature photonics ARTICLES
https://doi.org/10.1038/s41566-018-0154-z

Hybrid perovskite films approaching the radiative limit with over 90% photoluminescence quantum efficiency

Ian L. Braly, Dane W. deQuilettes, Luis M. Pazos-Outón, Sven Burke, Mark E. Ziffer, David S. Ginger and Hugh W. Hillhouse

Reducing non-radiative recombination in semiconducting materials is a prerequisite for achieving the highest performance in light-emitting and photovoltaic applications. Here, we characterize both external and internal photoluminescence quantum efficiency and quasi-Fermi-level splitting of surface-treated hybrid perovskite ($CH_3NH_3PbI_3$) thin films. With respect to the material bandgap, these passivated films exhibit the highest quasi-Fermi-level splitting measured to date, reaching 97.1 ± 0.7% of the radiative limit, approaching that of the highest performing GaAs solar cells. We confirm these values with independent measurements of internal photoluminescence quantum efficiency of 91.9 ± 2.7% under 1 Sun illumination intensity, setting a new benchmark for these materials. These results suggest hybrid perovskite solar cells are inherently capable of further increases in power conversion efficiency if surface passivation can be combined with optimized charge carrier selective interfaces.

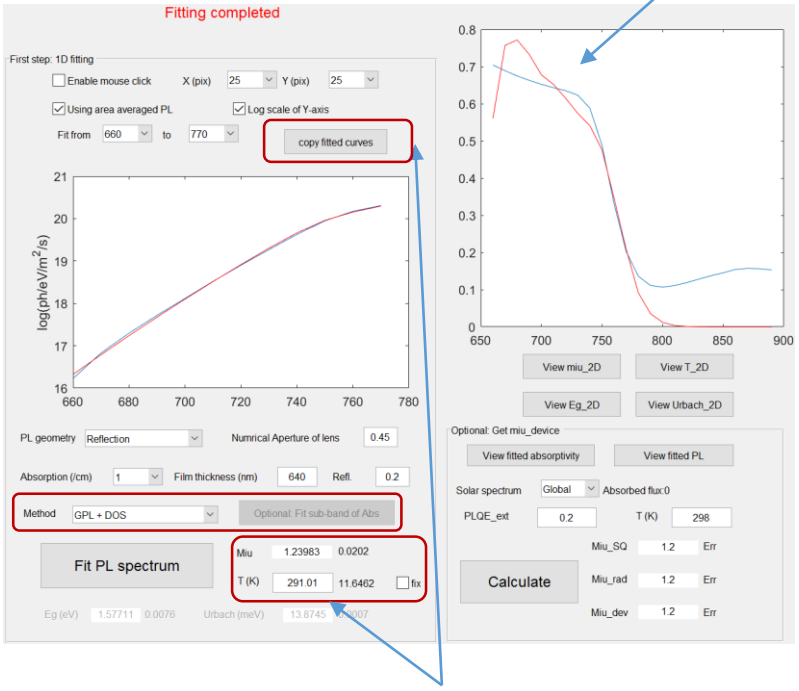
The expression of spectral absorptivity:

$$a(\varepsilon) = \frac{(1-R)(1-\exp(-\alpha d))}{1-R\exp(-\alpha d)}$$

PL curve fit -1D

Blue curve: absorptivity calculated from absorption coefficient
Red curve: absorptivity extracted from the PL spectrum with the help of fitted Miu and T

- **Fit Options**



Fitted result: QFLS (Miu) and Temperature (T)
Optional: fitting with fixed temperature
Optional: copy fitted curves to clipboard

GPL + DOS: only works for PL's left branch (high energy side)

$$I_{PL}(\varepsilon) = \left\{\frac{2\pi\varepsilon^2}{h^3c^2}\right\} \cdot \left\{\frac{1}{exp\left(\frac{\varepsilon-(E_F^{CB}-E_F^{VB})}{kT}\right)-1}\right\} \cdot \{a(\varepsilon, E_F^{CB}, E_F^{VB}, T)\}$$

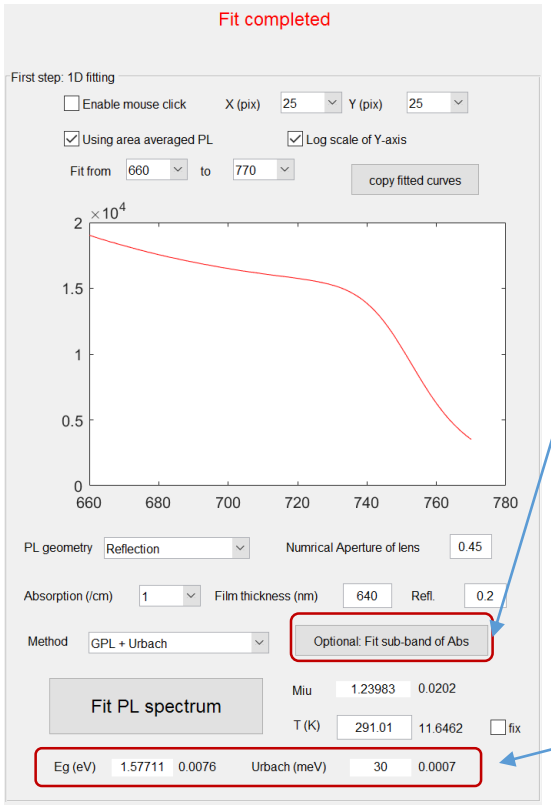
Where h is Planck's constant ($4.136\text{x}10^{-15}$ $eV{\cdot}s$), c is the speed of light ($2.998\text{x}10^{8}$ m/s), k is the Boltzmann constant ($8.617\text{x}10^{-5}$ eV/K), ε is the photon energy in eV, $a(\varepsilon, E_F^{CB}, E_F^{VB}, T)$ is the occupation and temperature dependent spectral absorptivity, and I_{PL} is the spectral photoluminescence emission flux in units of $photons/(m^2{\cdot}s{\cdot}eV)$.

The expression of spectral absorptivity with DOS:

$$a(\varepsilon) = \frac{(1-R)(1-\exp(-\alpha d \cdot (f_v - f_b)))}{1 - R\exp(-\alpha d \cdot (f_v - f_b))}$$

PL curve fit -1D

- **Fit Options**



Optional: fit to the measured absorption coefficient to get Eg and Eu (Only available for the methods of GPL + Urbach, GPL + Urbach +DOS)

Urbach energy: the sub-band tail of absorption coefficient can be described by exponential decay:

$$\alpha(E) \propto \exp\left(\frac{E - E_g}{E_u}\right)$$

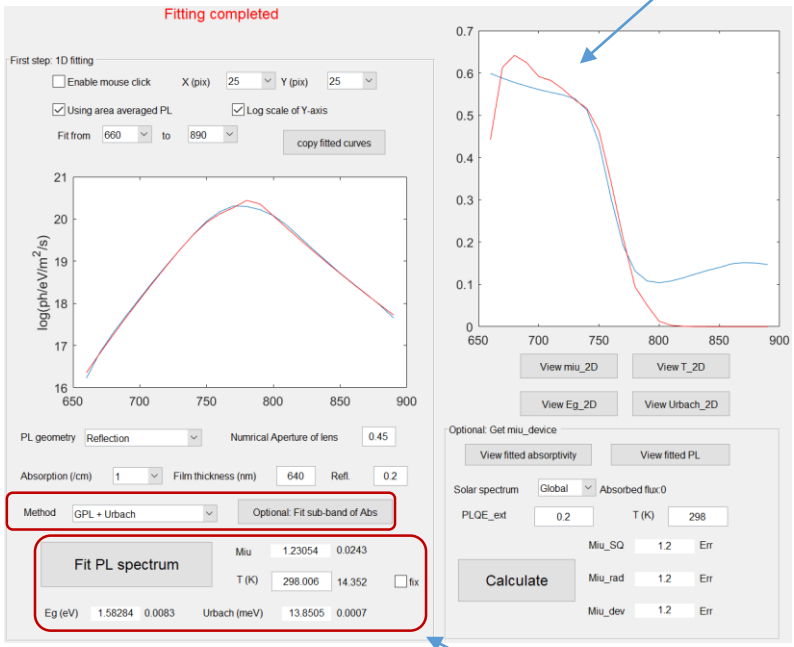
Note: E_g is an effective optical band gap (different from the energy gap)

Fitted result: absorption coefficient shows E_u is ~30 meV

PL curve fit -1D

Blue curve: absorptivity calculated from absorption coefficient
Red curve: absorptivity extracted from the PL spectrum with the help of fitted Miu, T, Eg and Eu

- **Fit Options**



Generalized Planck law + Urbach: works for the full PL spectrum.

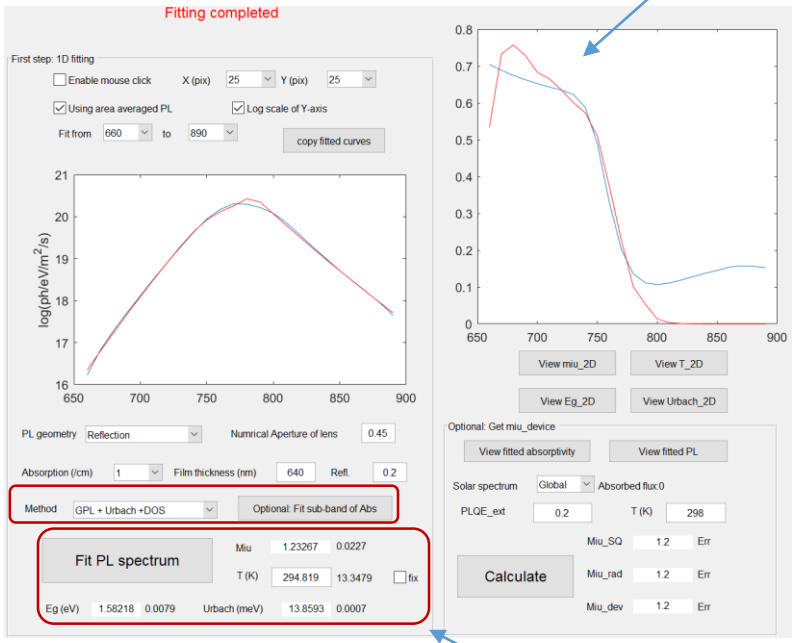
Left branch: fitted by GPL method
Right branch: fitted by Urbach method

Fitted result: PL spectrum shows Eu is ~13.85 meV

PL curve fit -1D

Blue curve: absorptivity calculated from absorption coefficient
Red curve: absorptivity extracted from the PL spectrum with the help of fitted Miu, T, Eg and Eu

- **Fit Options**



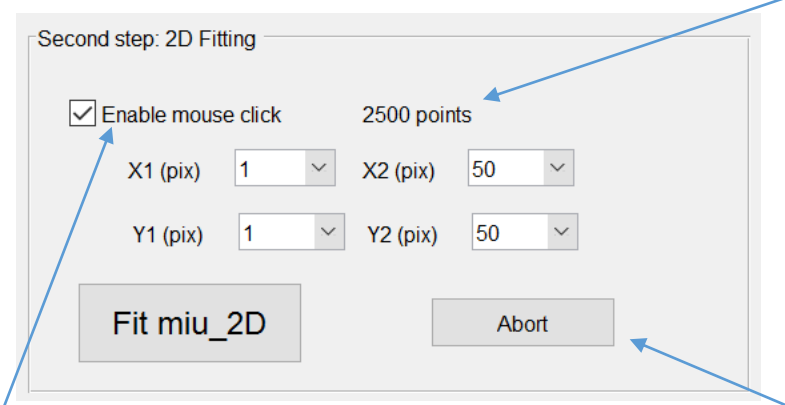
Generalized Planck law + Urbach + DOS: works for the full PL spectrum.

Left branch: fitted by GPL method
Right branch: fitted by Urbach method

Fitted result: PL spectrum shows Eu is ~13.86 meV

PL curve fit -2D

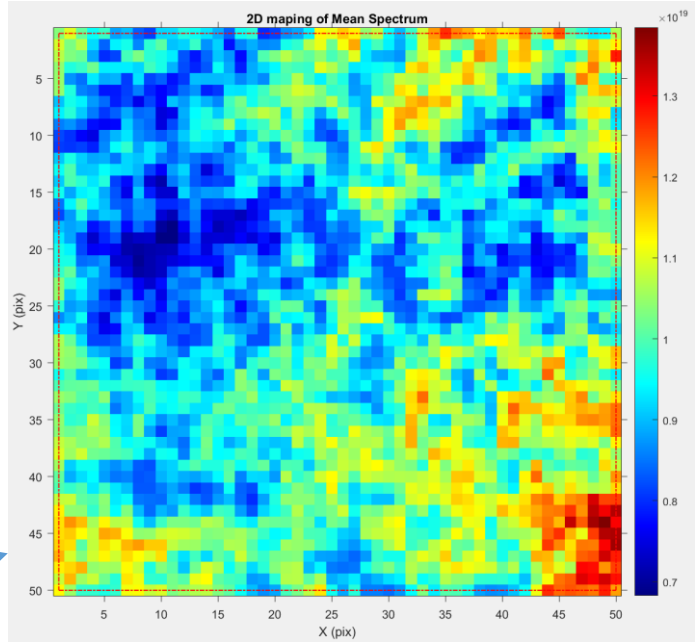
- **Fit Options**



Number of fitting loops

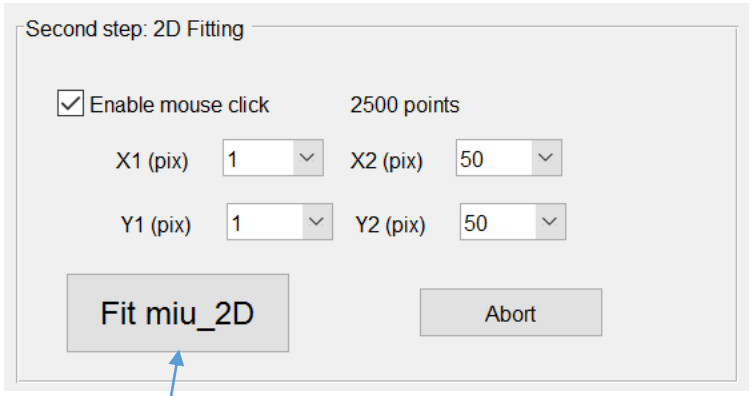
To abort the fitting

Edit fitting area by mouse click
First click: set the top-left point
Second click: set the bottom-right point
The selected area is indicated by the dashed square
(available if mouse click is enabled)



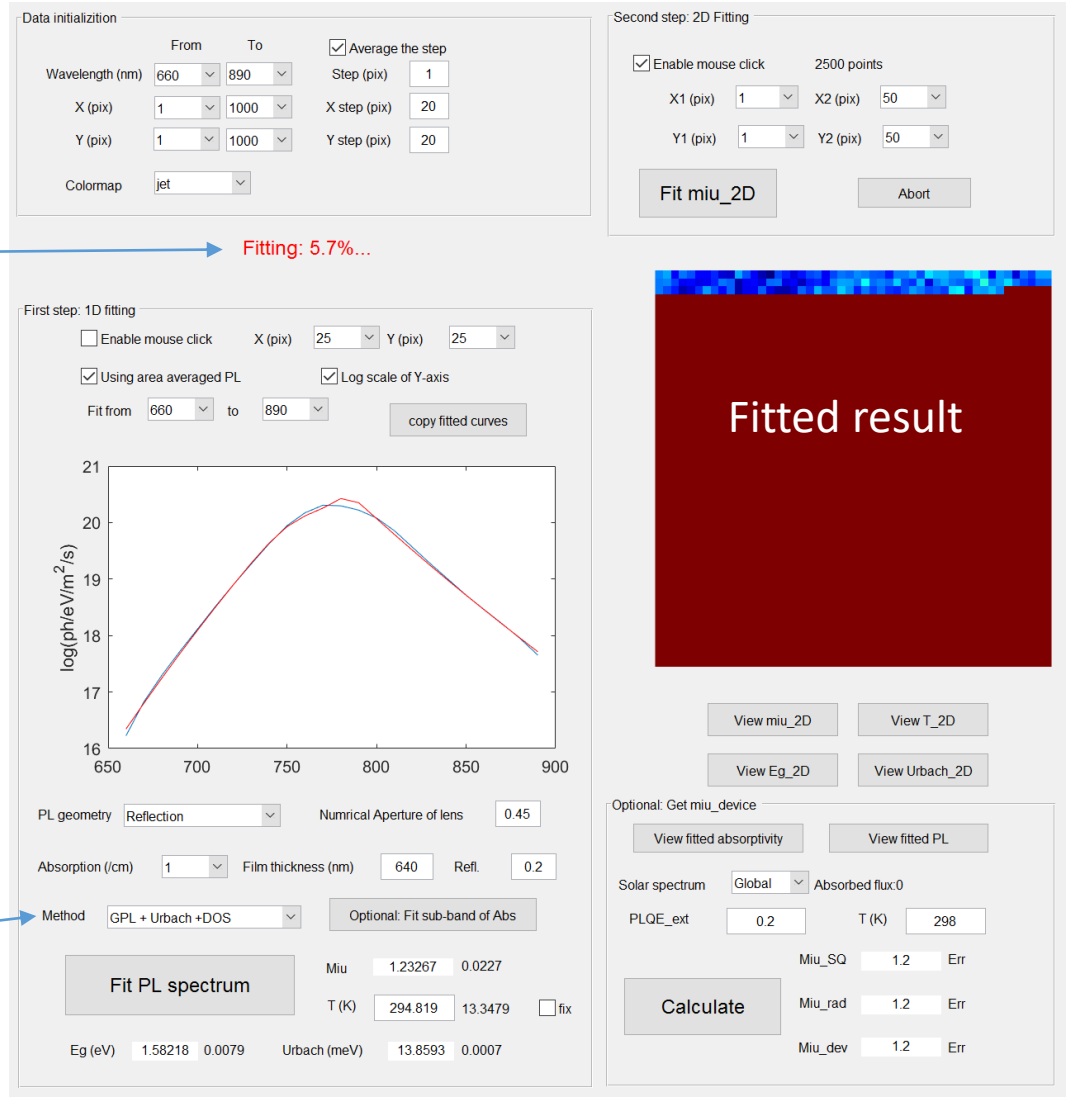
PL curve fit -2D

- **Fit Options**

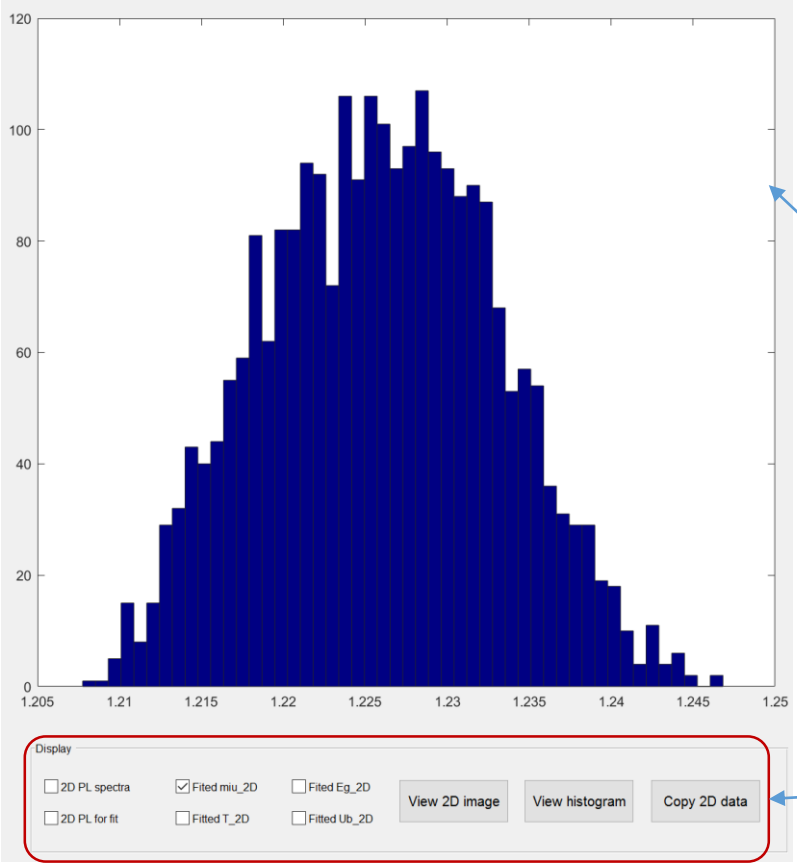


Press this button to start the 2D fit
The fitting method is in line with the 1D fit

Fitting progress

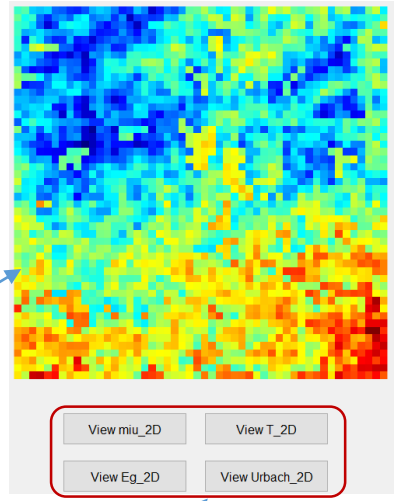


PL curve fit -2D



The fitted result shows miu~1.225±0.015 eV

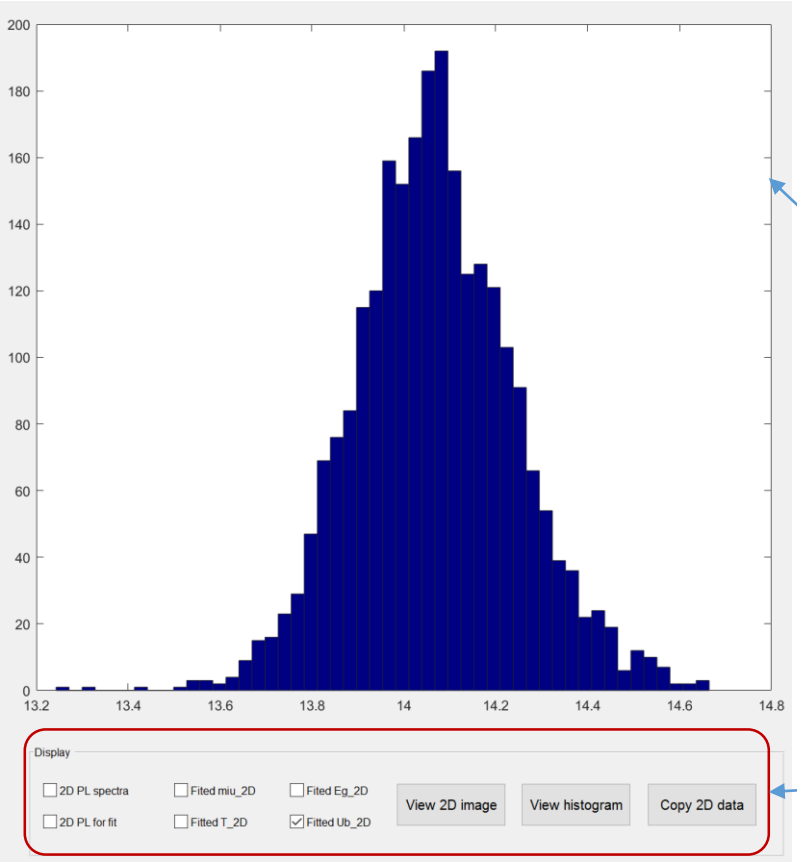
- This result is more accurate than the one got in page 21
- The width of miu is related to film's spatial inhomogeneity



View the fitted result: here miu_2D is displayed

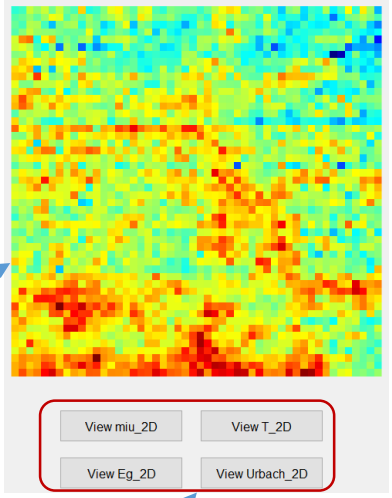
Data manipulation: here miu_2D is selected and displayed in histogram

PL curve fit -2D



The fitted result shows
Eu~14.1±0.3 meV

- This result is more accurate than the one got in page 21
- The width of Eu is related to film's spatial inhomogeneity



View the fitted result: here Eu_2D is displayed

Data manipulation: here Eu_2D is selected and displayed in histogram

PL curve fit -2D

A reference based on the study of 2D PL spectra

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Quantification of spatial inhomogeneity in perovskite solar cells by hyperspectral luminescence imaging†

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QFLS mapping

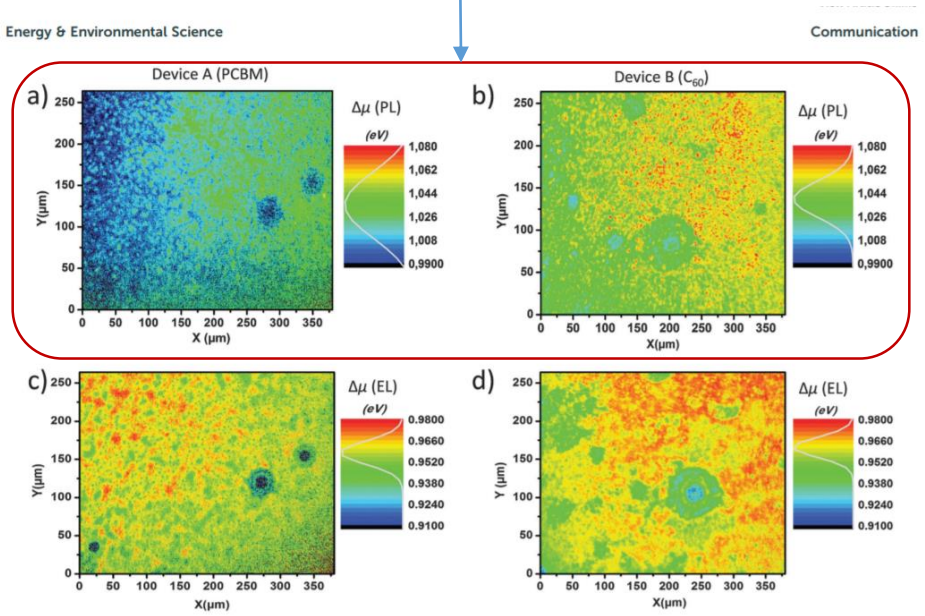
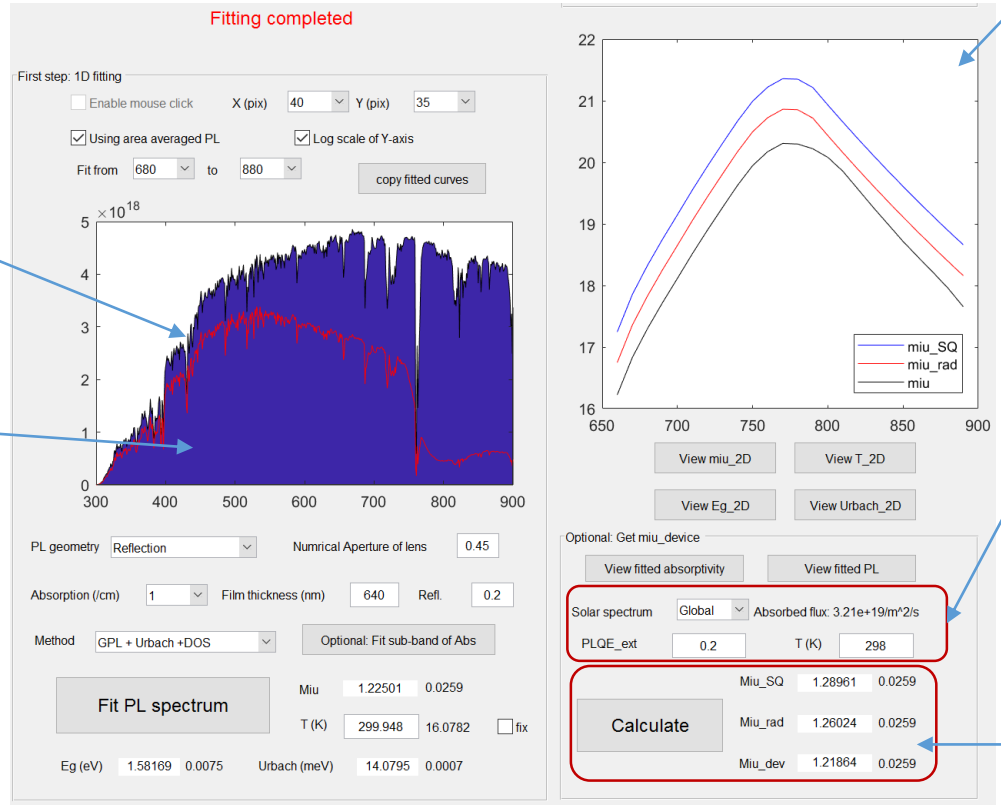


Fig. 3 (a) Absolute mapping of the quasi-Fermi level splitting derived from photoluminescence (a and b, top) and electroluminescence (c and d, bottom), for perovskite solar cells using PCBM (left, device A) or C_{60} (right, device B) as the ETL. The Gaussian distribution of the signal has been overlaid with the color scale as a guide to the eye.

Voc prediction

Red curve: absorbed solar spectrum under AM G1.5

AM G1.5



Simulated PL spectra with different type of QFLS

miu_SQ: PL at Shockley-Queisser limit
miu_rad: PL at radiative limit
miu: measured PL

Parameters for Miu_dev caculation

PLQE is also termed as PLQY

$$\mu_{dev} = \mu_{rad} - k_B T \left|\ln PLQE_{ext}\right|$$

Miu_dev is highly dependent on PLQE and Temperature

Voc prediction

A reference based on QFLS fitting:
Use high external PLQE to explain high Voc

There are amendments to this paper

LETTER

doi:10.1038/nature25989

Maximizing and stabilizing luminescence from halide perovskites with potassium passivation

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ARTICLES

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Hybrid perovskite films approaching the radiative limit with over 90% photoluminescence quantum efficiency

Ian L. Braly[1,4], Dane W. deQuilettes[2,4], Luis M. Pazos-Outón[3], Sven Burke[2], Mark E. Ziffer[2], David S. Ginger[2*] and Hugh W. Hillhouse[1*]

Reducing non-radiative recombination in semiconducting materials is a prerequisite for achieving the highest performance in light-emitting and photovoltaic applications. Here, we characterize both external and internal photoluminescence quantum efficiency and quasi-Fermi-level splitting of surface-treated hybrid perovskite ($CH_3NH_3PbI_3$) thin films. With respect to the material bandgap, these passivated films exhibit the highest quasi-Fermi-level splitting measured to date, reaching 97.1 ± 0.7% of the radiative limit, approaching that of the highest performing GaAs solar cells. We confirm these values with independent measurements of internal photoluminescence quantum efficiency of 91.9 ± 2.7% under 1 Sun illumination intensity, setting a new benchmark for these materials. These results suggest hybrid perovskite solar cells are inherently capable of further increases in power conversion efficiency if surface passivation can be combined with optimized charge carrier selective interfaces.