Predicting and Optimizing Solar Cell Performance with Material/Surface Characteristics

Yiheng Zhu, Allison Perna, Peter Bermel

Abstract—**Solar market share has grown rapidly in recent years. To further improve solar technology in terms of cost and efficiency and promote adoption, researchers often seek material and device level advancements. Photovoltaic simulation tools can be utilized to predict device performance before fabrication and experimentation, streamline research processes, and interpret experimental results. Therefore, we developed ContourPV, which simulates various combinations of values of different device characteristics to optimize and predict photovoltaic performance. ContourPV sweeps the inputted range of values for each chosen device or layer characteristic and obtains performance data by utilizing the drift-diffusion solver, ADEPT. ContourPV plots these metrics in contour plots as output. The parameters that can be swept include Shockley-Read-Hall recombination lifetime, doping concentration, radiative recombination coefficient, and surface recombination velocity for front and rear contacts. Open circuit voltage, short circuit current, fill factor and efficiency are available as output. This tool can provide researchers with intuitive simulation results to predict the performance of a solar cell design, determine material properties based on experimental current-voltage measurements, and help predict performance crossover regions between different device designs. Silicon and GaInP are investigated as example materials in ContourPV: silicon because it is the most common material for commercial solar panels, and GaInP because it is a strong candidate for high-efficiency multijunction solar cells. Furthermore, a wide range of other material systems can be simulated in this tool by users of ADEPT.**

I. INTRODUCTION

Particularly over the last decade, photovoltaic modules have been continually increasing their market share with dramatic reductions in installation cost and improvements in efficiency. This change has been driven partially by new solar cell architectures that have improved the efficiency of solar cell and cause the cost reduction of solar cell. According to IRENA's Renewable Power Generation Costs in 2017, by 2019, the best solar photovoltaics projects will deliver electricity for an LCOE equivalent of USD 0.03/kWh [1], which is extremely competitive with the projected cost of electricity generated by fossil fuels.

Silicon and III-V materials are common solar cell materials. Si single junction solar cells are a widespread, affordable photovoltaic technology, but the best efficiencies of modules may be limited to 26% [2]. Comparing to silicon solar cells, III-V solar cells are thinner and often have direct bandgaps instead of indirect. This improves efficiency by enhancing photon recycling, in which photons are recaptured to produce electron-hole pairs for light-generated current. Compared to perovskite solar cells, III-V solar cells are usually more chemically stable, resulting in longer lifetimes [3,4]. Also, the efficiencies of III-V solar cells can remain high upon scaling to large areas [5]. A key component of high-performance multijunction cells, the rear-heterojunction GaInP single junction solar cell, can achieve 20.8% efficiency on its own, which is not far from theoretical limits for its corresponding bandgap [6].

There are multiple loss mechanisms in solar cells that can reduce their efficiencies [5,7,8]. Major factors include non-radiative recombination, reflection off the surface of devices, incomplete absorption of above-bandgap photons, parasitic absorption, excess heating from below-bandgap photons, internal series resistance, and non-ideal device parameters [9]. Researchers are developing different architectures of devices to reduce recombination and increase solar absorption – two processes that increase device power output.

III-V multijunction solar cells consist of multiple semiconductor materials placed on top of each other with increasing bandgap energy [5]. Many researchers start to combine solar cells with different material into multijunction solar cell. Researchers have combined GaInP and Si solar cells to make GaInP/Si dual-junction tandem cells that have achieved 29.8% efficiency, which is a new record for the class of III-V/Si junction tandem solar cells [3]. If one uses three to six materials, it is possible for III-V multi-junction devices to yield record efficiencies above 44%.

The basic steps to investigate a new type of solar cell device include structure design, performance simulation, fabrication and characterization. Simulations are beneficial to research for several reasons. First, simulation is a cost-efficient method to test the design because simulation tool can provide result fast and users can model many cases. Second, simulations can predict the result without doing physical experiments or if physical experiments are impossible. Simulation tools provide virtual environment which is safe and easy to operate. Also, simulations can provide theoretical result which can be used as reference for further experiments. Many solar cell researchers first simulate their design before fabrication, and then compare the prediction with the measured results.

Many material/surface characteristics can affect the performance of solar cell. In the ContourPV simulation tool, we focus on Shockley-Read-Hall lifetime (from non-radiative recombination), doping concentration, radiative

recombination coefficient, and surface recombination velocity for front and back contacts. Recombination is a process by which high-energy conducting electrons lose energy and recombine with a hole, reducing the number of charge carriers available for electricity conduction [5]. Shockley-Read-Hall recombination is one type of recombination that dominates in silicon-based solar cells [5]. Lifetime is the average time that a carrier can spend in an excited state after electron-hole pair generated and before it recombines [5]. Lifetime strongly influences efficiency; usually solar cells made from material with longer lifetimes will have higher efficiencies, since fewer charges are lost during transport [5]. Doping is a technique to introduce free charge carriers by adding atoms with a different number of valence electrons than the underlying lattice. For instance, when group V atoms are doped by semiconductor materials from group VI, n-type materials are created [5]. Similarly, p-type materials are created when the dopants from group II atoms dope with semiconductor material from group III [5]. Radiative recombination is one type of recombination that is thermodynamically required, and strongest in direct bandgap semiconductors. Surface recombination can be caused by any defects or impurities within or at the surface of the semiconductor and surface recombination velocity describe the rate of the recombination at a surface of semiconductor [5]. Other parameters can also affect the solar cell performance but in ContourPV, we mainly focus on the above factors, which can have huge impact on PV device performance.

Four photovoltaic performance metrics, which can be used to predict the performance of solar cell device, are open circuit voltage, short circuit current, fill factor and solar cell efficiency. The open circuit voltage is the maximum voltage available from a solar cell, when the current is zero, and short circuit current is the current flowing through solar device under illumination when there is no voltage across the device [5]. Fill factor is defined as the ratio between the maximum power from the solar cell to the product of open circuit voltage and short circuit current, as shown in Fig 1 [5]:

$$\text{FF} = \frac{P_{MAX}}{P_T} = \frac{I_{MP} \cdot V_{MP}}{I_{SC} \cdot V_{OC}} \tag{1}$$

Efficiency is defined as the ratio of energy output from the solar cell device to input energy from the sun [5]:

$$\eta = \frac{V_{oc} \cdot I_{SC} \cdot FF}{P_{in}} \tag{2}$$

ContourPV utilizes an existing drift-diffusion solver, ADEPT 2.1, which simulates light current-voltage measurements, among other experiments, to output these photovoltaic performance metrics.
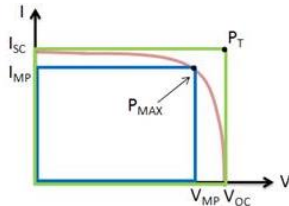

Fig 1. Photovoltaic performance metrics demonstration. Open circuit voltage is the voltage when there is no current and short circuit current is the current when there is no voltage. Fill factor is the ratio between product of Voc times Jsc and the maximum power [10]

ADEPT (A Device Emulation Program and Tool) is a detailed numerical device simulation program developed at Purdue University. Single solar cells, thin-film solar cells and multijunction solar cells can be modeled by ADEPT. ADEPT can provide Voc, Jsc, FF, efficiency numerical results to users. However, if users want to know trend of performance metrics, they have to run ADEPT many times, and replace the values in input file every time. In the backend of ContourPV tool, it will automatically run ADEPT many times using values within specified ranges. ADEPT can provide ContourPV with numerical values of performance metrics and ContourPV plots those values with respect to each device characteristic parameter [11].

ContourPV tool allows users to clearly identify how material/surface characteristics affect the solar cell performance in a single simulation run, which saves users with time comparing to using ADEPT.

II. METHODS

A. Overview of ContourPV tool

Our ContourPV includes a graphical user interface (GUI) developed with, Rappture, which is a toolkit in the nanoHUB workspace that provides basic infrastructure for a large class of scientific applications [12].

ContourPV tool consists of three pages, starting page, parameter page and simulation page. Starting page allows users to choose the proper setting depending on whether they already have the formatted input file. Parameter page allows users to upload input file or fill in information about input file, choose two device characteristic parameters and upload external absorption files. All the simulation results will be displayed in simulation page [13].
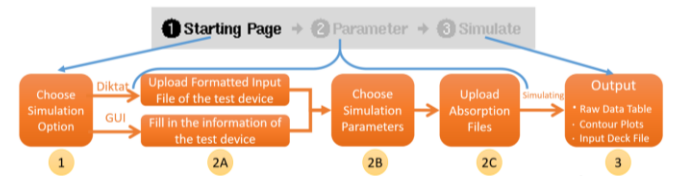

Fig 2. Flowchart of ContourPV tool, which contains three pages and fives states about data input and output

ContourPV GUI has three pages, starting page, parameter page, and simulate page. The starting page allows users to choose either default setting or custom setting based on whether they already have a formatted input file of their devices, and depending on default or custom setting, there will be different settings for input file in the parameter page. In default setting, there is an "Input File" tab, where user can upload input file which is already formatted or chose to run default files which are in the tool. Our default file is for simple c-Si solar cell under illumination. In custom setting, there is a "Layer" tab, where users can input value of each device characteristic parameter for each layer of their device and input some global values and ContourPV will generate a formatted input file in the backend.

B. Input data of device features

ContourPV tool uses the same format input file as ADEPT's. If the user already has a formatted input file,

choose "Upload Input Diktat" and upload the file to the input string text box. If the user does not have a formatted input file but has material properties data of the design, choose the "Use Graphical User Interface" and fill in the data into GUI. For the format of the input file, please refer to ADEPT 2.1 user manual, provided at: https://nanohub.org/resources/adeptnpt/supportingdocs.
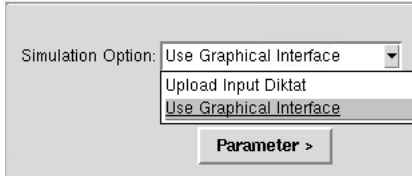

Fig 3. Users have to select one simulation option in starting page.
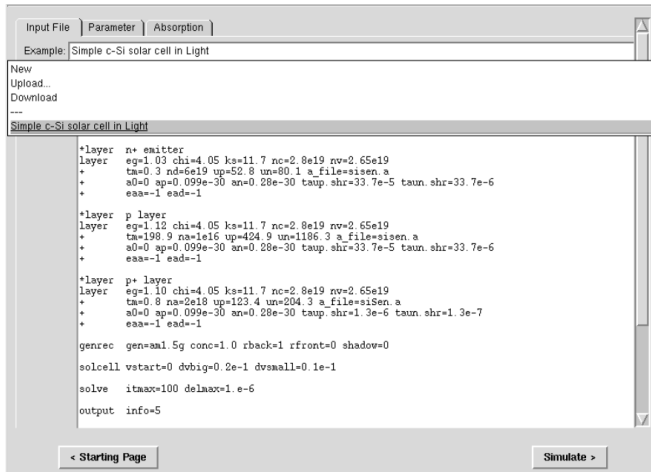
Fig 4. The text box where users can upload input file, choose to run a default example, or download what they input.
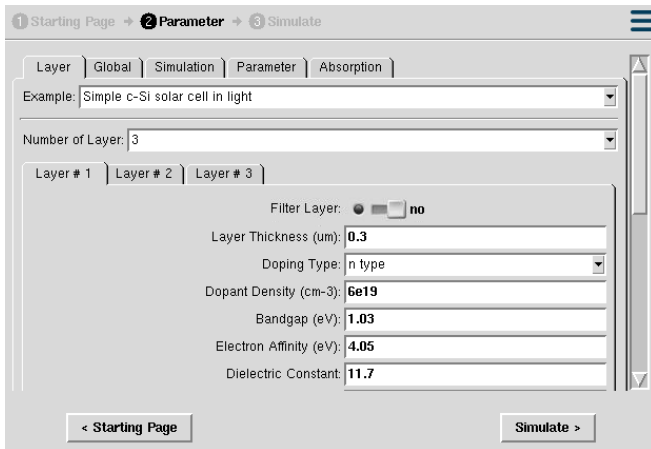

Fig 5. Here, the user provides detailed information about the material properties of each layer.
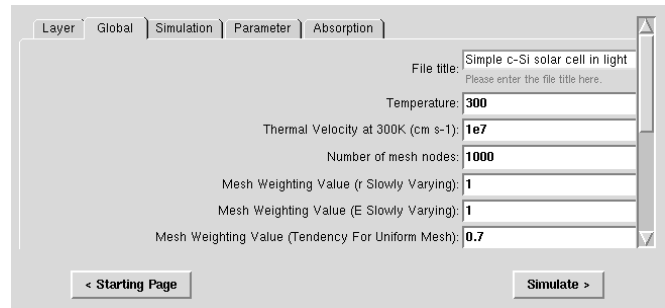

Fig 6. Here, the user provides information about the global device simulation conditions (e.g., operating temperature, grid spacing, etc.).
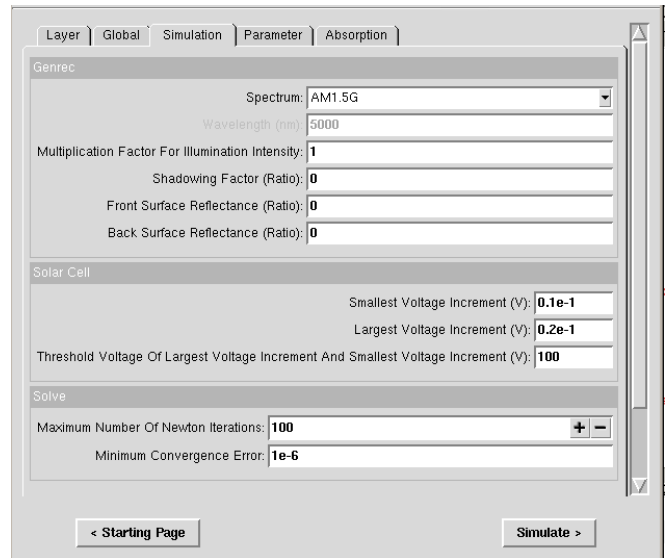

Fig 7. Here, the user provides additional information for running the simulation.

C. Select parameters to sweep

Users can choose two device characteristic parameters to sweep. "Parameter1" will be the parameter on x axis and "Parameter2" will be the parameter on y axis appeared in output contour plots. "SRH Lifetime", "Doping Concentration", "Radiative Recombination Coefficient", "Surface Recombination for Front Contact" and "Surface Recombination for Back Contact" are options for "Parameter Choice" in ContourPV tool. Users can select one option in "Parameter Choice" for each parameter, define a proper range and steps between the range, and choose swept layers. If the layer is chosen to be swept, the value of parameter in that layer will be same as the value in each combination set. If the layer is not chosen to be swept, the value of parameter in that layer will keep the same for simulating all combinations.
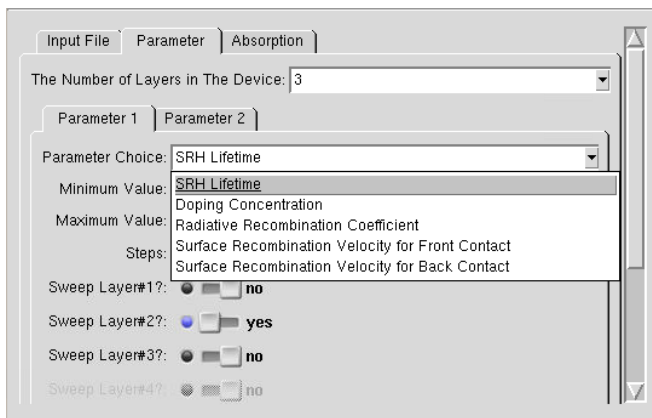
Fig 8. Here, the user selects one material/surface characteristics in "Parameter Choice", defines the range and the number of points generated, and chooses the swept layers.

C. Upload absorption files

If external absorption files are needed, then the user will choose the number of files needed, and upload the absorption files corresponding to the layer (formatted the same as in ADEPT). If the user chooses "Use Graphical User Interface", the external absorption file will follow the order of each layer. If the user chooses "Upload Input Diktat", external file parameters should be included in the input file and the names of absorption files in the input file should be consistent with the absorption files the user uploads. The detailed format of absorption files is provided in the ADEPT user manual, available via:
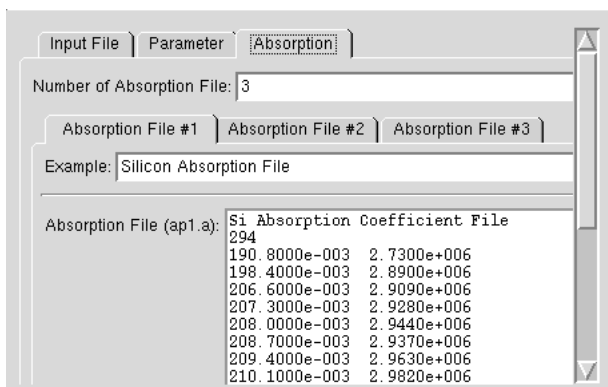https://nanohub.org/resources/adeptnpt/supportingdocs.

Fig 9. Here, the user can upload absorption files if requested in prior input dialog boxes, or use a default option, such as silicon.

D. Backend of ContourPV tool

ContourPV first makes a control file, referred to as a diktat, as template file for sweeping the value. Steps in "Parameter 1" and "Parameter 2" create numbers of combination set. For example, if "Steps" in "Parameter 1" is equal to 3 and "Steps" in "Parameter 2" is equal to 3, there will be 9 combinations. In every iteration, ContourPV runs each combination which is consisted by two values, each of which is from one of two chosen device characteristic parameters. Before simulating each combination set, in the control file, the parameter values of each chosen layer are replaced with values in the combination set, and an input file is generated and will be used as ADEPT input. ADEPT generates a ".sum" file which contains the values of photovoltaic performance. ".sum" file is read to extract the performance metric values and each of these values is saved in an array which stores one type of photovoltaic performance metric. After all the combination has been processed through ADEPT, a raw data table is displayed, and each contour plot is generated according to the values stored in each array.

E. Output

The output of ContourPV includes raw data text file of photovoltaics performance metrics from ADEPT 2.1 and one contour plot for each of PV performance metric. Each contour plot is shown as image and axis are in log scale to provide users with a more intuitive plot. Users can download the image of the plot to their local directory as well as the raw data to generate their own plots as desired.

III. RESULTS & DISCUSSION

Here, we ran our default example input file, "Simple c-Si solar cell in light," which has three layers. In "Parameter 1", "SRH lifetime" is chosen, the range is from 1e-8 to 1e-6 seconds with 10 steps, and all three layers are chosen to be swept. And in "Parameter 2", "Doping Concentration" is chosen, the range is from 1e15 to 1e17 cm^{-3} with 10 steps, and only the top layer is chosen to be swept. Since all three layers are silicon, all the external absorption files are the same silicon absorption file. The output is as follows.

A. Raw Data Table

Raw data table includes all the values plotted in the contour plots. The first two columns are device characteristic parameter values for the parameter on the x- and y-axes. The following four columns are PV performance parameters. Every row shows the input and output values each time ADEPT is called. Users can download the raw data table to generate their own contour plots.

B. Contour Plots

"Parameter 1" is on the x-axis, which is SRH Lifetime and "Parameter 2" is on the y-axis, which is doping concentration. For short circuit current plot, we can conclude SRH lifetime strongly affect short circuit current. For open circuit voltage, when SRH lifetime is short, doping concentration increases open circuit voltage and when SRH lifetime gets longer, the SRH lifetime increases open circuit voltage.
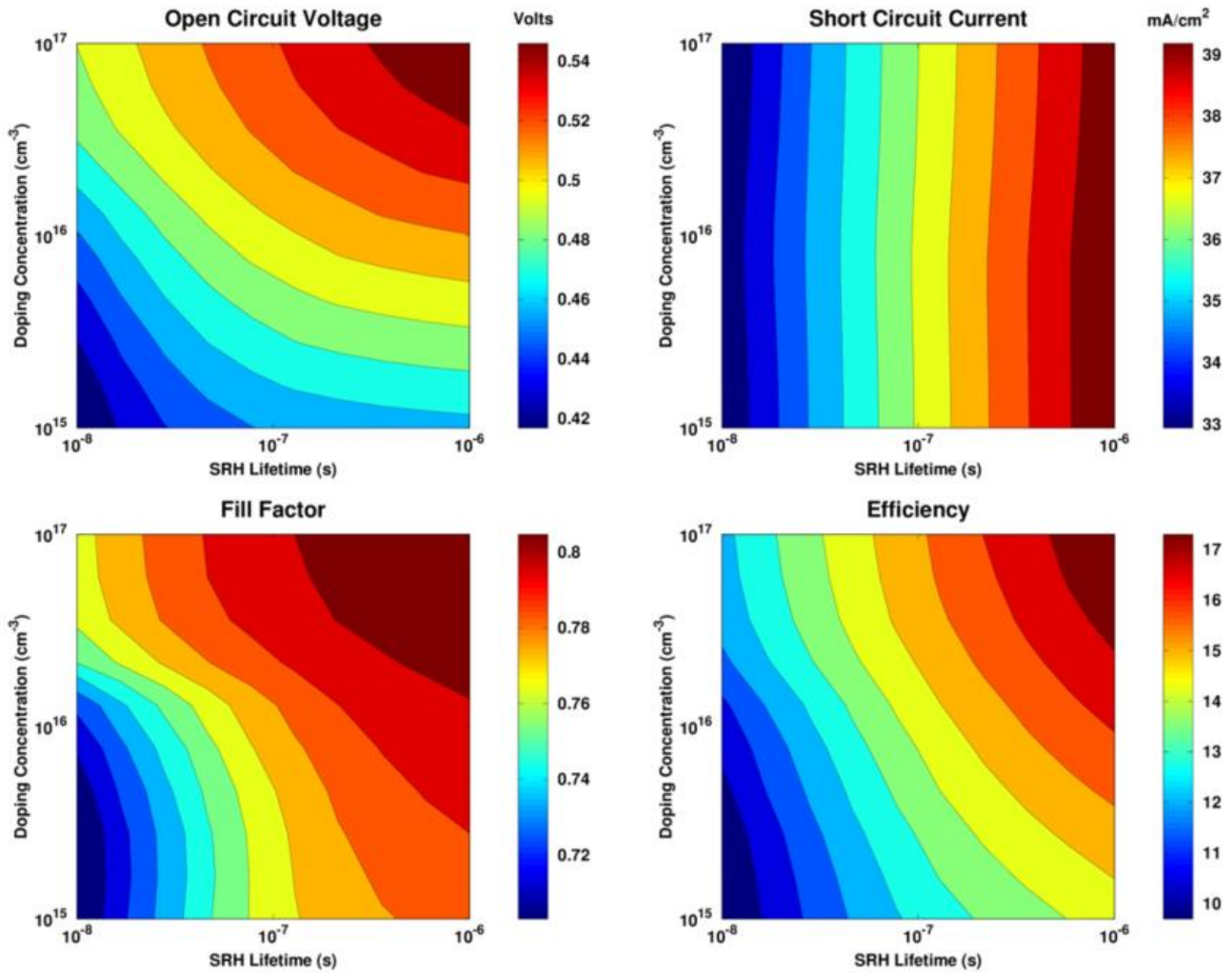
Fig 10. Contour plots output for default silicon example. As expected, the best overall performance is observed for a combination of higher doping and SRH lifetimes, which is driven by a combination of improved open-circuit voltages and enhanced photocurrent collection efficiencies (i.e., a higher short-circuit current).

C. Inputdeck

Inputdeck is an input file for ADEPT or ContourPV tool with placeholders in sweeping variables, to help the user identify them. Users can download this file and replace the placeholders with values to run ADEPT or ContourPV tool. Replacing the placeholders is not required for use with ContourPV.

IV. DISCUSSION

We used ContourPV tool to analyze GaInP for rear heterojunction and front homojunction. We used ContourPV tool to simulate GaInP rear heterojunction and front homojunction separately. In "Parameter 1", "SRH Lifetime" is chosen, the range is from 1e-9 to 1e-5 with 10 steps, and GaInP emitter layer (Layer#2) is chosen to be swept for rear heterojunction and both GaInP layers (Layer#2 and Layer#3) are chosen to be swept for front homojunction. And in "Parameter 2", "Doping Concentration" is chosen, the range is from 1e16 to 1e20 with 10 steps, and GaInP emitter layer is

chosen to be swept for both junctions. The corresponding external absorption files are uploaded.

After we simulated these two solar cells, we calculated the differences of Voc, Jsc, FF and Efficiency and plotted the differences in contour plots.

As can be seen from Fig 11, for rear heterojunction, SRH lifetimes strongly affect Voc, Jsc, and efficiency when SRH lifetimes are below 1e-7. When SRH lifetimes are above 1e-7, doping concentration strongly affect device performance. For front homojunction, SRH lifetimes dominate Voc and efficiencies. When SRH lifetime is below 1e-8, Jsc is strongly affected by SRH lifetime. When SRH lifetime is above 1e-8, Jsc is mostly influenced by doping concentration. Overall, front homojunction solar cell performances better than rear heterojunction solar cell, but for several cases rear heterojunction works better than front homojunction.
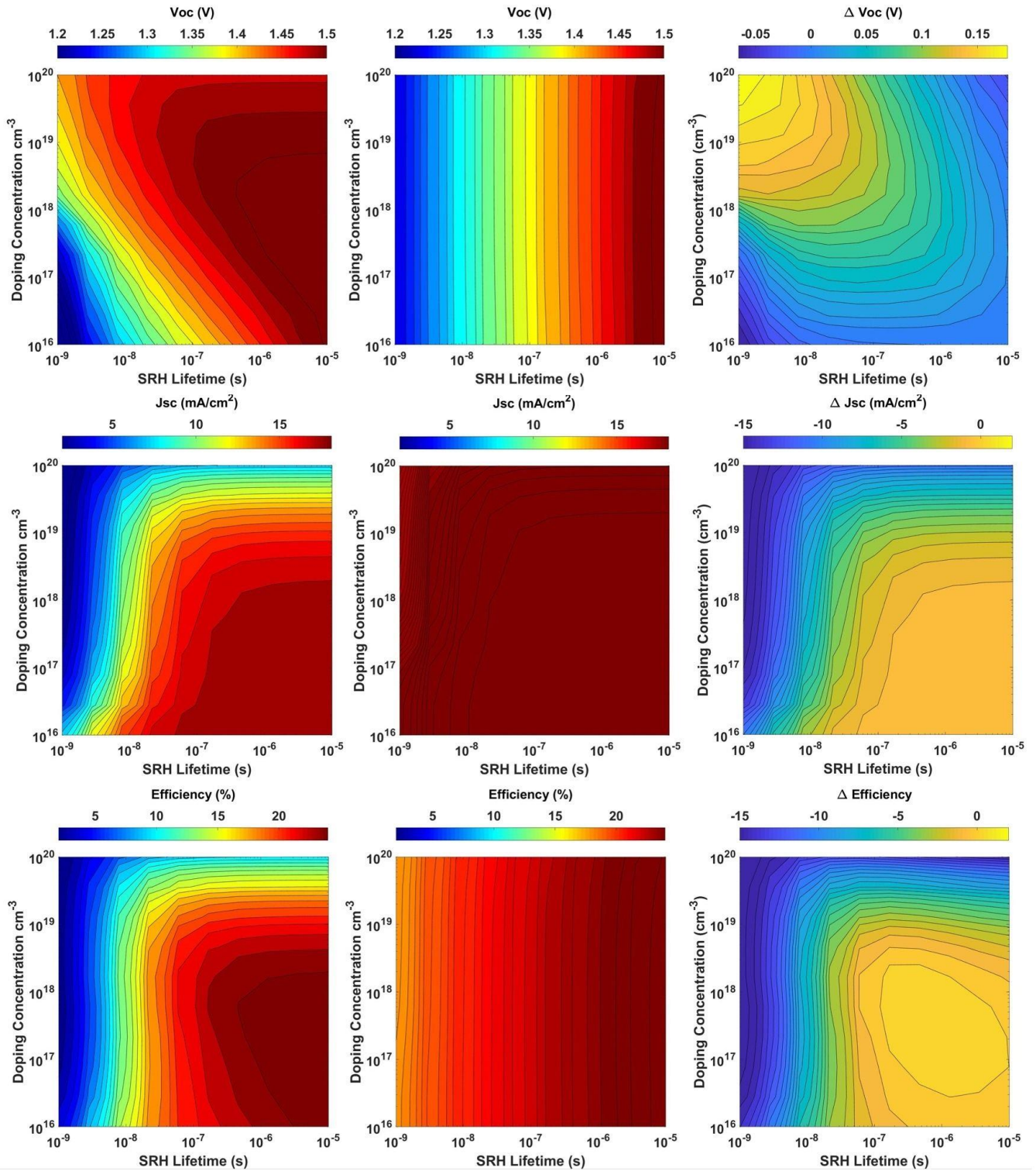
Fig 11. Contour plot of open circuit voltage Voc, short circuit current Jsc, and efficiency with SRH lifetime on x axis and doping concentration on y axis. Contour plots on left columns are for rear heterojunction. Contour plots in the middle columns are for front homojunction. Contour plots on the right columns are for difference (use values of rear minus those of front).

Generally, rear heterojunction has potentially higher built-in voltage than front homojunction and Voc is positively related to built-in voltage, but also requires enough current and band alignment.

Since the junction of rear heterojunction is in the back and free electrons are generated at the front. Electrons require relatively large SRH lifetime to be able to go through the junction before they recombine. If the SRH lifetime is too small, the diffusing length of electrons is shorter than travel distance that they are required to travel in order to be used in circuit and the free electrons recombine before they are used, which is not ideal. Larger SRH lifetime usually maintain better carrier collection and Jsc usually will be larger. If the doping concentration gets too large, since high doping

reduce Jsc because of lower mobility/carrier lifetimes, the Jsc will decrease.

For rear heterojunction, larger SRH lifetime and moderate doping concentration will have higher efficiencies. For front heterojunction, larger SRH lifetimes cause higher efficiencies.

V. CONCLUSION

ContourPV can provide researchers with more intuitive results about how material/surface characteristics affect photovoltaic performance. When we used ContourPV tool to compare rear heterojunction and front homojunction, for most case rear heterojunction performs better when doping concentration is high and SRH lifetime is low and for several cases with large SRH lifetime and moderate doping concentration, rear heterojunction has higher efficiencies than those of front homojunction.

In the future, we plan to add more options for material/surface characteristic parameters and reduce the ContourPV execution time. The ContourPV tool will also be applied to analyze GaInP front and rear heterojunction solar cells, thin-film/stratified (planar) layer-based solar cells (Perovskites, CIGS, CdTe, silicon, III-Vs, etc).

APPENDIX

We are showing the detailed instruction and notes about using ContourPV tool and users can also refer the user guide on tool website https://nanohub.org/resources/contourpv .

1) Starting Page User Instruction

Starting page screen shot is shown in Fig 3 and the instruction for how to choose "Simulation Option" is below.

- Choosing "Upload Input Diktat" or "Use Graphical Interface" depends on whether the user already has an input file which has the same format as ADEPT input file.
- "Upload Input Diktat" is for users who already have ADEPT format input put file.
- "Use Graphical Interface" is for users who only have data about their device.
- After choosing the simulation option, click "Parameter" to go to the next page.

2) Input data about the designed device and simulation condition

Depending on the type of "Simulation Option", users can upload input either using input file or fill in information using user interface.

a) "Uploading Input Diktat" chosen for "Simulation Option" to upload input file

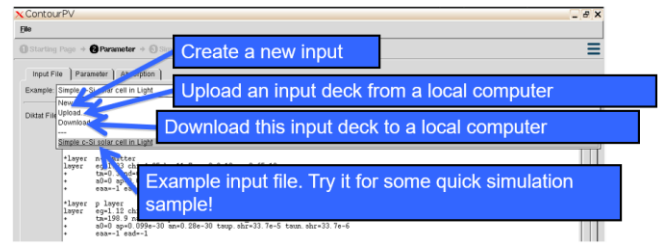Fig 12 shows the instruction of uploading diktat file.

Fig 12. Instructions of uploading diktat file

- Users can edit input file in the text box.
- Copy paste can be done by selecting "Upload" and a window will pop out.
- The format of the input file and variables here and in most subsequent slides is the same as ADEPT 2.1. For further detail, please refer to the ADEPT user guide: https://nanohub.org/resources/adeptnpt/supportingdocs
- After Upload the input file, click "Parameter" tab to fill more information.

b) Use Graphical User Interface to fill in the data about device and simulation conditions

Layer, Global and Simulation tabs are for "Use Graphical Interface" setting, which is the same as ADEPT "Use Graphical Interface" part. Fig 13 -15 shows some details about filling in the information in these three tabs.
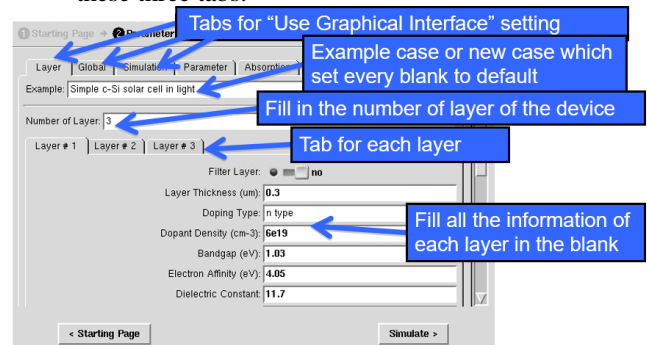

Fig 13. Fill in all the information about device in "Layer" tab

- Layer, Global and Simulation tabs are for "Use Graphical Interface" setting, which is the same as ADEPT "Use Graphical Interface" part.
- The maximum number of layers is 7 and "Layer #1" is the top layer of the device.
- After fill all the information for all the layers, click "Global" tab to fill more information.
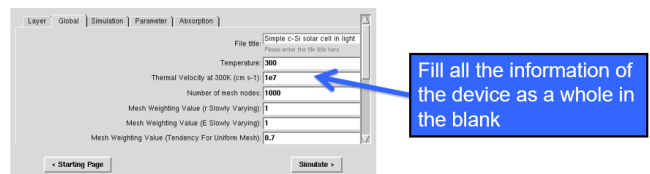

Fig 14. Fill in all the information about simulation condition in "Global" tab

- The Global tab contains the information for device as a whole.

- After filling in all the information in "Global" tab, click "Simulation" tab.
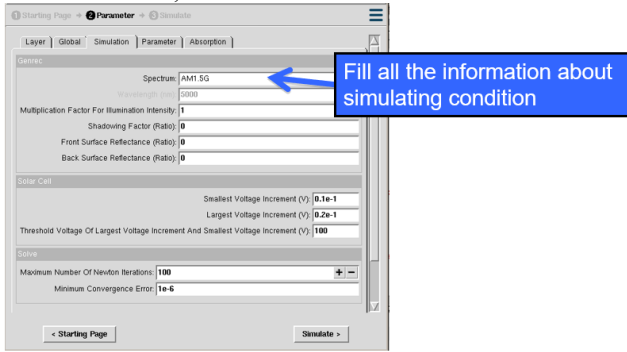

Fig 15. Fill in all the information about simulation parameters in "Simulation" tab.

- Information in Simulation tab is about simulating condition.
- ContourPV tool calculates the light IV for photovoltaic cells.
- After filling all the information in "Simulation" tab, click "Parameter" tab.

3) Select the material/surface characteristics in "Parameter" tab
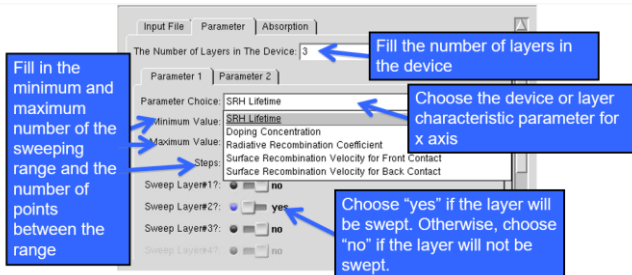

Fig 16. Select material/surface characteristics and related information in "Parameter" tab.

- "Parameter 1" is the parameter will appear on the x axis and "Parameter 2" is the parameter will appear on the y axis.
- If two parameters have the same parameter choice and sweeping layer, x axis in the contour plot will be meaningless.
- The range is the same for all layers which are chosen within one parameter.
- Click "Absorption" tab after filing all the information in "Parameter" tab.

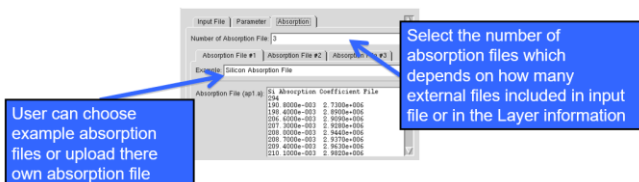4) Upload absorption file in "Absorption" tab

Fig 17. Upload absorption files for corresponding layers of the device in "Absorption" tab

- If no absorption file is needed, the number of absorption file will be 0.
- If "User Graphical Interface" setting is chosen at the starting page, the number of absorption files will be the total number of external files selected in "Layer". The order of absorption files should follow the order of layers which require absorption files.
- If "Upload Diktat" setting is chosen at the starting page, the input file has to have "a_file" variable if external absorption file is needed for the layer. The first absorption file is ap1.a and "a_file=ap1.a" has to be written. 1 means the 1st absorption file. Subsequent absorption files follow the same style and format as the ADEPT tool.
- Click "Simulate" after finishing filling in all the input data.
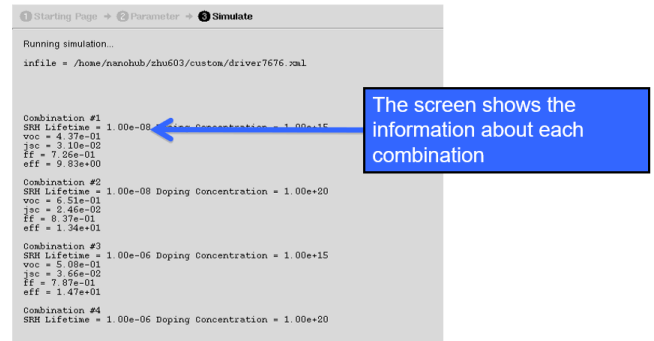
5) Screen during simulating

Fig 18. Screen during simulation process

- If the ADEPT gave an error about the combination of input parameters, the simulation process will stop.
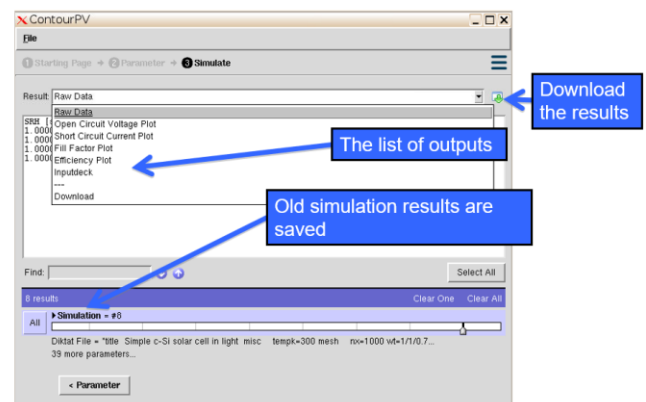
6) Output of ContourPV tool

Fig 19. Output of ContourPV tool

- Users can download the raw data and generate their own format contour plots.
- The inputdeck has a placeholder for the parameter it swept.
- Users can download the inputdeck which can be used as an input file for ADEPT or ContourPV tool

after replacing the placeholders with numbers. Placeholders can refer to Table 1.

Device Characteristic Parameter	Placeholder
SRH Lifetime	$[TAU]
Doping Concentration	$[ND]
Radiative Recombination Coefficient	$[RRC]
Surface Recombination Velocity for Front Contact	$[SRF]
Surface Recombination Velocity for Back Contact	$[SRB]

Table 1. Placeholders and corresponding device characteristic Parameters

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