

- **CASINO Simulation Package**

CASINO Monte Carlo Simulation package can be downloaded from the website below. In the URL, you will be able to gain knowledge on what CASINO simulation is about and how to construct the appropriate model for you device architecture.

<http://www.gel.usherbrooke.ca/casino/What.html>

- **Example of the Input File for CASINO Simulation**

In the package, you will be able to find an example file that can be loaded in CASINO software interface. The example here helps demonstrate how to construct the layering architecture for conventional halide perovskite solar cells, where it has TiO<sub>2</sub> as the ETL and carbon (the majority element of HTL) as the HTL. Using the example file, you will be able to perform CASINO simulation by setting the incident beam energy and CASINO will output the energy distribution profile in three dimensions along the x-, y- and z- axes.

- **Example of the Output File from CASINO Simulation**

An example of the CASINO output file is attached in the package so that user can see what the expected output file format looks like before loading it into the MATLAB app that we develop

- **Utilize the MATLAB App to Process the CASINO Output File**

The *LoadAndPlotCASINO.mlapp* is the MATLAB app built using MATLAB R2018b. The goal of the app is to import the simulated energy distribution from CASINO and plot the energy distribution in MATLAB as well as return a MATLAB workspace variable in .mat format.

Below is the screenshot of the user interface as shown in Figure 1. To start, it has the UI button allows user to select the file that they would like to process using this app. The selected file contains the energy distribution profile exported from CASINO.

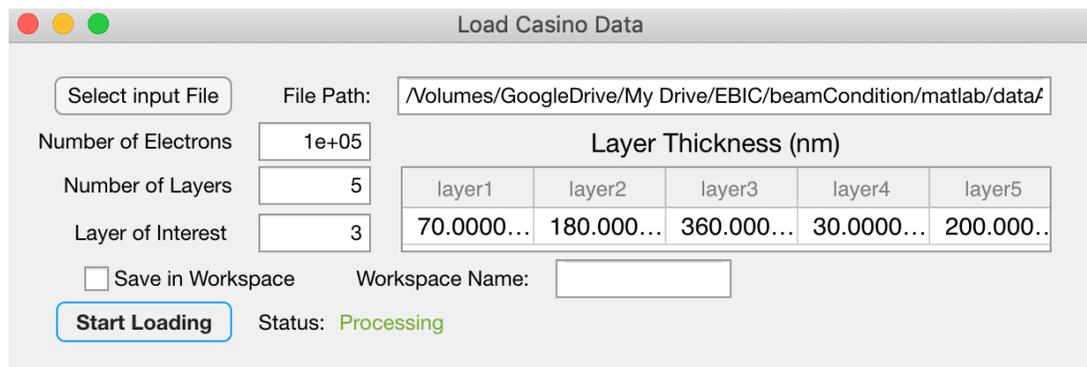


Figure 1. User interface of the LoadAndPlotCASINO.mlapp MATLAB app.

The other required fields are before the app can process the CASINO data:

**Number of Electrons:** number of electrons used in CASINO simulation

**Number of Layers:** total number of layers simulated in CASINO model

**Layer of Interest:** the layer that you will like the app to plot the energy distribution

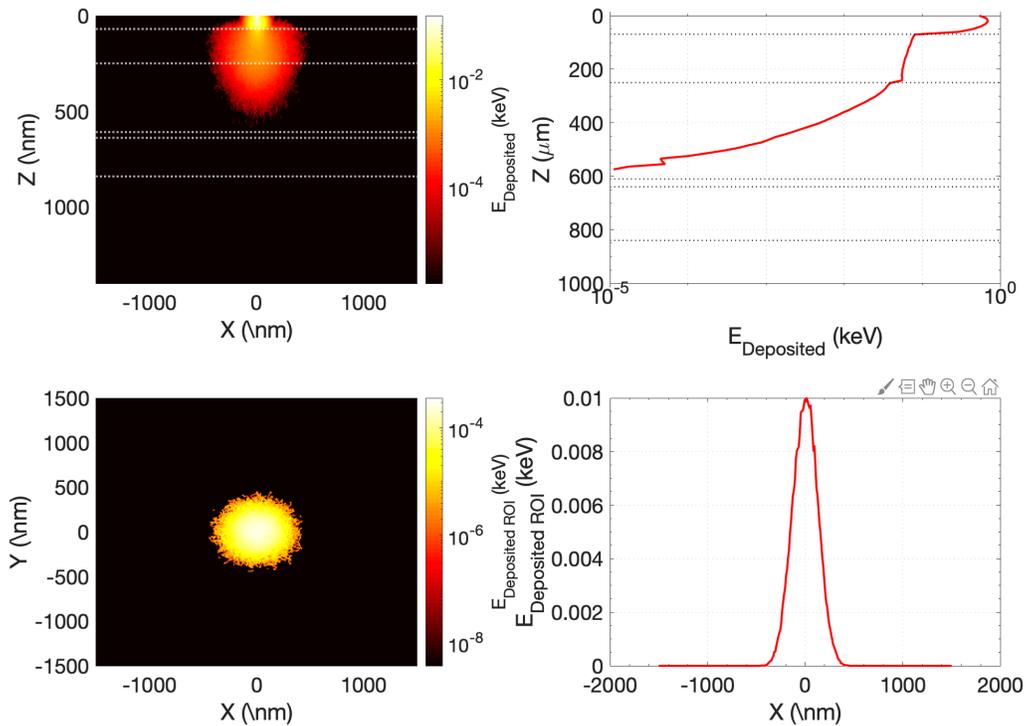
**Layer Thickness (nm):** specify the layer thickness in nanometer

**Save in Workspace:** the app saves the loaded/processed input file by checking this option.

The default saving directory is the same as the input file

**Workspace Name:** specify the file name of the workspace output that you would like to save as. The file will not be able to save if special symbols are used ( . , : ? / ). Also the file name should start with alphabet characters rather than numbers/integers.

Figure 2 displays the plotted energy distribution in the select layer of interest. It outputs four plots. First row shows the energy distribution in the XZ planes along with the energy deposited per incident electron in a cross-section view. Bottom row displays the energy deposition in the XY plane in the layer of interest. The plot in the bottom right can be used to estimate the full width half max (FWHM) of the beam profile in the layer



**Figure 2.** An example of output file from the MATLAB app.