

fcc_analyzer_PyQt5

a GUI to visualize \mathcal{FC} classes output

Javier Cerezo
javier.cerezo@uam.es

VERSION: 0.1
July 7, 2021

1 Description

`fcc_analyzer_PyQt5` is a graphical user interface (GUI) written in python3 and relying on the PyQt5 and matplotlib libraries. It reads the output from \mathcal{FC} classes (for a TI calculation), namely `fort.21/Assignments.dat` (assignments) and either `fort.22/Bin_Spectrum.dat` (spectral histogram) or `fort.18` (final convoluted spectrum), and opens an interactive plot that facilitates the analysis of the transitions, the investigation of different broadening schemes (if `fort.22/Bin_Spectrum.dat` is available) and the comparison with reference spectral data.

2 Installation

2.1 Precompiled binary

System-specific binaries generated with `cx-Freeze` or `pyinstaller` may be available from the author upon request.

2.2 Python script

The source can be run directly as a python script from any computer architecture where a python interpreter is available. The python script is located in `src/`. python version 3 is required along with following modules (the minimum version tested is specified):

- `matplotlib` (version $\geq 1.4.2$)
- `numpy` (version $\geq 1.9.1$)

PyQt binding are also needed, as provided through the module `PyQt5`¹

¹A version relying on PyQt4 is also available but is deprecated and no longer maintained. It requires python 2.7.

- PyQt5 (version $\geq 5.9.2$)

One of the most straightforward methods to get a working python environment is through the [conda](#) package manager, which allows to install and manage different python versions easily. Among the advantages, it can be installed at the user folders/account not requiring admin (or root) privileges and it is available for different operating systems as a simple installer. A very suitable package for conda is miniconda, a light-weight version that can be downloaded from <https://docs.conda.io/en/latest/miniconda.html>.

Once installed, the required modules to run the `fcc_analyzer_PyQt5` script can be installed through the command line (under any of the supported operating systems) by simply typing:

```
conda install pyqt numpy matplotlib python=3
```

The user is referred to the official `conda` documentation for further details.

3 Running the application

3.1 Launch the application

The application should be invoked in the folder where the `fort.21` and either `fort.22` or `fort.18` files that will be analysed reside, using the following syntax from the command line:

```
fcc_analyzer_PyQt5 [flags]
```

If no `fort.21` is found in the current directory, a dialog to set the path to the files will be opened (this is useful when the program is called by mouse-clicking, e.g. in Windows). The following optional flags can be used when called from the command line:

<code>-type (abs emi ecd cpl)</code>	Type of <i>FC classes</i> calculation performed.
<code>-maxC N</code>	Maximum class to be loaded ($N \leq 7$).
<code>-h</code>	Show help.

3.2 Using the application

The GUI consists of the following parts:

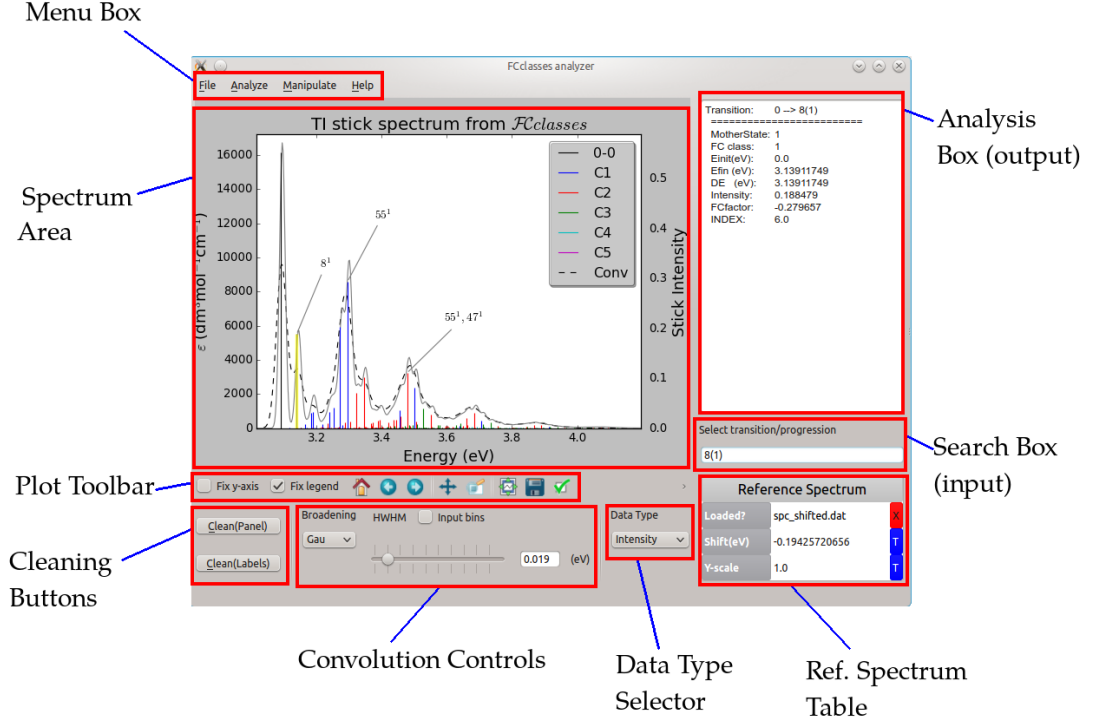


Figure 1: Screenshot of `fcc_analyzer_PyQt5` highlighting the different parts.

The interaction and analysis of the simulated spectrum are performed with the different widgets in the plot. Below, the different parts are described.

3.2.1 Menu Box

- File
 - Save plot: save plot to a png file.
 - Export to xmgrace: export plot data (including labels) to xmgrace file. A export assistant is first raised to select how to organize the plots:
 - * Overlaid graphs: place the stick and spectra in different graphs, that are overlaid, as in the matplotlib plot.
 - * Same graph: include sticks and spectra in the same graph. The spectra are normalized to the maximum stick intensity.
 - Import plot: Load reference spectrum to the Spectrum Area. Units: (eV|cm⁻¹|nm).
 - Quit: exit the application

- Analyse
 - Momenta: compute momenta of the convoluted and write to the Analysis Box.
- Manipulate
 - Shift to simulated: shift reference spectrum (if loaded) to match the convoluted spectrum.
 - Scale to convoluted: scale reference spectrum (if loaded) to match the convoluted spectrum.
- Help
 - Instructions: show a short guide to use the application.
 - About: show general info about the application.

3.2.2 Spectrum Area

This area is interactive. The following actions are possible:

- Right-mouse click on a stick: highlight and get info about the transition (written into Analysis Box).
- Left-mouse click on a stick: add label over the stick
- Right-mouse click on a label: drag the label
- Right-mouse click on a legend line: activate/deactivate plot
- Press “+”/“-” keys to browse back and forward between highlighted stick

3.2.3 Analysis Box

In this box, the information about the highlighted transitions is shown, as well as the analysis of the momenta. This box is not editable, but the info can be copied.

3.2.4 Search Box

Selector of transitions. The general syntax is the following:

```
Mode1'(Quanta1'),Mode2'(Quanta2')... --> Mode1(Quanta1),Mode2(Quanta2)...
```

where `Mode1'(Quanta1')` refer to mode `Mode1'` in the initial state that is excited `Quanta1'` quanta, and `Mode1(Quanta1)` are the equivalent entities for the final state.

The ground vibrational state is represented by a zero (0). When the initial state is in the ground state, the initial part, `0-->` can be omitted. Some examples:

- 8(1),9(2): select the transition from the ground initial state to the final state where mode 8 is excited 1 quantum and mode 9 is excited 2 quanta.
- 0-->8(1),9(2): same as above
- 8(1)-->0: select transition from initial state excited 1 quantum on mode 8 to the final ground state.
- 0-->0: select 0-0 transition

To select a progression in the final state, use P instead of the number of quanta. This keyword can only be used for one mode in the same selection. Some examples:





- 8(p): select progression of mode 8 in the final state.
- 0-->8(p),9(2): select progression of mode 8 in the final state when, simultaneously, mode 9 is excited 2 quanta.
- 1(1)-->8(p): select progression of mode 8 in the final state, starting from the initial state where mode 1 is excited one quantum.

3.2.5 Plot Toolbar

This is formed by two check boxes and the standard matplotlib toolbar with PyQt5 back-end. The check boxes are:

- Fix y-axis: whether or not scale y-axis when the convolution or the data type are updated.
- Fix legend: whether the legend can be displaced with the mouse or not.

The matplotlib toolbar include:

- : zoom into (left mouse click) or out (right mouse click) a rectangle.
- : move the spectrum (left mouse click) or zoom (right mouse click).
- : export image.
- : customize axes properties.

3.2.6 Cleaning Buttons

- Clean(Panel): remove highlight on transitions and clear the analysis box.
- Clean(Labels): clear all labels added to the spectrum

3.2.7 Convolution Controls

These controls are only active if the fort.22 file is available. Note that this is not present for old versions of *FCclasses*.

- Broadening selector [Gau|Lor]: type of broadening function
- HWHM slider and box: set the HWHM of the broadening function. The box is editable and allows a more precise selection of the value, even beyond the slider limits (0.01 to 0.1 eV).
- Input bins check box: use the bins given in the input fort.22 file. Otherwise, a new histogram with only 1000 bins is used (which is faster).

3.2.8 Data Type Selector

Select the type of spectrum: [Intensity|Lineshape].

3.2.9 Ref. Spectrum Table

Information about the reference spectrum (loaded with File->Import plot).

- Loaded?: whether reference spectrum is loaded. If so the file name is shown. The red button with the cross deletes the reference spectrum.
- Shift(eV): shift applied to the reference spectrum (in eV). This box is editable. The value always refer to the originally loaded value, unless the blue T button is pressed, which resets the reference value to the current one.
- Y-scale: scaling applied to the reference spectrum Y-axis. This box is editable. The value always refer to the originally loaded value, unless the blue T button is pressed, which resets the reference value to the current one.