Procedure for Fitting SWCNT Absorption Spectra

0. Save Data

Make sure that all .m files, reference files and absorption data files are stored in the same folder.

1. Load Absorption Data

An absorption measurement should have two header lines and two columns (1 - wavelength, 2 - absorption data), separated by a comma and must be saved as a .txt file.

2. Choose Wavelength Range to be Fitted

The option to specify a region corresponding to either S_{11} or S_{22} is provided later, but these regions must fall within the region specified for the background subtraction.

3. Select a Method of Background Subtraction

4. Load Reference Data

This data table must consist of 5 columns with one header line. The column order is: 1 - string that contains the (n,m) species, 2 - S_{11} position in nm, 3 - S_{22} position in nm, 4 – S_{11} position in eV and 5 – S_{22} position in eV. (n,m) species must be sorted in ascending S_{11} position. An example data set is provided in the file "Reference_Data_Bachilo.txt".

5. Select Type of Nanotube Transitions, Either S_{11} or S_{22}, and Define the Range to be Fitted

6. Choice of FWHM

7. Discard (n,m) Species That Are Not Expected

In this step a photoluminescence contour map can be of assistance.

8. Automatic Detection of Peaks in Measured Data

The code locates maxima in the measurement data; however these peaks do not necessarily correspond to nanotube transitions and could be exciton phonon sidebands. The user is now given the choice to remove these and later assign them to an exciton phonon sideband.

9. Manual Assignment of Peaks in Measured Data

The user is now given the option to add one or more additional peaks by specifying their wavelength value. In this assignment a photoluminescence contour map can be of assistance. At this point the exciton phonon sideband is not assigned.

10. Detected Peaks are Assigned to (n,m) Species and the User is Allowed to Change the Assignment

11. Assignment of Exciton Phonon Sidebands

The user is given the option to assign exciton phonon sidebands to various (n,m) species that were detected in the previous routines.

12. Choice of Line-Shape for the Nanotube Transitions

13. Extension of the Range to be Fitted

In the event that the S_{11} region was chosen the user is given the option to also fit the S_{22} region. If the user decides to also fit the S_{22} region, steps 7-10 are repeated for the S_{22} region.

14. Check the Quality of the Fit

The result of the fit is presented to the user along with the chi-square value of the fit. The user is then given the option to further optimize the fit by changing various fit parameters.

15. Generate Results Table

16. Export Fitting Results to a .txt File

17. Incorporation of Metallic SWCNTs

If the S_{22} region or the full spectrum was fitted, the user has the option to include metallic nanotubes in the S_{22} region. In order to do so, the steps 1-4 need to be repeated and the S_{22} region should be selected. The user is now given the choice to select the folder containing the results from the previous fit and the metallic SWCNT reference file. The user is presented with all metallic nanotubes in the selected range and is now prompted to discard the ones not represented in solution. The fit is performed and the user is given the choice to further optimize the fit by changing various fit parameters. Upon creating a results table, the option is presented to export the fitting results to a .txt file.

18. Film Fitting

The user is asked to select a film absorption measurement, which should have two header lines and two columns (1 - wavelength, 2 - absorption data), separated by a comma and must be saved as a .txt file. Following the background subtraction the folder containing the fit results from a previous solution fit has to be chosen. If the entire spectrum was fitted, the user is given the choice to either fit, S_{11} or S_{22} on their or the entire spectrum. The fit is performed and the user is given the choice to further optimize the fit by changing various fit parameters. Upon creating a results table, the option is presented to export the fitting results to a .txt file.