

Supplementary Materials

Berrada, Meryem^{1*}, McFall, Alan¹, and Chen, Bin¹

¹Hawaii Institute of Geophysics and Planetology, University of Hawaii at Manoa.

2500 Campus Rd, Honolulu, HI 96822

*Corresponding author

Code architecture:

Function outside the RamanAnalysis class

1. **gaussian(x, amp, mean, stddev)**: Represents a Gaussian function with amplitude, mean, and standard deviation parameters.
2. **lorentzian(x, amp, mean, gamma)**: Represents a Lorentzian function with amplitude, mean, and gamma parameters.
3. **voigt(x, amp, mean, stddev, gamma)**: Represents a Voigt profile function with amplitude, mean, standard deviation, and gamma parameters.
4. **pseudo_voigt(x, amp, mean, stddev, fraction)**: Represents a pseudo-Voigt profile function with amplitude, mean, standard deviation, and fraction parameters.

Function inside the Raman Analysis class (denoted with the “self” parameter)

5. **update_search(self, *args)**: Function to update search results based on a search term.
6. **show_results(self, search_term)**: Function to display search results in a listbox.
7. **hide_results(self)**: Function to hide the search results listbox.

8. **plot_selected_data(self):** Function to plot selected data based on the selected filename.
9. **on_select(self, event):** Function to handle the selection of items in the results listbox.
10. **enforce_minimum_size(self, event):** Function to enforce a minimum window size when resized.
11. **create_GUI(self):** Function to create the graphical user interface (GUI).
12. **toggle_axis_sync(self):** Method to toggle axis synchronization in the manual tab.
13. **toggle_axis_syncAuto(self):** Method to toggle axis synchronization in the auto tab.
14. **toggle_axis_sync(self):** This method toggles axis synchronization in the manual tab. It connects/disconnects the on_axis_change method to the xlim_changed event of ax4 based on whether synchronization is enabled or disabled.
15. **on_axis_change(self, event_ax):** This method updates the x-axis limits of ax5 when synchronization is enabled in the manual tab.
16. **toggle_axis_syncAuto(self):** This method toggles axis synchronization in the auto tab. It connects/disconnects the on_axis_changeAuto method to the xlim_changed event of ax1 based on whether synchronization is enabled or disabled.
17. **on_axis_changeAuto(self, event_ax):** This method updates the x-axis limits of ax2 when synchronization is enabled in the auto tab.
18. **database_tab_display(self):** This method displays text and instructions in the "Instructions" tab of the GUI, providing an overview of how to use the software.
19. **on_frame_configure(self, event):** This method adjusts the canvas size when the frame is configured.
20. **on_canvas_configure(self, event):** This method adjusts the canvas size based on the content of the table when the canvas is configured.

21. **save_table(self)**: This method retrieves data from the table and saves it to a file.
22. **fit_selected_model(self, event=None)**: This method fits a selected model (e.g., Gaussian, Lorentzian, Voigt, Pseudo-Voigt) to the loaded Raman spectrum, plots the fitted peak, and inserts the fitted parameters into the table.
23. **update_initial_amp(self, *args)**: Updates the initial amplitude guess based on user input.
24. **update_initial_mean(self, *args)**: Updates the initial mean guess based on user input.
25. **update_initial_stddev(self, *args)**: Updates the initial standard deviation guess based on user input.
26. **update_initial_gamma(self, *args)**: Updates the initial gamma guess based on user input.
27. **update_initial_fraction(self, *args)**: Updates the initial fraction guess based on user input.
28. **next_peak(self)**: Switches to the next peak in the dataset and updates entry fields for peak fitting.
29. **update_entry_fields(self)**: Updates entry fields with peak-specific values.
30. **update_arpls_parameters(self, event)**: Updates parameters for the arpls background subtraction method.
31. **arpls(self, y)**: Performs asymmetrically reweighted penalized least squares (arpls) background subtraction in the manual tab.
32. **update_arpls_parametersT3(self, event)**: Updates parameters for the arpls background subtraction method in a different context in the auto tab.
33. **arplsT3(self, y)**: Performs arpls background subtraction in the auto tab.

34. **subtract_backgroundFigure4(self)**: Toggles background subtraction for the loaded Raman spectrum in ax4.
35. **subtract_backgroundFigure1(self)**: Toggles background subtraction for the loaded Raman spectrum in ax1.
36. **load_file_t3(self)**: Loads a Raman data file for processing in the auto tab.
37. **load_file(self)**: Loads a Raman data file for processing in the manual tab.
38. **remove_selected_peaks(self)**: Removes selected peaks from the loaded Raman spectrum based on user input.
39. **undo_remove_peaks(self)**: Undoes the removal of previously removed peaks, restoring them to the loaded Raman spectrum.
40. **remove_selected_peaksT3(self)**: Removes selected peaks from the loaded Raman spectrum based on user input.
41. **undo_remove_peaksT3(self)**: Undoes the removal of previously removed peaks, restoring them to the loaded Raman spectrum.
42. **on_zoom(self, event)**: Allows for some labels to overlap the graph boundary because the rule is to hide when the peak is hidden. It handles zooming events in the graph.
43. **handle_prominence_entryT3(self, event)**: Handles the input of peak prominence threshold and updates the graph based on the specified threshold. It also updates the displayed value and clears the text field.
44. **auto_config_display(self)**: Sets up the GUI components for configuring and displaying Raman spectroscopy data.
45. **handle_prominence_entryT2(self, event)**: Handles the input of peak prominence threshold for a different graph and updates the graph accordingly.

46. **start_matching(self)**: Initiates the process of finding matches for peaks and displays the results.
47. **check_cancel(self)**: Checks if the matching process should be canceled and performs cleanup if necessary.
48. **handle_match_button(self)**: Handles the matching process by searching for mineral matches based on specified conditions and displays the results.
49. **populate_figure1(self)**: Populates the first subplot of a figure with Raman spectrum data, peaks, labels, and saves the figure.
50. **populate_figure2(self)**: Populates the second subplot of a figure with top matching files for each peak, allowing toggling visibility, and saves the figure.
51. **toggle_visibility(self, index)**: Toggles the visibility of a specific file line in the second subplot of the figure.
52. **populate_figure3(self)**: Populates the third subplot of a figure with bar charts showing mineral names and percentages for each peak.
53. **cancel_button_click(self)**: Cancels the ongoing search process and updates the interface accordingly.
54. **update_search(self, *args)**: Updates the search results based on the entered search term.