What is new in UNIFIT 2025?

Main focus of the advancement to the **UNIFIT 2025** was the rework, new design and optimization of the calculation of the transmission function. The pop-up and pull-down commands were improved. The windows-selection and the quantification menus were redesigned. The functions of the menus 'Plot Intensity Axis' and 'Plot Energy/Wavenumber Axis' were improved.

i) The special function 'Calibration Intensity Scale' was completely reworked and redesigned. A new iteration method was implemented. Former pull-down commands were redesigned. The following items were changed:

a) The pull-down menu of the three methods of the T(E) estimation were clearly separated (see Fig.1):

- Survey Spectra Approach (SSA)
- Quantified Peak-Area Approach (QPA)
- Approach Transmission Function *T*(*E*)



Fig. 1 Screen shot: Pull-down menu of the operation 'Calibration Intensity Scale'



Fig. 2 Screen shot of the start display of an approach of the Cu survey excited with Al twin, shown: $T(E) \cdot S_{cu}(E)$ (red), $M_{Cu}(E)$ (black) and the T(E)-input dialogue with the eight start parameters, iteration conditions

b) The operation dialogs of all methods were redesigned. The currently used method is displayed in the dialog title (see Fig. 2).

c) The normalization option was reworked (see Fig 2). If all parameters are fixed, then the normalization will be activated.

d) The iteration error and the estimation time were displayed.

e) The implemented iteration method 'Step by Step' of the QPA method was optimized. The calculation time was strongly reduced (see Fig 3). The reworked 'Step by Step' method is about 20 times faster with respect to UNIFIT 2024.



Fig. 3 Screen shots: left: presentation of the result of the 'Step by Step' method using UNIFIT 2024 and UNIFIT 2025

f) A new iteration method of the QPA method were developed and integrated. Now, the iteration method **'Step by Step'** and **'Randomize'** are offered (see Fig 4).

ii) The dialogues 'Plot Energy/Wavenumber Axis' and 'Plot Intensity Axis' were refreshed. New options were implemented (see Fig. 5).

iii) The dialogue 'Select Windows' was refreshed. New options were implemented.

iv) The dialogue 'Quantification' was refreshed. New options were implemented.

v) The design option 'Dark Mode' was implemented. All dialogues can be displayed in the 'Light Mode' or 'Dark Mode' (see Fig 6).

vi) Now, the appearance of the '**Reduction Lines**' is variable. The colour, thickness and line shape can be defined.



Fig. 4 Screen shots: left: Result presentation of the 'Randomize' method UNIFIT 2025

	Plot Energy/Wavenumber Axis
R(E)	Binding Energy / eV
from: 3500 to: 4800 Number of Increments: 5 Size of Increments: 260 Scaling for All Windows Fixed Decimal Places (max 4): 0 Decimal Places fix Zero Line	from:413to:392Number of Increments:6Size of Increments:3.5Fixed Decimal Places (max 4):0Decimal Places fix0Non-equidistant ScalingPlot Energy - Parameter Area
All None	 ☑ Labelling of Scale Lines □ Grid Lines
 ☑ Show Residual Plot Energy - Intensity Area ☑ Labelling of Scale Lines □ Grid Lines 	 Setting: All Std. Windows Save as Preferences XPS
□ Setting: All Std. Windows □ Save as Preferences I(E)	● Ebin/eV ○ Ekin/eV
○ Counts	Number of Points x2
Original Preview OK Cancel -DS DS+	Original Preview OK Cancel -DS DS+

Fig. 5 Dialogues 'Plot Intensity Axis' and 'Plot Energy/Wavenumber Axis'



Fig. 6 Dialogue 'Axes/Lines/Text', left: Dark mode, right: Light mode

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