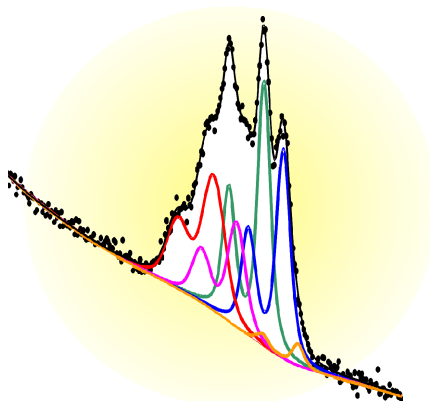


# unifit FOR WINDOWS



## Spectrum Processing, Analysis and Presentation Software for Photoelectron Spectra

### General Characteristics:

- Curve fitting algorithm of Marquardt
- Selection of product, sum or convolution of Gaussian and Lorentzian functions
- Background simulation by different models
- Calculation of inelastic electron scattering cross sections
- Valence-band edge and Fermi energy calculation
- Batch processing for treatment of parameter-dependent series
- Calibration of the transmission function and intensity scales
- Quantification using cross section and sensitivity factor data bases
- Data bases of binding energies, doublet data, Auger parameters
- 32-bit and 64-bit MS Windows based program
- Simultaneous display and handling of up to 300 windows
- Individual preferences (language, export format, curve fitting, graph display and design, printing, etc.)
- I/O routines on user demand
- Extensive graphical design tools
- Fit parameter and 3D plots including quantification results
- Comfortable data export from all windows presentations
- High resolution export (1200 dpi) for all window presentations, the quantification table and fit-parameter table
- Copy – Paste function for transferring processing results to other generally used softwares (Word<sup>®</sup>, Excel<sup>®</sup>, Origin<sup>®</sup>)
- Saving and loading of projects

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## UNIFIT - an Universal Program for XPS Peak Fitting, Analysis and Presentation Based on WINDOWS

An adequate modelling of experimental photoelectron spectra containing several different components has remained a challenge all the time, regardless of the achieved level for energy resolution and sensitivity of spectrometers. The higher the resolution, the more detailed information can be gained on binding energies and intensities of components with decreasing energetic distance. In order to obtain the desired information from photoelectron spectra in the past several computer codes have been developed that base on the description of experimental data by synthesis of theoretical model functions.

The typical advantages of commercially available software are comfortable handling and extensive graphical design options. However, they often exhibit severe restrictions in data modelling. Furthermore, user-developed programme codes are very often tailor-made for single spectrometers and special applications. In many cases they have been written for use by insiders only.

In order to fill this gap, a programme for peak shape analysis of core level photoelectron spectra has been developed, tested and used intensively by the author's group for years. The result is UNIFIT FOR WINDOWS, which involves appropriate description of the spectra by adequate models, excellent numerical performance for fast calculations, convenient data handling, and versatile opportunities for data transfer and representation.

UNIFIT has been designed to accept experimental data of several different formats. Simultaneous handling of up to 300 windows is possible.

**Individual preferences** can be selected for the mathematical background of the model function (product, sum or convolution of Lorentzian and Gaussian functions), fit parameters (absolute or relative), language (German or English), text style of dialogs and exported tables, details of presentation (line colours, line form, thickness of lines, text style of annotation) on the desktop as well as for printing. There are two methods for the error analysis of the calculated fitting results. In a special menu the parameters of the excitation satellites for MgK $\alpha$  and AlK $\alpha$  can be edited and saved in up to five sets of data.

**An extended input routine** allows the direct reading of measurement data of different kinds. The fast transfer of the data achieved in the spectra analysis to the standard spreadsheet software (i.e. Excel<sup>®</sup>, Origin<sup>®</sup>) is given by an export routine. All processing steps of all opened windows as well as the quantification table may be stored in one project. The original measurement data are saved in a separate directory. Auger parameters can easily be presented as Wagner plot.

**The active window presentation can be copied or exported** as an image with different resolutions (400 dpi, 600 dpi, 800 dpi, 1200 dpi) and formats (tiff, gif, emf, jpg, bmp, etc.) The output to a printer is made in a way that all important information are clearly shown. The provided test spectra give the user the possibility to test the different functions of the programme without measured data.

For the spectra modification menu there are options for charge correction of the active window, several procedures for the background calculation, satellite subtraction, smoothing, differentiation, and spike correction as well as the chance for spectra manipulation and operation. Additionally, a normalisation routine with four different methods is available.

**The peak fit is based on the non-linear least squares curve-fitting algorithm of Marquardt.** The programme allows choosing product, sum or convolution of Gaussian and Lorentzian functions for the calculation of the model function. All peak parameters may be varied freely, varied within a chosen interval or fixed at certain values. Moreover, parameters may be determined on absolute scales or they may be treated as relative parameters i.e. related to the leading peak of a doublet or to the first out of a group of peaks. Different options are available, enabling the user to keep, e.g. energy distances, peak widths or relative intensities of peaks constant during iteration. Furthermore, it is possible to include the background parameters in the fit routine. Besides this inclusion in the minimization procedure, the background can be simulated by five different methods (or combinations of them) and subtracted from the experimental curve before initiating the peak fit. The fit-parameter table can be saved, copied or exported. Two separate subprogrammes permit the estimation of valence-band edges or Fermi edges.

**The error of the fit parameters** can be calculated. The curve-fit results can be printed including fit, acquisition parameters, and additional comments, or exported for further treatment and presentation.

**A batch-processing submenu** was supplemented for fast analysis of parameter-dependent series of spectra (e.g. depth profiles, angle dependent measurements). All options for spectra modification and the peak fit can be included in batch processing. Six different presentations of the parameter-dependent measurement are available. Additionally, the estimated fit parameters can be plotted with respect to the window numbers, batch parameters or a freely chosen values.

**The quantitative analysis** is possible from survey or single spectra using cross sections as given by Scofield, empirical sensitivity factors by Wagner or defined individually by the user. The quantification table may be copied or exported as an image (600 dpi). A parameter-plot function allows the presentations of the peak areas or atom percentages with respect to the window numbers, batch parameters or manual chosen values. Remarks and comments may be included in the spectrum presentation. **The integrated data bases** of photoelectron lines and Auger parameters can be used for peak identification, labelling and chemical-state plot (Wagner plot) respectively. A project comment can be used for specifying the individual treatment of the sample. The data banks integrated in UNIFIT can be shown, edited and extended directly with special subprogrammes.

**The subroutine "Annotation/Design"** gives the user the manual controlling of the scaling and labelling of the energy, intensity, and parameter axis. The energy axis in every window is drawn with increasing kinetic energy (or decreasing binding energy) from the left to the right and significant information for the user in the title bar. Additionally, the spectrum may be entitled and labelled. Optionally a grid for all axes can be plotted. For standard spectra and parameter plots a legend for specifying the plotted curves can be shown.

**The menu "Calibrate Intensity Scale"** allows the determination of the transmission function of the spectrometer in two different ways. The calculated functions can be shown, saved and used for quantification.