



## Title

The New Software UNIFIT 2024 for Universal XPS/AES/XAS/RAMAN Spectrum Processing, Peak Fit, Quantitative Surface Analysis and Presentation of the Results

## Appointment

By Arrangement

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## Organizer and Chairman

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## Group of participants and aim of the course

The crash course is offered to users of X-ray photoelectron spectroscopy (XPS), Auger electron spectra (AES) and X-ray absorption spectroscopy (XAS) (analysts, chemists, physicists, and engineers) from research facilities and industry, who deal with the quantitative analysis and the chemical state of solid state surfaces and thin layers. The course participants are instructed in the spectrum treatment and analysis programme UNIFIT 2024 and in particular to the peak fit of XPS, AES and XAS spectra. Amongst other topics, the usage of data banks for the qualitative, quantitative and chemical analysis of XPS and AES spectra and a practical calculation of the uncertainties of the fit parameters are demonstrated.

The batch processing (e.g. as 3D presentations) of fit results of line scans and multipoint measurements gives detailed information about the homogeneity of chemical composition of analyzed sample surface.

An appropriate model for the XPS data fit of inhomogeneous samples is introduced and discussed. Test spectra and real XPS measurements are fitted with the new peak-fit routine. Examples of the peak fit of RAMAN spectra are demonstrated.

The course syllabus is also suitable for user of older versions of the programme UNIFIT. Additionally, improvements and new features of the version UNIFIT 2024 are demonstrated.

## Meeting Place

Faculty of Chemistry and Mineralogy of the University of Leipzig, Wilhelm-Ostwald-Institute, Linnéstr. 02, 04103 Leipzig

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## Outline

09.00 – 16.30

### Structure and Handling of the Software UNIFIT 2024

- Import of measurement data and export of processing data as well as processed graphics
- Spectrum processing and peak fit of XPS, AES, XAS and RAMAN data
- Quantification and thickness estimation of XPS and AES measurements
- Presentation of the results
- Improvements and additional features of the new software version

### Exercises

- Programme handling
- Spectrum processing, peak-fit and calculation of the spectral background using different model functions for XPS, AES and XAS
- Peak-fit using absolute or relative fit parameters
- Estimation of the uncertainties of the peak-fit parameters of XPS measurements
- Estimation of the transmission function
- Quantitative, qualitative and chemical XPS/AES analysis: line identification, estimation of the atomic concentration and chemical analysis
- Batch processing of sputter depth profiles, line scans (estimation of the recording size) and multipoint measurements (generation of different chemical 3D plots)
- Data export and presentation of the results

(subject to modifications)

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### Course Fee and registration, eligibility requirements

The course fee is 300 Euro. The fee is including course material, lunch at the Mensa, coffee breaks and conference drinks. Please order a course via mail.

A cancellation free of charge is only possible previous to the deadline for application.

The deposited fees are refunded completely in the event of cancellation of the course by the Unifit Scientific Software GmbH. Other claims of recourse against the organizer are excluded.

The number of participants is limited between 2 to 6.

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