Unifit Scientific Software

Title

The New Software UNIFIT 2027 for Universal XPS/AES/XAS/RAMAN Spectrum Processing, Peak Fit, Quantitative Surface Analysis and Presentation of the Results

Appointment

25th – 26th of March 2027

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 2027 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 2027 are demonstrated.

Meeting Place

Faculty of Chemistry and Mineralogy of the University of Leipzig
Johannisallee 29, 04103 Leipzig

Outline

Thursday, March 25th, 10.30 – 18.30

Introduction

- Fundamentals of the photoelectron spectroscopy (XPS) and Auger electron spectroscopy (AES)
- Fundamentals of the X-ray absorption spectroscopy (XAS)

Theoretical Basics of the Peak-shape Analysis of XPS, AES and XAS Data

- Basics of the peak-shape analysis: mathematical modelling of XPS, AES and XAS peaks as well as the spectral background function
- Estimation of the uncertainties: correctness and significance of the peak-fit results of XPS and AES data

Quantitative Analysis of XPS and AES data

- Estimation of transmission functions of electron spectrometers
- Influence of the photoelectron ionization cross section and scattering effects

Structure and Handling of the Software UNIFIT 2027

- 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

Friday, March 26th, 8.45 – 15.30

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)

Accommodation

The reservation of the lodgings lies in the responsibility of the course participant and is not carried out by the organizer of the course. The course participant is liable for ordered and not taken rooms.

Course Fee and registration, eligibility requirements

Registration: Course Fee:

	Early Bird Before 01. January 2027	**Regular Before 01. March 2027**	**Late After 11. March 2027**
Regular:	400 Euro	450 Euro	500 Euro
Student:	300 Euro	350 Euro	400 Euro

Registration: Course Fee Plus Single Licence Unifit 2027:

	Early Bird Before 01. January 2027	**Regular Before 01. March 2027**	**Late After 11. March 2027**
Regular:	1400 Euro	1450 Euro	1500 Euro
Educ. Disc.:	900 Euro	950 Euro	1000 Euro

Registration: Course Fee Plus Research Group Licence Unifit 2027:

	Early Bird Before 01. January 2027	**Regular Before 01. March 2027**	**Late After 11. March 2027**
Regular:	2400 Euro	2450 Euro	2500 Euro
Educ. Disc.:	1800 Euro	1850 Euro	1900 Euro

The fee is including course material, Thursday evening dinner, coffee breaks and conference drinks, excluding lodging and lunch.
Please register via e-mail until March 11th 2027.
After reception of your registration, you will receive a registration confirmation/invoice. You will receive additional detailed information about the event before March 18th 2027.

A cancellation free of charge is only possible previous to the deadline for application. No refund is paid in case of cancellations after this deadline or nonappearance of the participant. The cancellation needs to be in written form. A representation of the participant can be sent free of charge, if announced in written form.

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 to 15.