



TUTORIAL

X-ray Photoemission Spectroscopy Analysis using CasaXPS

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X-ray photoelectron spectroscopy (XPS) data are quantified by applying bell-shaped curves to the spectra [1]. As with most measurements, there are multiple levels of information that can be extracted from XPS analysis, including the most basic, elemental identification and quantitation, and more complex fitting that can yield in-depth chemical state composition. The consequences of transmission function [2] and escape depth will consider.

Proceeding an X-ray Photon Emission Spectroscopy big data set could be time consuming. Function of your samples and measured core levels, you will need different base line, different functions for fitting. You could also need to fit your background at the same time as your core level [3], fit with yours line shape form reference samples.

In this course, some examples of background determinization, peak fitting and statistic uncertainties [4] on big data set will be explain using CasaXPS [5]. Some examples will use PCA projection [6], and linear least square fit [7,8].

[1] G. H. Major, N. Fairley, V. Fernandez, and M. R. Linford, 'Introduction to Chemical State Analysis by XPS with Examples', in *Catalytic Science Series*, vol. 21, WORLD SCIENTIFIC (EUROPE), 2023, pp. 51–70. doi: 10.1142/9781800613294_0003.

[2] B. P. Reed *et al.*, 'Versailles Project on Advanced Materials and Standards interlaboratory study on intensity calibration for x-ray photoelectron spectroscopy instruments using low-density polyethylene', *Journal of Vacuum Science & Technology A*, vol. 38, no. 6, p. 063208, Dec. 2020, doi: 10.1116/6.0000577.

[3] S. Saini *et al.*, 'Deriving Stable Peak Models to Fit Complex XPS Data From Cu Contaminated Pt Electrocatalysts', *Surface & Interface Analysis*, vol. 57, no. 6, pp. 455–469, Jun. 2025, doi: 10.1002/sia.7401.

[4] P. J. Cumpson and M. P. Seah, 'Random uncertainties in AES and XPS: II: Quantification using either relative or absolute measurements', *Surface and Interface Analysis*, vol. 18, no. 5, pp. 361–367, May 1992, doi: 10.1002/sia.740180509.

[5] N. Fairley *et al.*, 'Systematic and collaborative approach to problem solving using X-ray photoelectron spectroscopy', *APPLIED SURFACE SCIENCE ADVANCES*, vol. 5, Sep. 2021, doi: 10.1016/j.apsadv.2021.100112.

[6] V. Fernandez, D. Morgan, P. Bargiela, N. Fairley, and J. Baltrusaitis, 'Combining PCA and nonlinear fitting of peak models to re-evaluate C 1s XPS spectrum of cellulose', *Applied Surface Science*, vol. 614, p. 156182, Mar. 2023, doi: 10.1016/j.apsusc.2022.156182.

[7] G. H. Major, V. Fernandez, N. Fairley, E. F. Smith, and M. R. Linford, 'Guide to XPS data analysis: Applying appropriate constraints to synthetic peaks in XPS peak fitting', *Journal of Vacuum Science & Technology A*, vol. 40, no. 6, p. 063201, Dec. 2022, doi: 10.1116/6.0001975.

[8] V. Fernandez, N. Fairley, and J. Baltrusaitis, 'Unraveling spectral shapes of adventitious carbon on gold using a time-resolved high-resolution X-ray photoelectron spectroscopy and principal component analysis', *Applied Surface Science*, vol. 538, p. 148031, Feb. 2021, doi: 10.1016/j.apsusc.2020.148031.