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peakR: An Open-Source Nonlinear Curve Fitting Package

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peakR is an open-source package for nonlinear peak fitting that was developed using the popular statistical programming language, R. By utilising a modified Levenberg-Marquardt algorithm, the sum of both nonlinear and linear functions fitted to experimental data can be solved. The package consists of a set of R functions and an RStudio Addin that allows the user to analyse their dataset through either an interactive graphical user interface (GUI) or by using programming code to enable a smooth data analysis workflow irrespective of the user's analysis preference. As nonlinear peak fitting is a commonly used post-acquisition data analysis procedure in surface science, peakR specialises in analysing X-ray photoelectron spectroscopy (XPS) spectra. In particular, it enables chemical peak identification and labelling by comparing and matching experimental values to the built-in "Element Binding Energy" database.

Primary author: Mr QUITALES, Ramon

Presenter: Mr QUITALES, Ramon

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