Perspective Article

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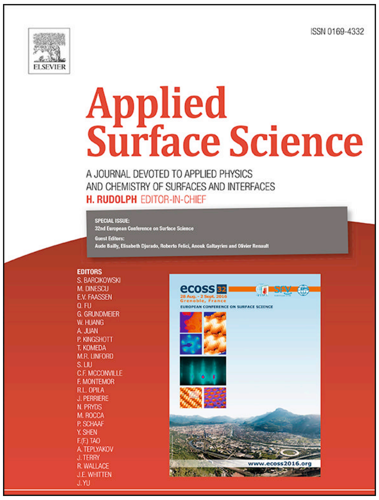

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The Gaussian-Lorentzian Sum, Product, and Convolution (Voigt) Functions in the Context of Peak Fitting X-ray Photoelectron Spectroscopy (XPS) Narrow Scans

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Abstract

X-ray photoelectron spectroscopy (XPS) is arguably the most important vacuum technique for surface chemical analysis, and peak fitting is an indispensable part of XPS data analysis. Functions that have been widely explored and used in XPS peak fitting include the Gaussian, Lorentzian, Gaussian-Lorentzian sum (GLS), Gaussian-Lorentzian product (GLP), and Voigt functions, where the Voigt function is a convolution of a Gaussian and a Lorentzian function. In this article we discuss these functions from a graphical perspective. Arguments based on convolution and the Central Limit Theorem are made to justify the use of functions that are intermediate between pure Gaussians and pure Lorentzians in XPS peak fitting. Mathematical forms for the GLS and GLP functions are presented with a mixing parameter *m*. Plots are shown for GLS and GLP functions with mixing parameters ranging from 0 to 1. There are fundamental differences between the GLS and GLP functions. The GLS function better follows the 'wings' of the Lorentzian, while these 'wings' are suppressed in the GLP. That is, these two functions are not interchangeable. The GLS and GLP functions are compared to the Voigt function, where the GLS is shown to be a decent approximation of it. Practically, both the GLS and the GLP functions can be useful for XPS peak fitting. Examples of the uses of these functions are provided herein.

Key words: XPS, GLS, GLP, Voigt function, Gaussian function, Lorentzian function