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RESEARCH ARTICLE

The x- and y-Symmetrization of XPS Spectra, and the Creation of Models From x-Symmetrized Spectra for the Visually Impaired

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ABSTRACT

We describe the x-symmetrization of *X*-ray photoelectron spectroscopy (XPS) spectra as a possible alternative approach for viewing them. In x-symmetrization, the counts at each binding energy in a spectrum are symmetrized or centered about the *x*-axis, altering the appearance of the spectrum. X-symmetrized XPS spectra may accentuate background variations and other spectral features that may be less naturally emphasized in conventionally plotted spectra. They may also help identify when backgrounds have been appropriately placed across XPS narrow scans. An x-symmetrized spectrum can be rotated about the *x*-axis to create a three-dimensional depiction of it. 3D printed versions of such spectra may increase the accessibility of XPS spectra for the visually impaired. In y-symmetrization, an XPS spectrum is symmetrized about the *y*-axis or at another binding energy. A comparison of a background-subtracted peak to its y-symmetrized rendition may help identify asymmetry in XPS peaks.

1 | Introduction

X-ray photoelectron spectroscopy (XPS) is the most important method for chemically analyzing surfaces [1–4]. XPS is based on the photoelectric effect, which was explained by Einstein in 1905 [5], later demonstrated with X-rays by Robinson [6–9], and ultimately developed into a practical technique by Siegbahn and coworkers in the 1960s [10, 11]. By conservation of energy, the fundamental equation of XPS states that, for conductors, the energy of the incident X-ray ($h\nu$) is partitioned between the binding energy of the photoelectron, as measured at the shared Fermi level of the sample and spectrometer (BE_F), the kinetic energy of the photoelectron, as measured at the spectrometer (KE_{spec}), and the work function of the spectrometer (Φ_{spec}), as follows:

$$h\nu = BE_F + KE_{spec} + \Phi_{spec} \quad (1)$$

In the case of insulators, Equation (1) can be rewritten as:

$$h\nu = BE + KE + \Phi, \quad (2)$$

where the final term (Φ) in Equation (2) accounts for uncertainties in the sample surface potential and binding energy reference point [12].

While the fundamental instrumentation needed for XPS has been around for decades [13], it continues to advance significantly [14]. For example, hard XPS (HAXPES) sources are increasingly found on instruments. These probe more deeply into materials than conventional, monochromatic Al Kα sources [15]. Gas cluster ion sources, which effectively clean many inorganic samples in situ and depth profile through some organic samples without damaging them, are routinely found on instruments [16]. Recent reports indicate that, compared to conventional depth profiling with ion beams, depth profiling with femtosecond lasers results in essentially no sample damage, e.g., oxides are not reduced during this form of depth profiling [17]. Near