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Insufficient reporting of x-ray photoelectron spectroscopy instrumental and peak fitting parameters (metadata) in the scientific literature

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ABSTRACT

This study was motivated by earlier observations. It is a systematic examination of the adequacy of reporting of information (metadata) necessary to understand x-ray photoelectron spectroscopy (XPS) data collection and data analysis in the scientific literature. The information for this study was obtained from papers published in three high-quality journals over a six-month period in 2019 and throughout 2021. Each paper was evaluated to determine whether the authors had reported (percentages of the papers properly providing the information are given in parentheses) the spectrometer (66%), fitting software (15%), x-ray source (40%), pass energy (10%), spot size (5%), synthetic peak shapes in fits (10%), backgrounds in fits (10%), whether the XPS data are shown in the main body of the paper or in the supporting information (or both), and whether fitted or unfitted spectra were shown (80% of published spectra are fit). The Shirley background is the most widely used background in XPS peak fitting. The Al Kα source is the most widely used x-ray source for XPS data collection. CASAXPS is the most widely used fitting program for XPS data analysis. There is good agreement between the results gathered during the two years of our survey. There are some hints the situation may be improving. This study also provides a list of the information/parameters that should be reported when XPS is performed.

I. INTRODUCTION

We report a survey of reported x-ray photoelectron spectroscopy (XPS) metadata with a focus on parameters associated with data collection and peak fitting. The outcome of this study highlights inadequacies in reporting that contribute to the propagation of incorrect analyses appearing in the scientific literature. Building from this survey, a list of important parameters is provided to assist newer users in recording and reporting XPS data in a manner that will be useful and informative to the research community.

XPS is a surface analysis method that is based on the photoelectric effect. XPS identifies the elements and the chemical states of the elements at surfaces. The use of XPS has increased dramatically over the last four decades to the point that it is now a well-established technique.[1] XPS continues to bring in new users and widen its scope of influence in other fields.[2–6] The increasing