Update on Tools to Encourage and Facilitate Generation and Reporting of Reliable and Reproducible Information using Surface Analysis Methods

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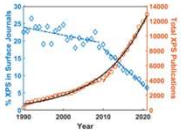
The Challenge with XPS as an example

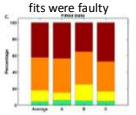
As use of XPS in publications is expanding at nearly an exponential rate, much of it outside of surface- and interface-analysis community. There is a growing range of applications and XPS instrumentation is evolving with new capabilities



Publication and report problems limit value of XPS data reported

1. Inappropriate/incorrect analysis
2. Incomplete parameter reporting in publications and data sets

In one study 40% of peak fits were faulty



Parameters about peak fitting and instrument operation often missing

Peak Fitting Information and Parameters 50 Papers in three journals	
Parameter/Information	*% Papers Including Information*
Software Used	35% to 50%
Background applied	5% to 40%
Peak Shape used	10% to 65%
Fitting process described	0% to 10%
Identification of Fitting Constraints used	10% to 30%

Instrument Specification Information and Parameters from 90 papers in three Journals	
Parameter/Information	*% Papers Including Information*
Instrument Identification	82% to 95%
X-rays Used	65% to 75%
Pass Energy	5% to 35%
Charge Neutralization used or not	0% to 10%
Emission Angle Identified	5% to 25%
Acquisition time noted	0% to 5%

Problem not unique to XPS or Surface Analysis. Open publications, requirements for data access, and artificial intelligence needs are also altering the ways data needs to be collected, stored and archived.

Multiple resources have been and are being developed to assist those unfamiliar with, but needing surface analysis, and analysts in doing analysis of appropriate quality. Listed here are two focused topic collections in JVSTA, Notes and Insite papers in Surface and Interface Analysis, Instrument Overview papers in Surface Science Spectra. This poster not intended to be read but a photograph or use of QR codes can provide access to the information for you to use as needed.

New **JVSTA Topical Collection Reproducibility Challenges and Solutions II with a focus on surface and interface analysis**
https://pubs.aip.org/jva/collection/1441/Reproducibility-Challenges-and-Solutions-II-with-a

Paper Categories and Topics	First Author	DOI https://doi.org/
Selecting an appropriate surface analysis method, optimizing GCIBs, and roles of AI and ML		
Selecting the best surface analysis method for your materials/samples	Kye J. Robinson	10.1116/6.0003576
Challenges in porosity characterization of thin films: Cross-evaluation of different techniques	Mikhail R. Baklanov	10.1116/6.0002793
Materials characterization: Can artificial intelligence be used to address reproducibility challenges?	Miu Lun Lau	10.1116/6.0002809
Application of machine learning to spectrum and image data	Satoka Aoyagi	10.1116/6.0002858
Sputter rates, depth resolution, and ion yields: A practical guide to choosing the best GCIB	N. Sano	10.1116/6.0002864
SIMS – Quantification, Data Analysis and Interpretation		
Novel principal component analysis tool based on python for analysis of complex spectra of TOF-SIMS	Yadong Zhou	10.1116/6.0003355
Best practices for performing quantitative TOF-SIMS analyses	Alan M. Spool	10.1116/6.0003660
SIMS applications - batteries, nanoparticles and semiconductors		
VAMAS TWA interlaboratory comparison: Surface analysis of TiO_2 nanoparticles using ToF-SIMS	Francesca Bennet	10.1116/6.0002814
ToF-SIMS in battery research: Advantages, limitations, and best practices	Teo Lombardo	10.1116/6.0002850
OrbiSIMS depth profiling of semiconductor materials—Useful yield and depth resolution	Yundong Zhou	10.1116/6.0003821
Scanning Probe – STM Tips and Nanoindentation		
In situ plasmonic tip preparation and validation techniques for scanning tunneling microscopy	Benjamen N. Taber	10.1116/6.0002807
Some considerations in nanoindentation measurement and analysis by atomic force microscopy	Irit Rosenhek-Goldian	10.1116/6.0003136
UPS Work Function Determination and Immersion Ellipsometry of Ultrathin Films.		
Immersion ellipsometry for uncorrelated determination of ultrathin film thickness and index of refraction	Samira Jafari	10.1116/6.0003511
Work function measurement by ultraviolet photoelectron spectroscopy: A versailles interlaboratory study	Jeong Won Kim	10.1116/6.0002852
XPS Data Analysis Quality and Reporting Issues		
Insufficient reporting of XPS instrumental and peak fitting parameters (metadata) in the literature	George H. Major	10.1116/6.0002714
Perspective on improving the quality of data analysis in the literature with a focus on XPS	George H. Major	10.1116/6.0002437
XPS extracting information - approaches to data collection, analysis and peak fitting		
The case for denoising/smoothing X-ray photoelectron spectroscopy data by Fourier analysis	Alvaro J. Lizarbe	10.1116/6.0004167
Guide to XPS data analysis: Applying appropriate constraints to synthetic peaks in XPS peak fitting	George H. Major	10.1116/6.0001975
Double Lorentzian lineshape for asymmetric peaks in photoelectron spectroscopy	Alberto Herrera-Gomez	10.1116/6.0002602
Chemical significance of x-ray photoelectron spectroscopy binding energy shifts: A Perspective	Paul S. Bagus	10.1116/6.0003081
Angle resolved xps assessment of the structure and composition of nanofilm using the multilayer model	Alberto Herrera-Gomez	10.1116/6.0002981
Practical guides for XPS: Use of argon ion beams for sputter depth profiling and cleaning	Alexander G. Shard	10.1116/6.0003681
Practical guide on chemometrics/informatics in XPS. I. Introduction to methods useful for large or complex datasets	Tahereh G. Avval	10.1116/6.0002082
Practical guide on chemometrics/informatics in XPS. II. Example applications of multiple methods to the degradation of cellulose and tartaric acid	Tahereh G. Avval	10.1116/6.0001969
Practical guide to understanding goodness-of-fit metrics used in chemical state modeling of x-ray photoelectron spectroscopy data by synthetic line shapes using nylon as an example	Neal Fairley	10.1116/6.0002196
More from XPS: Informative but underused approaches to XPS data collection & analysis	Donald R. Baer	10.1116/6.0004543
XPS - HAXPES and NAP-XPS		
Introduction to reproducible laboratory hard x-ray photoelectron spectroscopy	Kateryna Artyushkova	10.1116/6.0003740
Current Trends in NAP-XPS. Degree of Reporting of Instrument Parameters	Matthew R. Linford	(Still in final review)
XPS Application to Specific Types of Materials and Systems – catalysts, oxides insulators, iron and steels, actinides, radiation sensitive materials		
Examination of the use of XPS O 1s to characterize oxygen vacancies in catalytic materials and beyond	Christopher D. Easton	10.1116/6.0004686
Assignment of atomic charges in metal oxides based on core-level XPS spectra: The case of Ti in $SrTiO_3$(001)	Scott A. Chambers	10.1116/6.0004210
Following the propagation of erroneous XPS peak fitting through the literature. A genealogical approach	B. Maxwell Clark	10.1116/6.0004093
Reevaluation of XPS Pt 4f peak fitting: Ti 3s plasmon peak interference and Pt metallic peak asymmetry in Pt@TiO_2 system	Min-Ju Choi	10.1116/6.0003973
Interpretation of complex x-ray photoelectron peak shapes. I. Case study of Fe 2p3/2 spectra	A. E. Hughes	10.1116/6.0003804
Interpretation of complex x-ray photoelectron peak shapes. II. Case study of Fe $2p_{3/2}$ fitting applied to austenitic stainless steels 316 and 304	A. E. Hughes	10.1116/6.0003842
Review of actinide core-level photoemission	Alaina Thompson	10.1116/6.0003534
XPS guide for insulators: Electron flood gun operation and optimization, surface charging, controlled charging, differential charging, useful FWHMs, problems and solutions, and advice	B. Vincent Crist	10.1116/6.0003439
Photoemission spectroscopy on photoresist materials: A protocol for analysis of radiation sensitive materials	Faegheh S. Sajjadian	10.1116/6.0002808

New Material to be posted on AVS Webpages by the Recommended Practices Committee

The material in this poster and other information about additional papers, standards and websites will be posted in the Technical Resources tab under that title Guides, Standards and Recommended Practices. It can be found using the above QR code or under Technical Resources on the AVS home page https://avs.org/. Suggestions for material to add to the information are welcome (don.baer@PNNL.gov).

JVSTA Topical Collection Reproducibility Challenges and Solutions with a focus on XPS
https://pubs.aip.org/jva/collection/1440/Special-Topic-Collection-Reproducibility

Paper Categories and Topics	First Author	DOI
Experimental Information and Planning		I
First steps in planning, conducting, and reporting XPS measurements*	Baer, Donald R	10.1116/6.0000873
Introduction to X-Ray Photoelectron Spectroscopy (XPS)	Stevie, Frederick A.	10.1116/6.0000412
Sample Handling, Preparation and Mounting for XPS	Stevie, Frederick A.	10.1116/6.0000421
Standards and metrology as tools to address reproducibility XPS	Unger, Wolfgang E. S.	10.1116/1.5131074
Common errors in XPS analysis and reporting	Major, George H.	10.1116/6.0000685
Instrument Set Up and Data Collection		
A rapid proceduredrecheck XPS instrument performance	Wolstenholme, John	10.1116/6.0000224
Intensity calibration for XPS instruments using low-density polyethylene	Reed, Benjaman	10.1116/6.0000577
Extension of Intensity calibration to multiple instrument geometries.	Shard, Alexander G.	10.1116/6.0000578
Introduction to lateral resolution and analysis area measurements in XPS	Unger, Wolfgang E. S.	10.1116/6.0000398
XPS Guide: Charge neutralization and binding energy referencing for insulating samples	Baer, Donald R	10.1116/6.0000057
Peak Identification, Peak Fitting and Quantitative Analysis		
A Tutorial on Interpreting X-ray Photoelectron Spectroscopy (XPS) Survey Spectra*	Shah, Dhruv	10.1116/1.5043297
Guides to Quantitative XPS	Shard, Alexander G.	10.1116/1.5141395
Perspective on quantitation accuracy in XPS	Brundle, Christopher R.	10.1116/1.5141897
Introductory guide to backgrounds in XPS spectra	Engelhard, Mark H.	10.1116/6.0000359
Practical guide for curve fitting in X-ray photoelectron spectroscopy	Major, George H.	10.1116/6.0000377
Uncertainties in photoemission peak fitting	Herrera-Gomez, Alberto	10.1116/1.5143132
Interpreting the Carbon 1s Spectrum	Gengenbach, Thomas R.	10.1116/6.0000682
Correcting Peak Overlaps in Quantitative Auger Electron Spectroscopy of Cr-Containing Oxides	Burrell, Michael C	10.1116/1.5128901
Path Lengths and Depth Information		
A Practical Guide to Path Lengths in XPS	Powell, Cedric J.	10.1116/1.5141079
Experimental determination of electron attenuation lengths	Chambers, Scott A.	10.1116/6.0000291
Practical Guide to the Use of Backgrounds in Quantitative XPS	Tougaard, Sven	10.1116/6.0000661
Data and Reporting		
Data curation, archiving and storage	Suzuki, Mineharu	10.1116/1.5128408
Role of consistent terminology in XPS reproducibility	Baer, Donald R	10.1116/6.0000016
Technological or Scientific Applications		
Achieving reproducibility in semiconductor technology	Conard, Thierry	10.1116/1.5140746
Consistency and Reproducibility in Atomic Layer Deposition	Sønsteby, Henrik H	10.1116/1.5140603
Guides for XPS Analysis of Polymers	Easton, Christopher D.	10.1116/1.5140587
Guides to XPS study of catalysts	Davies, Philip R.	10.1116/1.5140747
Guide to XPS measurements of Epitaxial Films and Heterostructures	Chambers, Scott A.	10.1116/6.0000465
Guide to XPS Measurements on Nanoparticles	Baer, Donald R.	10.1116/1.5141419

New **Surface Science Spectra Instrument Papers to assist instrument parameter reporting**

Instrument parameter reporting is often woefully insufficient for either assessment of results or replication of measurements. A new series of Surface Science Spectra (SSS) papers has been initiated to help address the need. Some instrument parameters, such as geometry, remain constant for a specific family of instruments. Other important parameters for XPS spectrometers, such as pass energies, have impacts that vary with instrument design and a simple number does not necessarily provide useful information to a journal reader. The SSS papers provide a level of information about systems not generally available. The papers also describe common modes of operation that authors can reference, providing the needed details without the need for a full description.

Two instrument papers (SPECS EnviroESCA (NAP-XPS), and IONTOF Qtac (LEIS)) are published or undergoing review after minor revisions, one (Phi VersaProbe) is in SSS review, and two (Kratos Supra and Surpra+ and ThermoFisher NEXA G20 are in preparation.

- Paul M. Dietrich, et al.; Description and operation characteristics of SPECS EnviroESCA. *Surf. Sci. Spectra* 2025; 32 (1):013001 https://doi.org/10.1116/6.0003878
- Philipp Brüner et al.; Description and Operation Characteristics of IONTOF Qtac High Sensitivity Low Energy Ion Scattering Spectrometer, Resubmitted to *Surf. Sci. Spectra* after minor revision August 15, 2025.
- Noeb Biderman, et al.; Description and Operating Characteristics of PHI *VersaProbe* XPS Instruments Submitted to *Surf. Sci. Spectra* August 29, 2025.

New **Surface and Interface Analysis Notes and Insight papers were initiated in 2022 as short single topic papers to assist analysts in addressing important analysis topics. Currently > 30 papers**

Paper Categories and Topics	First Author	DOI 10.1002
Technique Basics – XPS, LEIS, Terminology		
Importance of standard terminology in surface chemical analysis: ISO 18115-1:2023, general terms and terms used in spectroscopy.	Shard, AG	10.1002/sia.7284
XPS Insight Note: Coster–Kronig Broadening	Isaacs, M	10.1002/sia.7410
XPS Insight Note: Multiplet Splitting in X-Ray Photoelectron Spectra.	Isaacs, M	10.1002/sia.7383
Much Ado About Nothing? Background Anomalies Without Accompanying Primary Peaks in XPS and LEIS.	Pinder, J	10.1002/sia.7378
Instrument Related – set up, operation, damage, X-ray source, charge control		
Surface science insight note: Optimizing XPS instrument performance for quantification of spectra.	Fernandez, V	10.1002/sia.7296
Detector Linearity and Deadtime Correction for Modern Photoelectron Spectrometers—Surface Analysis Insight Note.	Reed, B	10.1002/sia.7411
Insight Note. Complications of Magnesium Achromatic X-Rays in XPS: A Historical and Practical Perspective.	Jafari, S	10.1002/sia.7377
XPS insights: Sample degradation in X-ray photoelectron spectroscopy.	Morgan, DJ	10.1002/sia.7205
Leadley SR. HAXPES binding energy scale linearity check.	Leadly, SR	10.1002/sia.7156
Surface science insight note: Charge compensation and charge correction in XPS.	Mendoza-Sánchez, B	10.1002/sia.7309
XPS Analysis, Quantification, Depth Information		
Surface Analysis Insight Note: Uncertainties in XPS Elemental Quantification.	Shard, AG	10.1002/sia.7398
Surface analysis insight note: Differentiation methods applicable to noisy data for determination of sp2- versus sp3-hybridization of carbon allotropes and AES signal strengths.	Fairley, N	10.1002/sia.7157
Surface analysis insight note: Straightforward concentration depth profiling by angle-resolved X-ray photoelectron spectroscopy using a Tikhonov regularization algorithm.	Murdoch, BJ	10.1002/sia.7240
Enhancing Oxygen Spectra Interpretation by Calculating Oxygen Linked to Adventitious Carbon	Henderson, J	10.1002/sia.7376
XPS Imaging		
Surface science insight note: Imaging X-ray photoelectron spectroscopy.	Fernandez, V.	10.1002/sia.7337
Surface analysis insight note: Initial, statistical evaluation of X-ray photoelectron spectroscopy images.	Moeini, B.	10.1002/sia.7218
Surface analysis insight note: Multivariate curve resolution of an X-ray photoelectron spectroscopy image.	Moeini, B	10.1002/sia.7260
Surface analysis insight note: Analysis of X-ray photoelectron spectroscopy images with summary statistics.	Moeini, B	10.1002/sia.7248
Surface analysis insight note. Principal component analysis (PCA) of an X-ray photoelectron spectroscopy image. The importance of preprocessing. A-15	Moeini, B	10.1002/sia.7252
Surface analysis insight note: An example of a cluster analysis of spectra from an X-ray photoelectron spectroscopy image. A- 16	Moeini, B	10.1002/sia.7270
XPS Peaks Shape and Fitting		
Surface analysis insight note: Synthetic line shapes, integration regions and relative sensitivity factors.	Fernandez, V	10.1002/sia.7155
XPS insights: Asymmetric peak shapes in XPS.	Morgan, DJ	10.1002/sia.7215
Insight note: XPS peak fitting of the Al 2p peak from electrically isolated aluminum foil with an oxide layer.	Lizarbe, AJ	10.1002/sia.7238
XPS and SIMS of Specific Samples or Sample Types		
Surface science insight note: A linear algebraic approach to elucidate native films on Fe3O4 surface.	Bargiela, P	10.1002/sia.7290
Surface analysis insight note: Illustrating the effect of adventitious contamination on Pt photoemission peak intensities.	Fairley, N	10.1002/sia.7276
Surface analysis insight note: Accounting for X-ray beam damage effects in positive electrode-electrolyte interphase investigations.	Fantin, R	10.1002/sia.7294
Surface Analysis Insight Note: Observations relating to photoemission peak shapes, oxidation state, and chemistry of titanium oxide films.	Bargiela, P	10.1002/sia.7283
Surface analysis insight note: XPS analysis of battery electrodes—Challenges with nickel–manganese–cobalt and Li examples using an Al Kα x-ray source.	Strange, LE	10.1002/sia.7237
TOF-SIMS and XPS protocol for the analysis of organic multilayers.	Guyot, C	10.1002/sia.7277

New **ISO standard on reporting about sample preparation and handling**

ISO Surface Analysis Standards | Terminology | 20579 Part 1 summary

The International Organization for Standardization (ISO) Technical Committee 201 on Surface Chemical Analysis (TC201) has developed a variety of useful standards and guidelines dealing with terminology, instrument operation and data analysis. The terminology is freely available at ISO Online Browsing Platform by searching for "surface analysis vocabulary" or 18115 (https://www.iso.org/obp/ui). Several standards deal with parameter reporting for instrument use and sample preparation. A new standard 20579 part 1 indicates the information someone wanting surface analysis should report to the analyst doing the work. 20579 part 2 indicates what an analyst should record and report regarding sample handling and preparation. A summary of 20579 part 1 has been in Surface and Interface published on September 13 *Importance of sample handling and preparation for surface analysis: A summary of ISO Standard 20579 part 1, Documenting and reporting the handling of specimens prior to analysis.* DOI: 10.1063/SIA.70016.