CHEMICAL INTERPRETATION OF CORE-LEVEL X-RAY PHOTOEMISSION SPECTRA THROUGH A DATA-DRIVEN PROCESS

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DEVELOPMENT STATUS

Demonstration model

CATEGORIES

//Physical sciences

BACKGROUND

In research and industrial processes, the exact phase content of a given sample (area) has often to be characterized. While a stoichiometric characterization of the elements present is rather easy, finding out which chemical phases are present in which quantity is rather hard. Sensitive to the chemical environment are core-level binding energies, which are accessible by X-ray photoemission (XPS) measurements. For the chemical characterization these XPS spectra have to be interpreted which is not always conclusive. First principle methods, so called ab-initio methods, allow for the calculation of spectral properties. Our ab-initio data-driven approach solves the XPS interpretation process for a wide range of material compounds.

PROBLEM

In detail, the problem lies in a consistent interpretation of X-ray photoemission spectra. For this, a sum of peak functions is fitted to the experimental spectrum. This interpretation process with current approaches only works robustly for simple phases containing one chemical environment with a large enough shift in its core-level binding energy. Additionally, literature data of binding energies and/or single crystal spectra of possible phases have to be available for the interpretation. In the current state of the art often, either the spectra are to complex to reach a reasonable conclusion or there is not enough reference data in the literature available to compare with.

SOLUTION

Our process allows a consistent evaluation of core-level X-ray photoemission spectra of more complex phases and samples containing mixtures of phases, which might even be linear dependent on each other. To do so, theoretical core-level spectra for all possible phases, containing the elements known to be present in the sample, are constructed. These theoretical spectra are then fitted directly to the measured spectral data to yield a chemical interpretation. The theoretical spectra are constructed from a database of ab-initio core-level shifts

and binding energies on a wide range of materials, calculated with the FLEUR (www.flapw.dehttps://www.inventionstore.de/https://www.inventionstore.de/) program implementing methods of density functional theory.

ADVANTAGES

The process allows for a consistent chemical interpretation where this has been not possible before. The fit optimization process usually needs less free parameters as the usual approach and allows to incorporate further constrains in the optimization of the fit, reducing the degrees of freedom. Furthermore, the evaluation process allows the systematic handling of linear dependencies between phases, since shifts in binding energies do not have to be unique for a certain phase.

SCOPE OF APPLICATION

Chemical interpretation of X-ray photoemission spectra of samples containing compounds of which high-quality ab-initio data is available.

SERVICE

Development Status and Nex Steps:

Demonstration application in use with data available on all known binary metallic compounds.
Extent to wider range of materials and spectral methods.