

Beyond Chemical Composition: How Surface Science Can Measure Electronic Properties

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X-ray photoelectron spectroscopy (XPS) is a widely used technique to analyze surface composition and chemistry. Often, scientists and engineers aiming to optimize material performance in a device require complementary information about the material's optical and electronic properties. This combined information is necessary in fields such as semiconductors, photovoltaics, (opto)electronics, batteries, and other chemical redox applications.

Fortunately, modern XPS spectrometers offer additional techniques to study the behavior of electrons in a system in addition to the chemical makeup of atoms and molecules in the surface. Reflection electron energy loss spectroscopy (REELS) can be used for optical band gap measurements as well as hydrogen content and carbon hybridization, additional chemical information beyond XPS. Ultraviolet photoelectron spectroscopy (UPS) is a similar method to XPS but with lower-energy UV photons instead of X-rays and higher spectral resolution, illuminating finer details of the valence band structure including work function and ionization potential. Inverse photoemission spectroscopy (IPES), as the name implies, uses the opposite process of XPS and UPS to probe the conduction band of metals and other conductive materials for insight into unoccupied band structure and measuring the electron affinity. Low-energy IPES (LEIPS) is uniquely suited to studying electronic structure of e-beam-sensitive organics that can be damaged by the traditional IPES method [1]. Combined, UPS and IPES/LEIPS can be used to calculate the electronic band gap for conductive materials, an invaluable property for studying charge transfer across an electrochemical interface.

This presentation will discuss the unique information that each of these techniques yields on electronic states in a surface. Guidance will also be shared on choosing an appropriate technique for a given analytical question, how to prepare and mount samples appropriately for the various analyses, and common pitfalls to avoid in data acquisition and interpretation.

[1] Yoshida, H. Chem. Phys. Lett. **539-540**, 180-185 (2012).

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