Localization of d-orbital electrons in transition metals determined

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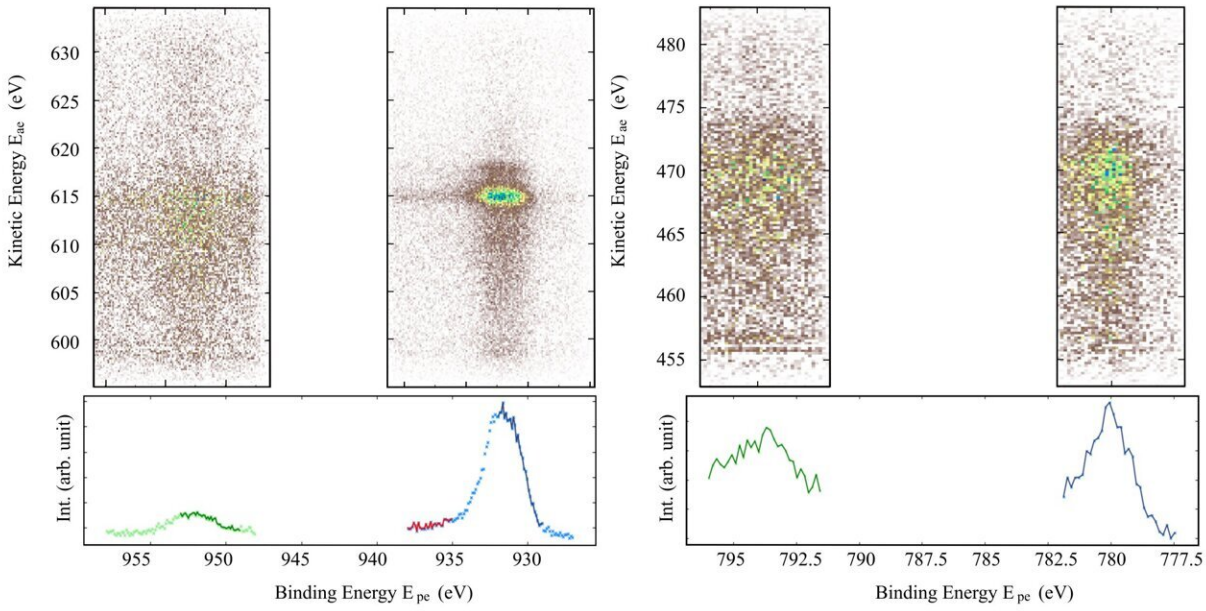

L_3 and L_2 photoelectron $L_{2,3}VV$ Auger electron coincidence maps of Cu (a) and Co (b) together with the coincident photoelectron spectrum acquired by the integration of the maps along the Auger electron kinetic energy. The regions chosen for closer analysis are marked as solid color lines in the binding energy sum spectra (green, red and blue).

Transition metals and non-ferrous metals such as copper, nickel and cobalt are not only suitable as materials in engineering and technology, but also for a wide range of applications in electrochemistry and

catalysis.

Their chemical and physical properties are related to the occupation of the outer d-orbital shells around the atomic nuclei. The energetic levels of the electrons as well as their localization or delocalization can be studied at the X-ray source BESSY II, which offers powerful synchrotron radiation.

Copper, nickel, cobalt

The team of the Uppsala-Berlin Joint Lab (UBjL) around Prof. Alexander Föhlisch and Prof. Nils Mårtensson has now published new results on copper, nickel and cobalt samples. They confirmed known findings for copper, whose d-electrons are atomically localized, and for nickel, in which localized electrons coexist with delocalized electrons.

In the case of the element cobalt, which is used for batteries and as an alloy in fuel cells, however, previous findings were contradictory because the measurement accuracy was not sufficient to make clear statements.

Spectroscopy combined with highly sensitive detectors

At BESSY II the Uppsala-Berlin joint Lab has set up an instrument which enables measurements with the necessary precision. To determine electronic localization or delocalization, Auger photo-electron coincidence spectroscopy (APECS) is used.

APECS requires the newly developed "Angle resolved Time of Flight" (ArTOF) electron spectrometers, whose detection efficiency exceeds that of standard hemispherical analyzers by orders of magnitude. Equipped with two ArTOF electron spectrometers, the

CoESCA@UE52-PGM end station supervised by UBjL scientist Dr. Danilo Kühn is unique worldwide.

Analyzing (catalytical) materials

In the case of the element cobalt, the measurements now revealed that the d-electrons of cobalt can be regarded as highly delocalized. "This is an important step for a quantitative determination of electronic localization on a variety of materials, catalysts and (electro)chemical processes," Föhlisch points out.

The Royal Society of Chemistry has selected the paper as a HOT Article 2022 because this measurement method might arouse interest in the broader research community. The end station is also available to international users at BESSY II, who can apply for beamtime twice a year.

The research was published in *Physical Chemistry Chemical Physics*.

More information: Artur Born et al, The degree of electron itinerancy and shell closing in the core-ionized state of transition metals probed by Auger-photoelectron coincidence spectroscopy, *Physical Chemistry Chemical Physics* (2022). DOI: 10.1039/D2CP02477B

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