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Valence band of tungsten compounds probed using 2p5d RIXS

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Heavy transition metals of 5*d* series are important additives in a wide spectrum of industrial applications, due to high melting temperatures, good surface stability, excellent mechanical strength, and corrosion resistance. They are common ingredients in catalytic converters as well as opto- and spin electronics devices.

Electronic structure of the late 5*d* elements is routinely probed *in-situ* using X-ray absorption spectroscopy (XAS), due to high sensitivity of the $L_{2,3}$-edge spectral shape to the occupation of *d* orbitals. However, in the case of the early 5*d* elements the XAS spectral changes are less pronounced, due to smaller relative change in the occupation of empty states upon electron transfer, which makes difficult the quantitative analysis. There, X-ray emission spectroscopy (XES), a technique probing density of occupied valence states, is more appropriate. It gives an element and symmetry sensitive insight into the electronic structure of occupied bands. A combination of the two techniques, namely 2*p* Resonant X-ray Emission Spectroscopy (RXES) and 2*p*5*d* Resonant Inelastic X-ray Scattering (RIXS), provide researchers with detailed information on electronic structure of core levels and valence band, respectively, with bulk sensitivity.

In this contribution we present an overview of the evolution of tungsten electronic structure in a series of tungsten compounds – oxides, carbides, silicates and sulphides – as revealed by RIXS and RXES upon excitation at W $L_{2,3}$-edge. We observe that electronic structure of core levels, even the shallow ones, is insensitive to the local environment. Also the bandwidth of valence band does not reveal significant differences among the compounds studied, except for WO_2 (see Fig.1). However, the intensity and fine structure of the spectra reveal small differences among all the studied compounds, that can be related to local structure and coordination type. The experimental spectra can be nicely reproduced using multiple-scattering approach (FEFF 9 or FDMNES) providing a way for their detailed analysis and leading to potential use of the technique in chemical characterization of a wide class of technologically relevant materials.

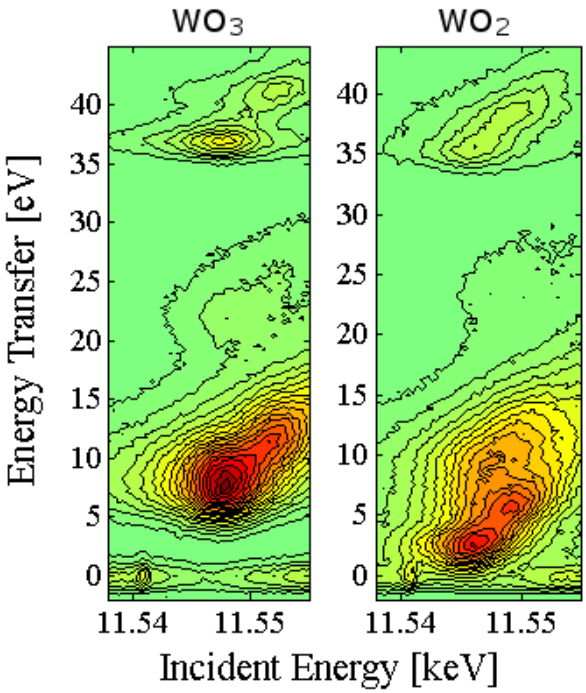

Figure 1. Contour plots of the valence band RIXS in WO_2 and WO_3 probed at W L_2-edge.

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