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Determination of electronic structure of iron compounds using resonant X-ray emission spectroscopy

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X-ray spectroscopy is dynamically developing and powerful tool to examine electronic structure of materials. Coupling this method with unique properties of synchrotron radiation allows to study more subtle effects and gather information with high precision

Resonant X-Ray Emission Spectroscopy (RXES) is a scattering experiment that is extremely useful in electronic properties studies. In proper experimental geometry with dispersive spectrometer it allows simultaneously record X-ray emission (XES) and absorption (XAS) spectra. This way both occupied and unoccupied electronic levels in material can be examined. Additionally, resonantly excited absorption and emission offers a possibility to study electronic states in very high resolution, much higher than in conventional Total Fluorescence Yield XAS or XES experiment [1].

Using RXES method iron foil, α-Fe_2O_3 (hematite) and $Fe(NO_3)_3$ were examined. Experiment was performed at SuperXAS beamline (Swiss Light Source,Paul Scherrer Institut, Villigen, Switzerland). RXES measurements were carried out around the Fe K-edge and X-ray detection was performed using a wavelength-dispersive spectrometer in the von Hamos geometry [2].

Data was obtained in a form of 2D RXES planes for each compound. From each plane non- and high resolution XAS and XES spectra were extracted and compared with calculated Density of States (lDOS) functions to identify electronic structure of studied materials. XAS, XES spectra and corresponding lDOS functions were calculated in FeFF9.6 software [3] using Full Multiple Scattering approach. Results for α-Fe_2O_3 (hematite) are shown in Fig. 1. Analysis was focused on valence to core and pre-edge regions of XES and XAS spectra, respectively. The contribution of molecular orbitals of iron and neighbouring atoms to the absorption and emission spectra was established, giving the insight into occupied and unoccupied states of studied compounds.

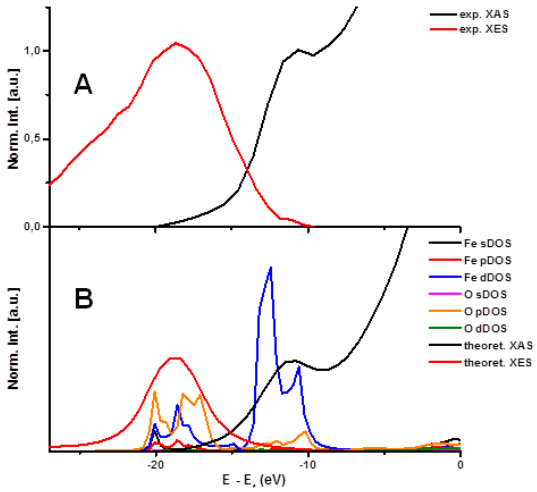

Figure 1. Example results for α-Fe_2O_3 (hematite) extracted from 2D RXES plane **A** - Experimental XES spectrum and XAS spectrum in valence to core and pre-edge region respectively. **B** – Theoretically calculated spectra and corresponding lDOS functions.

The results showing that the combination of RXES method with theoretical calculations that allow fast and accurate examination of electronic structure of materials will be presented.

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