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## Direct spectroscopic identification of reactive metal-oxygen species

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In transition metal-oxygen species, the way the oxygen atoms are bonded to the metal center is found to play a significant role in their reactivity, in view of different types of oxygen ligands and unusual oxidation states.<sup>[1,2]</sup> In particular, finding of compounds that present transition metals with unusual oxidation states or reactive oxygen species (superoxido, peroxido and oxygen centered radical) is of great scientific and technological interests, as they have key applications as oxidizing agents, catalysts, or reaction intermediates.<sup>[1,2]</sup>

Here, we use X-ray absorption spectroscopy (XAS) at the oxygen K and metal L<sub>3</sub>, M<sub>3</sub> or N<sub>3</sub> edges of [MO<sub>n</sub>]<sup>+</sup> systems (M = transition metal, *n* = integer) to identify the spectroscopic signatures of oxygen ligands and assign the oxidation state of the metal.<sup>[3,4]</sup> The [MO<sub>n</sub>]<sup>+</sup> species in the gas phase are produced by argon sputtering of a metal target in the presence of oxygen. The cationic species are mass selected and accumulated in an ion trap. X-ray absorption spectra are then recorded in partial ion yield mode.<sup>[5]</sup> Our ion trap instrument is installed at the undulator beamline UE52-PGM at the Berlin synchrotron radiation facility BESSY II.

Reactive species, such as the superoxido, the ozonido, the oxygen centered radical and species containing high-valent transition metals, are analysed in stable conditions in the ground state inside the cryogenic ion trap. This method is here demonstrated to be an important tool to identify oxygen ligands, offering direct access to element specific electronic structures.

### References

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### Category

Other

**Authors:** DA SILVA SANTOS, Mayara (Helmholtz-Zentrum Berlin für Materialien und Energie); FLACH, Max (Helmholtz-Zentrum Berlin für Materialien und Energie); S. ABLYASOVA, Olesya (Helmholtz-Zentrum Berlin für Materialien und Energie); TIMM, Martin (Helmholtz-Zentrum Berlin für Materialien und Energie); VON ISSENDORFF, Bernd (Albert-Ludwigs-Universität Freiburg); HIRSCH, Konstantin (Helmholtz-Zentrum Berlin für Materialien und Energie); ZAMUDIO-BAYER, Vicente (Helmholtz-Zentrum Berlin für Materialien und Energie); STÜKER, Tony (Freie Universität Berlin); RIEDEL, Sebastian (Freie Universität Berlin); LAU, Tobias (Helmholtz-Zentrum Berlin für Materialien und Energie)

**Presenter:** DA SILVA SANTOS, Mayara (Helmholtz-Zentrum Berlin für Materialien und Energie)

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