universität innsbruck

Innsbruck Physics Colloquium

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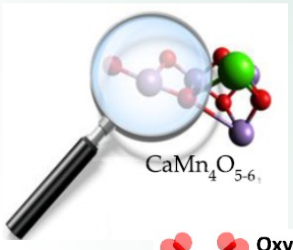
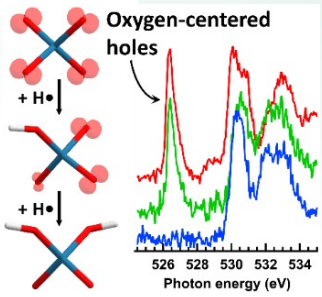
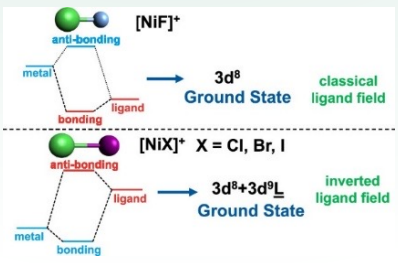
Spin states, oxidation states, and oxygen-centered radicals in transition-metal oxide clusters

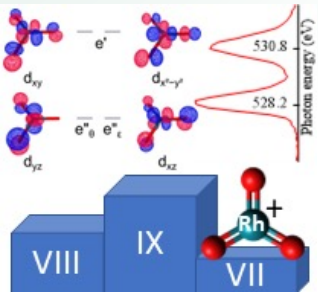
For key reactions like water splitting and dioxygen formation in the oxygen-evolving complex, the characterization of reactive intermediates would be an important step towards identification of reaction mechanisms. In particular, knowledge about spin states or oxidation states of transition metal centers, or the involvement of oxygen-centered radicals, is essential. While short-lived reactive intermediates are still difficult to observe directly, reactive species have long been prepared in cold ion traps, and X-ray spectroscopy is a valuable tool for identifying spin and oxidation states of transition metal centers, or for detecting reactive oxygen species. Combining both methods, we prepare and investigate clusters as model systems to study transition metal centers in highest or unusual oxidation states. Examples will be given of how oxidation states can be measured, [1] and how oxygen centered radicals can be detected by a characteristic spectroscopic fingerprint. [2] Recent highlights include the discovery of rhodium(VII), [3] the detection of inorganic (di)radicals, [4] or the identification of high-spin high-valent manganese (V) in mononuclear transition metal oxide species. [5] With polynuclear clusters, these model systems become even more relevant to chemical reactions.

[1] M. Flach et al., Inorg. Chem. 63 11812 (2024)
[2] M. da Silva Santos et al., ChemPhysChem, 24, e202300390 (2023)
[3] M. da Silva Santos et al., Angew. Chem. Int. Ed. 61, e202207688 (2022)
[4] M. da Silva Santos et al., Chem. Methods e202400023 (2024)
[5] O. S. Ablyasova et al., Phys. Chem. Chem. Phys., 26, 5830 (2024)









Tuesday, 10.12.2024, at 16:30 h, HS C (Technik)

Innsbruck Physics Colloquium,
Organisation: K. Erath-Dulitz, H.-C. Nägerl, T. Schrabback