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# (POS-21) Unraveling \(e_g\) Orbital Splitting in $TiO_2$: The Role of Local Distortion in Ligand Field Multiplet Theory

*Tuesday 10 June 2025 18:20 (2 minutes)*

Transition metals (TM) are d-block elements with partially or completely filled d-orbitals. They display unique and complex behaviors, including variable oxidation states, strong electron correlations, and intricate crystal field effects. Transition metal compounds are technologically and fundamentally important and exhibit a number of interesting effects that can be exploited in applications. Our techniques are ideally suited to studying these effects by probing the electronic structure (for example, crystal field and multiplet effects) in detail.
This presentation provides a comprehensive study of two titanium oxide ($TiO_2$) polymorphs, anatase and rutile. We utilize advanced spectroscopic techniques, including X-ray absorption spectroscopy (XAS) and resonant inelastic X-ray scattering (RIXS), along with ligand field multiplet theory (LFMT).
Our measurements are compared with theoretical insights. By examining the relationship between $L_3$-edge spiting and the distortion parameters $D_s$ and $D_t$, we show that the splitting of the $e_g$ orbitals is strongly influenced by distortions in local symmetry.

## Keyword-1

X-ray Spectroscopy

## Keyword-2

Ligand field multiplet theory

## Keyword-3

Titanium Oxide

**Author:** UFONDU, Peter (University of Saskatchewan)

**Co-authors:** MOEWES, Alexander (University of Saskatchewan); BOYKO, Teak (Canadian Light Source)

**Presenter:** UFONDU, Peter (University of Saskatchewan)

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