

XAS & Degeneracy Lifting in Manganites

Beamline: U4B

Category of Researcher:

GU

Technique: XAS

Researchers & Affiliations:

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Publication: Han-Jin Noh et al., "Jahn-Teller effect in spinel manganites probed by soft x-ray spectroscopy," *Appl. Phys. Lett.* **88**, 081911 (2006)

Motivation: The Jahn-Teller (JT) effect is a prototypical phenomenon demonstrating lifting of degeneracy to lower energy. XAS is an ideal tool to examine the modifications to the JT splitting energy. Systematic variations in sample composition were combined with XAS and multiplet modeling of the spectra to estimate the JT splitting energy.

Results:

- Range of polycrystalline samples, predominantly Mn^{3+}
- Scraped *in-situ* to prepare surface
- XAS scans acquired with linear polarization
- Multiplet model: fix $10Dq$ (CF), $V_{pd\sigma}$ (hybrid.), U (Coulomb), Δ (charge transfer) & vary Q_2 (JT splitting energy)
- Q_2 varies from 0 eV (no JT distortion) to 1.9 eV
- apical / in-plane bond length ratio (from XRD) closely correlated with Q_2
- XAS an ideal tool to examine the electronic configuration following a structural distortion

