Electronic structure of Fe oxides revealed by soft X-ray inelastic scattering

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Outline

Mixed valence and different orbital symmetry

- Jahn-Teller distortion driven magnetic polarons in magnetite
- RIXS study on the multiferroic Fe$_2$Mo$_3$O$_8$

picture from Nat. Mater. 16, 797 (2017)
AGM-AGS RIXS beamline in TLS (BL05A)

Resolving power: 8000-10000
$E_{in}: 500 - 1000 \text{ eV}$

Fe$_3$O$_4$

Verwey transition

Fe$^3+$

Fe$^{2+}$ & Fe$^{3+}$

trimeron

M. S. Senn et al., Nature 481, 173 (2012)
Jahn-Teller distortion driven magnetic polarons

Fe $L_3$-edg Resonant inelastic X-ray scattering

Spectral evidence of polaronic distortion
Resonant inelastic X-ray scattering of Fe$_3$O$_4$

$T = 80$ K
Scattering angle 90°
$\pi$ incident polarization

H. Y. Huang et al., Nat. Commun. 8, 15929 (2017)
Resonant inelastic X-ray scattering of Fe$_3$O$_4$

$T = 80$ K  
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H.-Y. Huang et al., Nat. Commun. 8, 15929 (2017)
Multiplet RIXS calculations for B-site Fe$^{2+}$

Calculated results

Multiplet RIXS calculations for B-site Fe\textsuperscript{2+}

Spin moment of Fe\textsuperscript{2+} + Jahn-Teller polaronic distortion $\Delta_{t_{2g}}$

Magnetic Polarons in LT phase of Fe\textsubscript{3}O\textsubscript{4}

Temperature dependent spin-orbital excitations
Temperature dependent spin-orbital excitations

Short-range ordering of the Jahn-Teller distortion
Polar magnet $\text{Fe}_2\text{Mo}_3\text{O}_8$

Figures from Nat. Mater. 16, 797 (2017)

Pyroelectric $P6_3mc$

- Hidden ferrimagnetism

Polar magnet $\text{Fe}_2\text{Mo}_3\text{O}_8$

Pyroelectric $P6_3mc$

- Hidden ferrimagnetism
- Ferrimagnetic order stabilized by Zn doping

Figures from Nat. Mater. 16, 797 (2017)

Fe₃O₄

Fe₂Mo₃O₈
Multiplet calculation

Quanty
Multiplet ligand-field theory using Wannier orbitals
M.W. Haverkort, M. Zwierzcki, and O.K. Andersen
Summary

Fe$_3$O$_4$:

- *dd* excitons in magnetite have an energy centroid 200 meV and are best explained as magnetic polaron.
- The local distortion of magnetite already exists above the Verwey transition temperature and even up to 550 K, and could be attributed to the precursor of the monoclinic phase across the Verwey transition.

Fe$_2$Mo$_3$O$_8$

- Crystal fields of tetrahedral and octahedral Fe sites are obtained by RIXS measurements.
- The ferrimagnetism in Fe$_2$Mo$_3$O$_8$ is confirmed by XMCD.

**Local electronic structures of compounds with mixed-valence (Fe$_3$O$_4$) and different orbital symmetry (Fe$_2$Mo$_3$O$_8$) can be revealed by RIXS.**
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Thank you for your attention!