



• HAXPES Experiments

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- HAXPES Experiments
- X-ray magnetic circular dichroism



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- Resonant Scattering

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Reading Assignment: Chapter 8.5-8.7



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Reading Assignment: Chapter 8.5-8.7

Homework Assignment #06: Chapter 6: 1,6,7,8,9 due Friday, November 15, 2024



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Homework Assignment #06: Chapter 6: 1,6,7,8,9 due Friday, November 15, 2024 Please send me your choices for General User proposal and final exam presentation. I need to approve them by the end of the week!





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the core states are used to fingerprint the chemical composition of the sample

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The electric field between the two hemispheres of radius R_1 and R_2 has a R^2 dependence from the center of the hemispheres





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Electrons with different azimuthal exit angles ω will map to different positions on the 2D detector









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the electron dispersion curve can be fully mapped by sample rotations



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ability to measure bulk photoemission and buried interfaces as well as the surface

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HAXPES is used to probe the thickness of a $CoFe_2O_4/La_{0.66}Sr_{0.34}MnO_3$ heterostructure by varying both angle of incidence and photon energy



The thickness of the CoFe $_2O_4$ overlayer measured as 6.5 \pm 0.5 nm by TEM was probed in two ways:

B. Pal, S. Mukherjee, and D.D. Sarma, "Probing complex heterostructures using hard x-ray photoelectron spectroscopy (HAXPES)," J. Electron Spect. Related Phenomena 200, 332-339 (2015).

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Both results give consistent results with proper normalization and also show the uniformity of the $CoFe_2O_4$ overlayer

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Energy dispersive measurements can provide depth profiling of spherical nanoparticles



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By fitting the S 2p and Se 3p photoemission line the structure is revealed to be CdSe at the core and ZnCdS in the outer shell

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Si nanoparticle anodes suffer from the accumulation of the SEI layer which reduces performance. The SEI is formed by electrochemical decomposition of the electrolyte at the anode surface.

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HAXPES is used to determine the elemental distribution and compounds present as a function of depth in the cycled Si anode.

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- pure FEC shows less change with cycling than EC containing electrolytes

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Using HAXPES data from Si, C, and F, a picture of SEI evolution dependence on electrolyte emerges

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as SEI grows, there is growth of Li_xSiO_y underneath as product of lithiation/delithiation

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The FEC acts to stabilize the SEI composition and prevent the change with depth that occurs with EC.

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scattering experiments

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this measurement is sensitive to the internal/external magnetic fields which split the levels according to the Zeeman effect





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XMCD and electron sum rules

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$$\mu^{-}(\mathcal{E}) = \frac{1}{x} \ln \left(\frac{I_{t}^{-}}{I_{t}^{-}} \right)$$





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these absorption coefficients can be used at the L_3 and L_2 edges to compute the orbital (m_{orb}) and spin (m_{spin}) magnetic moments in μ_B /atom

The XMCD experiment requires a source capable of switching the polarization (quarter wave plate) or a sample whose magnetic splittings can be inverted by flipping an external magnetic field

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The XMCD experiment requires a source capable of switching the polarization (quarter wave plate) or a sample whose magnetic splittings can be inverted by flipping an external magnetic field

XMCD and electron sum rules

The absorption coefficient is first measured for both relative orientations of magnetic splitting and circular po-

these absorption coefficients can be used at the L_3 and L_2 edges to compute the orbital (m_{orb}) and spin (m_{spin})

magnetic moments in μ_B /atom



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XMCD and electron sum rules

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magnetic moments in μ_B /atom

 $\mathbf{r} = \int_{U_{1}}^{U_{1}} (\mu^{+} + \mu^{-}) d\mathcal{E}$





The Zintl compounds exhibit interesting magnetic properties including colossal magnetoresistance which can be of value for spintronics applications



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Mn provides the bulk of the magnetic moment and appears to be in the divalent state. Sb provides a small antiferromagnetic component to the overall magnetic moment

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This will produce the resonant scattering term but not the XANES and EXAFS, which are purely quantum effects.

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Consider an electron under the influence of an oscillating electric field $\vec{E}_{in} = \hat{x}E_0e^{-i\omega t}$.

V

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$$\ddot{x} + \Gamma \dot{x} + \omega_s^2 x = -\left(\frac{eE_0}{m}\right)e^{-i\omega t}$$

Consider an electron under the influence of an oscillating electric field $\vec{E}_{in} = \hat{x}E_0e^{-i\omega t}$.

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The amplitude of the response has a resonance and dissipation

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Radiated field



The radiated (scattered) electric field at a distance R from the electron is directly proportional to the electron's acceleration with a retarded time t' = t - R/c (allowing for the travel time to the detector).

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which is an outgoing spherical wave with scattering amplitude

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$$f_s = \frac{\omega^2}{(\omega^2 - \omega_s^2 + i\omega\Gamma)}$$



The scattering factor can be rewritten

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$$f_s = \frac{\omega^2 + (-\omega_s^2 + i\omega\Gamma) - (-\omega_s^2 + i\omega\Gamma)}{(\omega^2 - \omega_s^2 + i\omega\Gamma)}$$



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and since $\Gamma \ll \omega_s$

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The scattering factor can be rewritten

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the second term being the dispersion correction

$$\chi(\omega) = f'_s + if''_s = \frac{\omega_s^2}{(\omega^2 - \omega_s^2 + i\omega\Gamma)}$$



The scattering factor can be rewritten

and since $\Gamma \ll \omega_s$

the second term being the dispersion correction whose real and imaginary components can be extracted

$$\begin{split} f_{s} &= \frac{\omega^{2} + \left(-\omega_{s}^{2} + i\omega\Gamma\right) - \left(-\omega_{s}^{2} + i\omega\Gamma\right)}{\left(\omega^{2} - \omega_{s}^{2} + i\omega\Gamma\right)} \\ &= 1 + \frac{\omega_{s}^{2} - i\omega\Gamma}{\left(\omega^{2} - \omega_{s}^{2} + i\omega\Gamma\right)} \approx 1 + \frac{\omega_{s}^{2}}{\left(\omega^{2} - \omega_{s}^{2} + i\omega\Gamma\right)} \end{split}$$

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$$\begin{split} f_{s} &= \frac{\omega^{2} + \left(-\omega_{s}^{2} + i\omega\Gamma\right) - \left(-\omega_{s}^{2} + i\omega\Gamma\right)}{\left(\omega^{2} - \omega_{s}^{2} + i\omega\Gamma\right)} \\ &= 1 + \frac{\omega_{s}^{2} - i\omega\Gamma}{\left(\omega^{2} - \omega_{s}^{2} + i\omega\Gamma\right)} \approx 1 + \frac{\omega_{s}^{2}}{\left(\omega^{2} - \omega_{s}^{2} + i\omega\Gamma\right)} \end{split}$$

$$\chi(\omega) = f'_{s} + if''_{s} = \frac{\omega_{s}^{2}}{(\omega^{2} - \omega_{s}^{2} + i\omega\Gamma)}$$

$$\chi(\omega) = \frac{\omega_s^2}{(\omega^2 - \omega_s^2 + i\omega\Gamma)} \cdot \frac{(\omega^2 - \omega_s^2 - i\omega\Gamma)}{(\omega^2 - \omega_s^2 - i\omega\Gamma)}$$



The scattering factor can be rewritten

and since $\Gamma \ll \omega_s$

the second term being the dispersion correction whose real and imaginary components can be extracted

$$\begin{split} f_s &= \frac{\omega^2 + (-\omega_s^2 + i\omega\Gamma) - (-\omega_s^2 + i\omega\Gamma)}{(\omega^2 - \omega_s^2 + i\omega\Gamma)} \\ &= 1 + \frac{\omega_s^2 - i\omega\Gamma}{(\omega^2 - \omega_s^2 + i\omega\Gamma)} \approx 1 + \frac{\omega_s^2}{(\omega^2 - \omega_s^2 + i\omega\Gamma)} \end{split}$$

$$\chi(\omega) = f'_{s} + if''_{s} = \frac{\omega_{s}^{2}}{(\omega^{2} - \omega_{s}^{2} + i\omega\Gamma)}$$

$$\chi(\omega) = \frac{\omega_s^2}{(\omega^2 - \omega_s^2 + i\omega\Gamma)} \cdot \frac{(\omega^2 - \omega_s^2 - i\omega\Gamma)}{(\omega^2 - \omega_s^2 - i\omega\Gamma)} = \frac{\omega_s^2(\omega^2 - \omega_s^2 - i\omega\Gamma)}{(\omega^2 - \omega_s^2)^2 + (\omega\Gamma)^2}$$





The scattering factor can be rewritten

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$$\begin{split} f_{s} &= \frac{\omega^{2} + \left(-\omega_{s}^{2} + i\omega\Gamma\right) - \left(-\omega_{s}^{2} + i\omega\Gamma\right)}{\left(\omega^{2} - \omega_{s}^{2} + i\omega\Gamma\right)} \\ &= 1 + \frac{\omega_{s}^{2} - i\omega\Gamma}{\left(\omega^{2} - \omega_{s}^{2} + i\omega\Gamma\right)} \approx 1 + \frac{\omega_{s}^{2}}{\left(\omega^{2} - \omega_{s}^{2} + i\omega\Gamma\right)} \end{split}$$

$$\chi(\omega) = f'_{s} + if''_{s} = \frac{\omega_{s}^{2}}{(\omega^{2} - \omega_{s}^{2} + i\omega\Gamma)}$$

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$$f'_s = \frac{\omega_s^2(\omega^2 - \omega_s^2)}{(\omega^2 - \omega_s^2)^2 + (\omega\Gamma)^2}$$

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The scattering factor can be rewritten

and since $\Gamma \ll \omega_s$

the second term being the dispersion correction whose real and imaginary components can be extracted

$$\begin{split} f_{s} &= \frac{\omega^{2} + \left(-\omega_{s}^{2} + i\omega\Gamma\right) - \left(-\omega_{s}^{2} + i\omega\Gamma\right)}{\left(\omega^{2} - \omega_{s}^{2} + i\omega\Gamma\right)} \\ &= 1 + \frac{\omega_{s}^{2} - i\omega\Gamma}{\left(\omega^{2} - \omega_{s}^{2} + i\omega\Gamma\right)} \approx 1 + \frac{\omega_{s}^{2}}{\left(\omega^{2} - \omega_{s}^{2} + i\omega\Gamma\right)} \end{split}$$

$$\chi(\omega) = f'_{s} + if''_{s} = \frac{\omega_{s}^{2}}{(\omega^{2} - \omega_{s}^{2} + i\omega\Gamma)}$$

$$\chi(\omega) = \frac{\omega_s^2}{(\omega^2 - \omega_s^2 + i\omega\Gamma)} \cdot \frac{(\omega^2 - \omega_s^2 - i\omega\Gamma)}{(\omega^2 - \omega_s^2 - i\omega\Gamma)} = \frac{\omega_s^2(\omega^2 - \omega_s^2 - i\omega\Gamma)}{(\omega^2 - \omega_s^2)^2 + (\omega\Gamma)^2}$$
$$f'_s = \frac{\omega_s^2(\omega^2 - \omega_s^2)}{(\omega^2 - \omega_s^2)^2 + (\omega\Gamma)^2} \qquad f''_s = -\frac{\omega_s^2\omega\Gamma}{(\omega^2 - \omega_s^2)^2 + (\omega\Gamma)^2}$$



Single oscillator dispersion terms

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These dispersion terms give resonant corrections to the scattering factor

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These dispersion terms give resonant corrections to the scattering factor

$$f'_{s} = \frac{\omega_{s}^{2}(\omega^{2} + \omega_{s}^{2})}{(\omega^{2} - \omega_{s}^{2})^{2} + (\omega\Gamma)^{2}}$$



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Single oscillator dispersion terms

These dispersion terms give resonant corrections to the scattering factor

$$f'_{s} = \frac{\omega_{s}^{2}(\omega^{2} + \omega_{s}^{2})}{(\omega^{2} - \omega_{s}^{2})^{2} + (\omega\Gamma)^{2}}$$

$$f_s'' = -rac{\omega_s^2 \omega \Gamma}{(\omega^2 - \omega_s^2)^2 + (\omega \Gamma)^2}$$



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