Today's outline - November 09, 2021

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- HAXPES Experiments

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Reading Assignment: Chapter 8.4

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Reading Assignment: Chapter 8.4

Homework Assignment #06:
Chapter 6: 1,6,7,8,9
due Tuesday, November 16, 2021

Today's outline - November 09, 2021

- HAXPES Experiments
- X-ray magnetic circular dichroism
- Resonant Scattering

Reading Assignment: Chapter 8.4

Homework Assignment #06:
Chapter 6: 1,6,7,8,9
due Tuesday, November 16, 2021

Homework Assignment #07:
Chapter 7: 2,3,9,10,11
due Tuesday, November 30, 2021

Final projects & presentations

In-class student presentations on research topics

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- Choose a research article which features a synchrotron technique

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- Think of a research problem (could be yours) that can be approached using synchrotron radiation techniques
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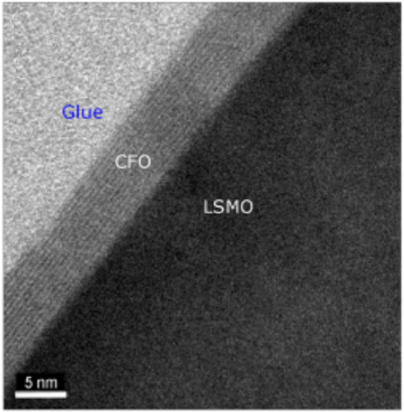
- Must be different techique than your presentation!

HAXPES of buried interfaces

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 ± 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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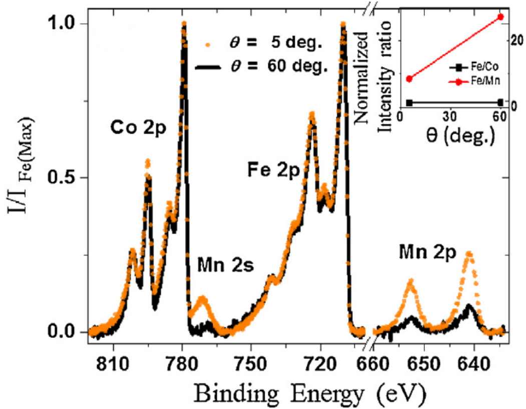

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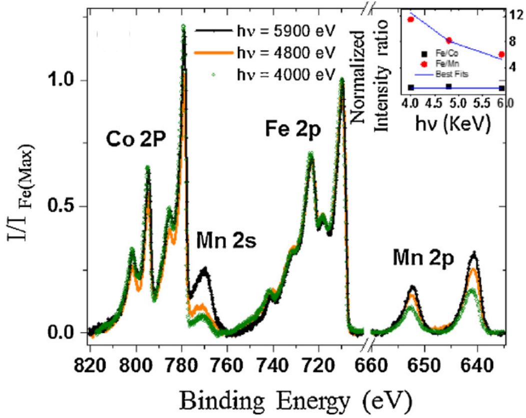

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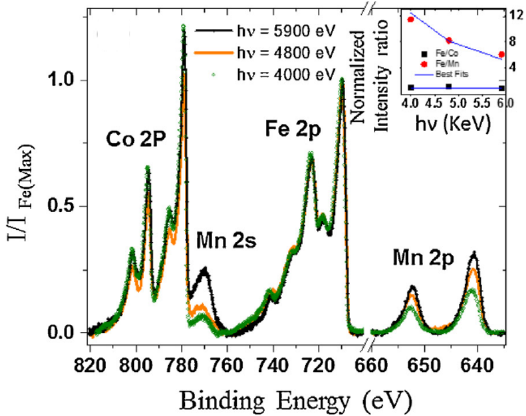

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Both results give consistent results with proper normalization and also show the uniformity of the $CoFe_2O_4$ overlayer

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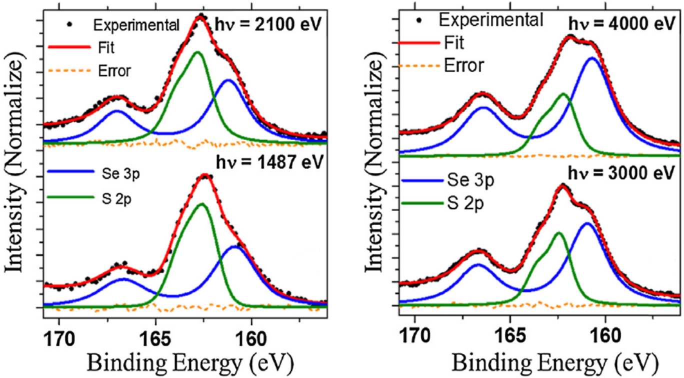
Energy dispersive measurements can provide depth profiling of spherical nanoparticles



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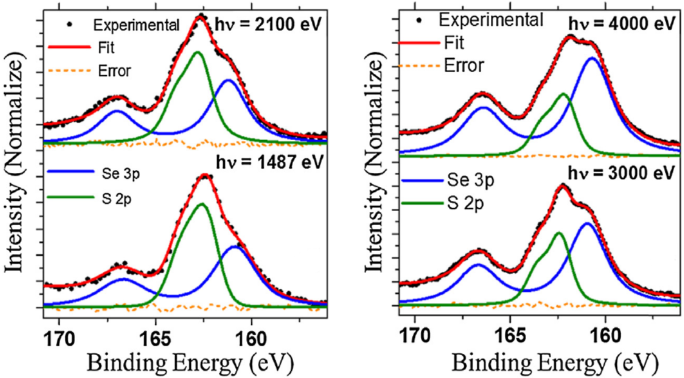

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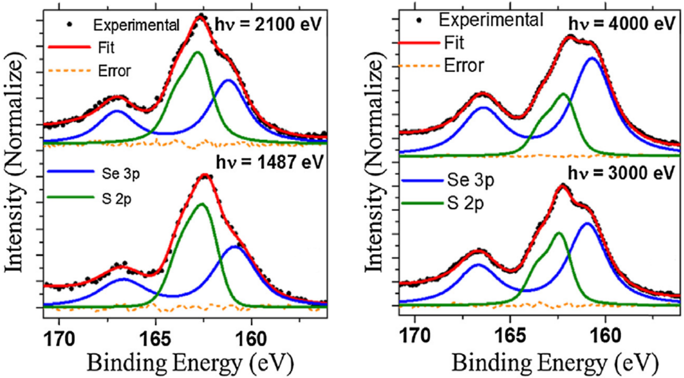

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By fitting the S 2*p* and Se 3*p* photoemission line the structure is revealed to be CdSe at the core and ZnCdS in the outer shell

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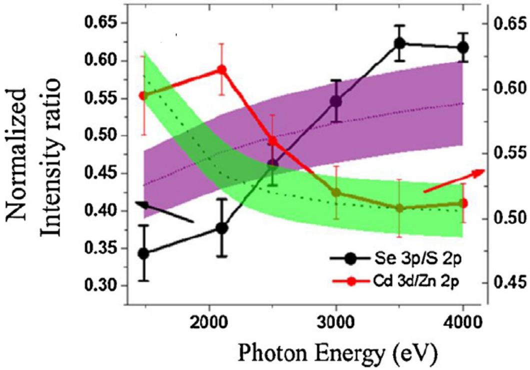

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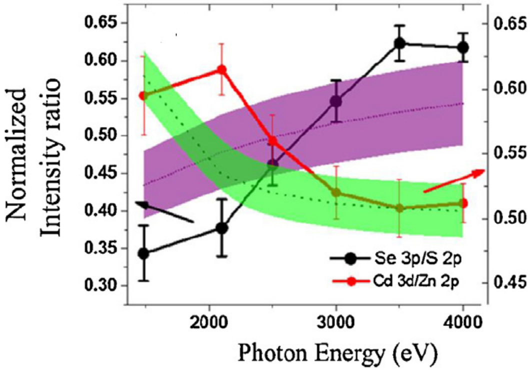

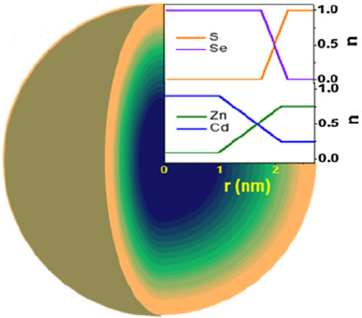

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HAXPES of Si anodes

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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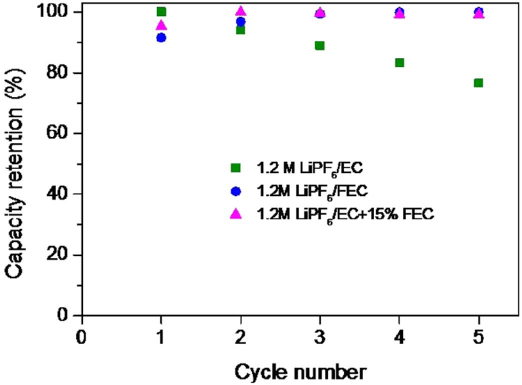

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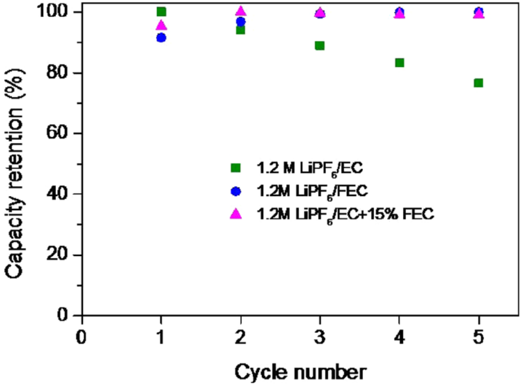

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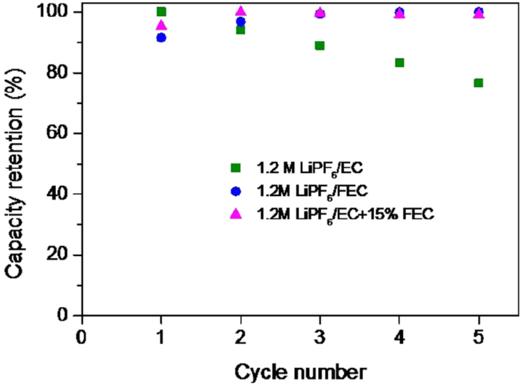

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HAXPES is used to determine the elemental distribution and compounds present as a function of depth in the cycled Si anode.

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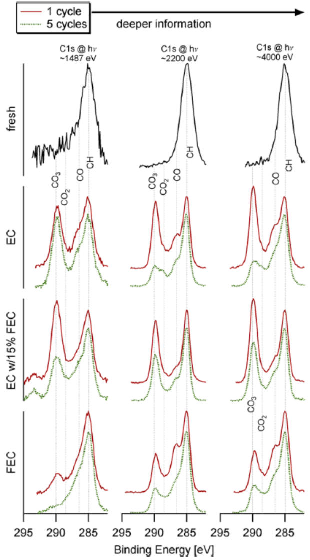

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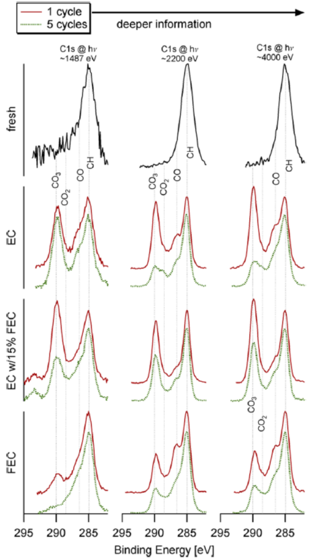

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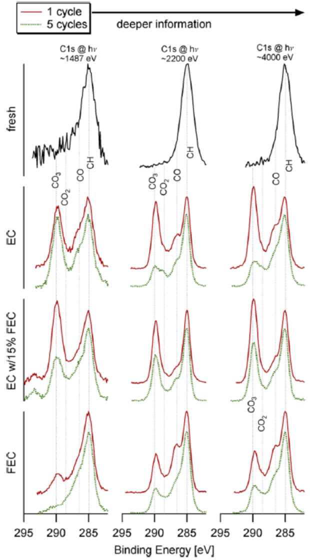

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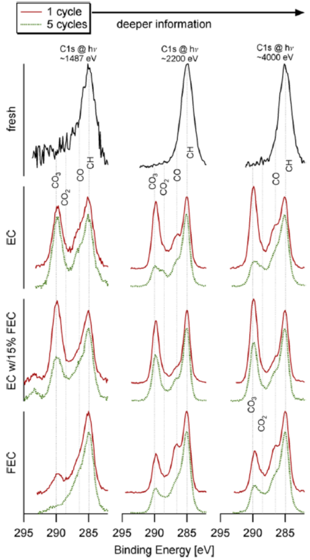

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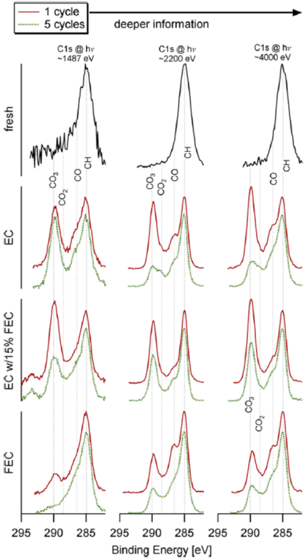

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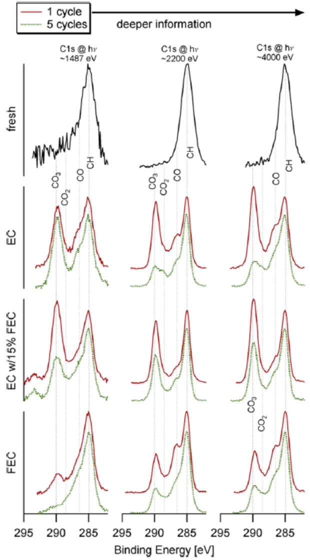

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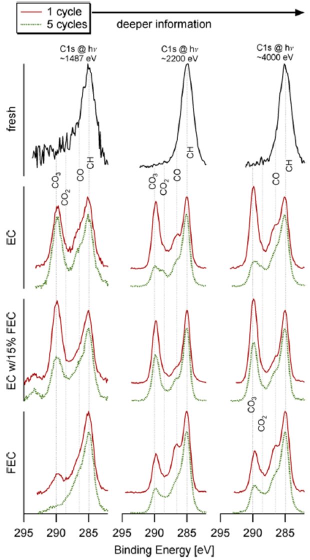

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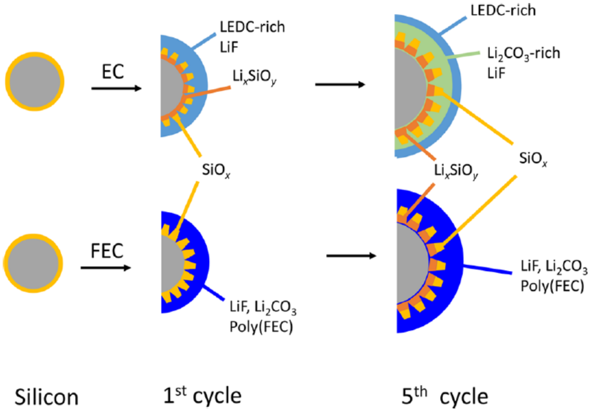

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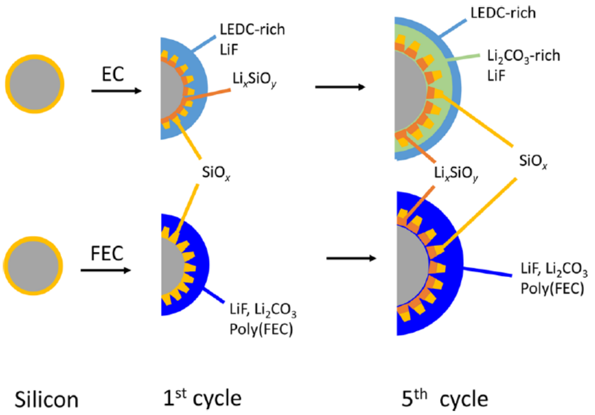

as SEI grows, there is growth of Li_xSiO_y underneath as product of lithiation/delithiation

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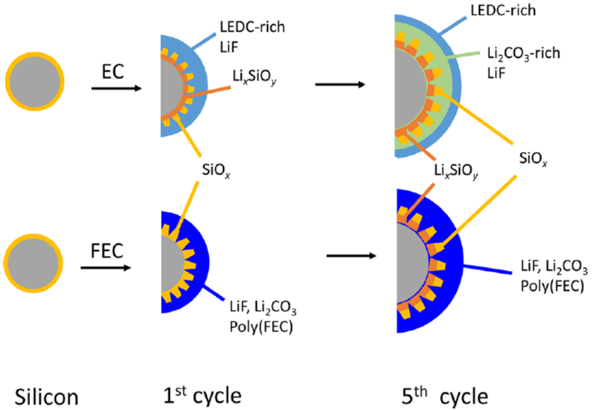

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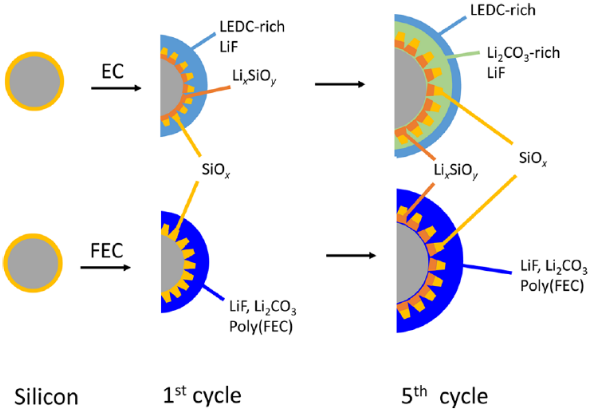

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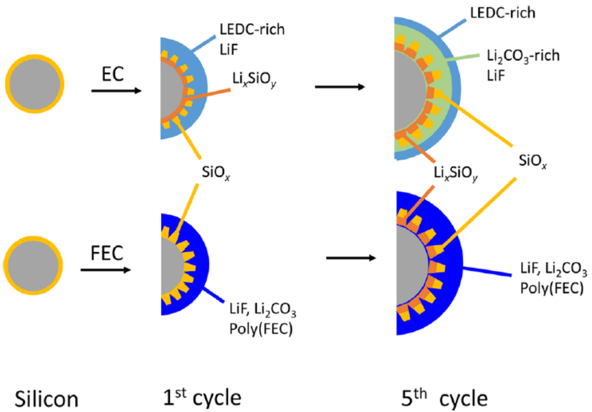

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The FEC acts to stabilize the SEI composition and prevent the change with depth that occurs with EC.

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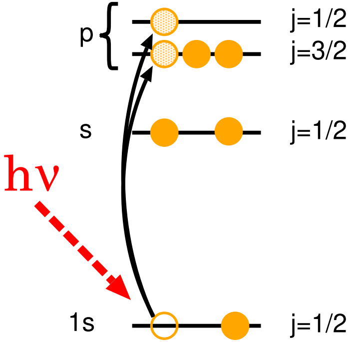

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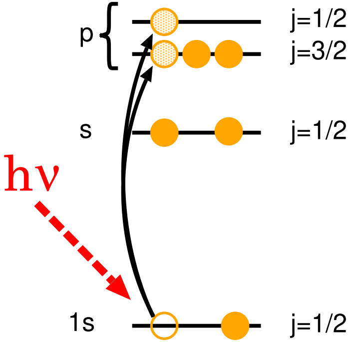

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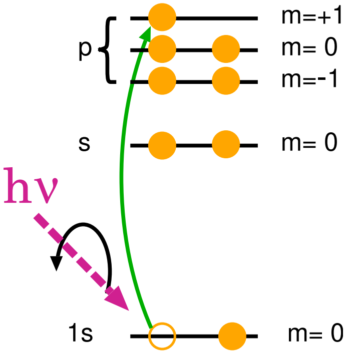

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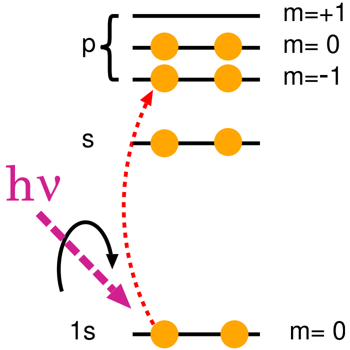

X-ray magnetic circular dichroism

The interaction x-rays with magnetic systems is generally weak and not considered in scattering experiments

One exception is the absorption coefficient of circularly polarized x-rays

in a normal x-ray absorption event, the selection rules for a transition are $\Delta l = \pm 1$, $\Delta m = 0, \pm 1$

if circularly polarized x-rays are used, however, the selection rules for m depend on the "handedness" of the radiation

$\Delta m = +1$ for "right-handed"

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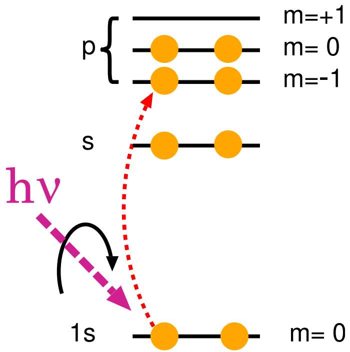
this measurement is sensitive to the internal/external magnetic fields which split the levels according to the Zeeman effect



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XMCD of $Yb_{14}MnSb_{11}$

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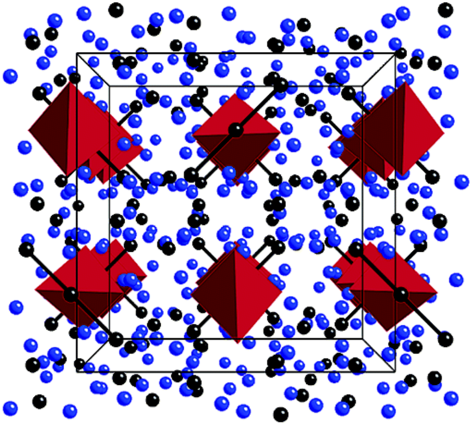

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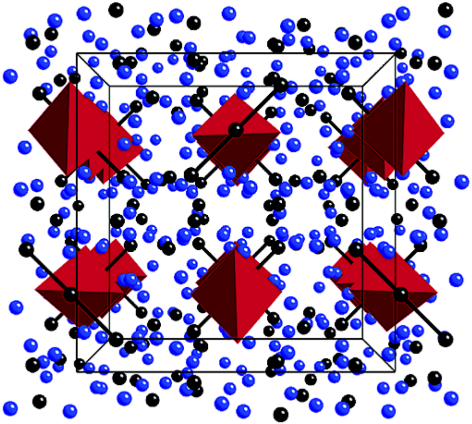

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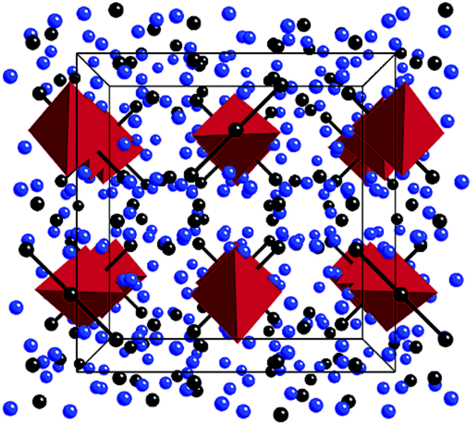

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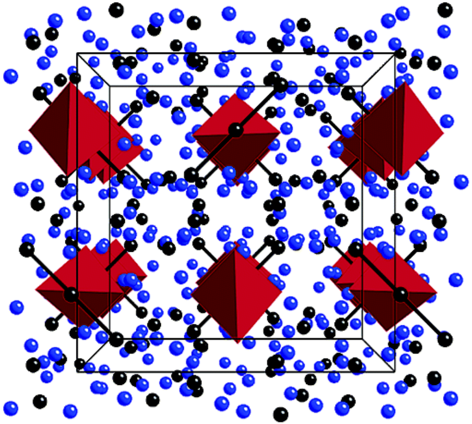

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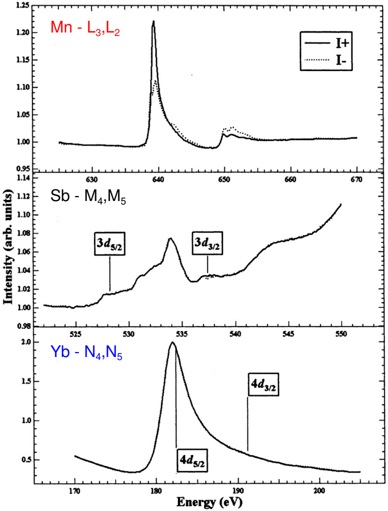

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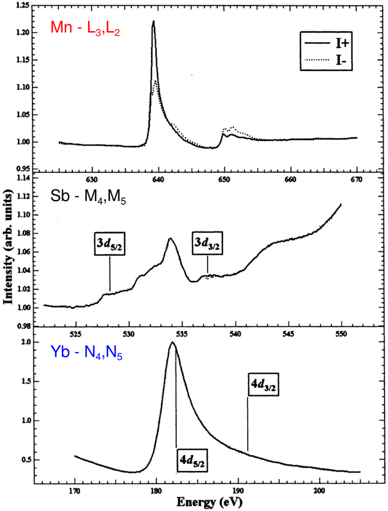

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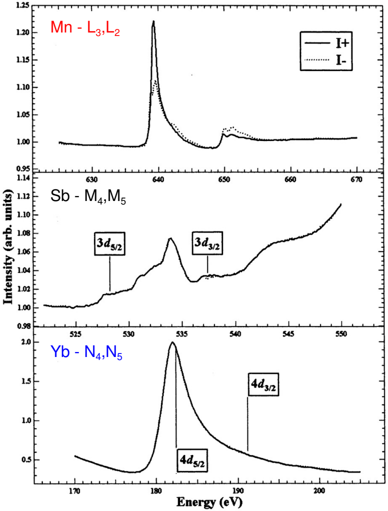

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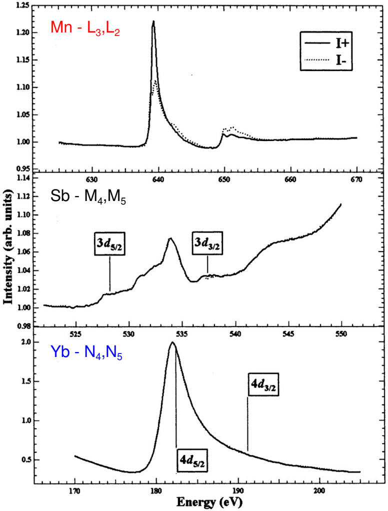

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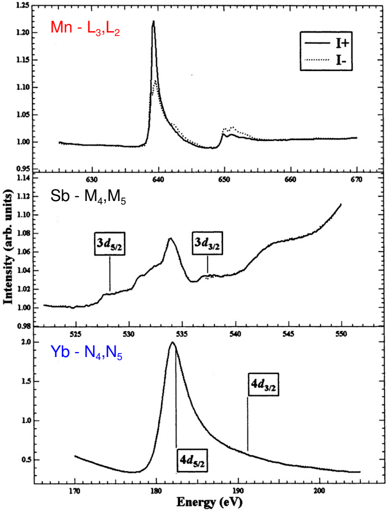

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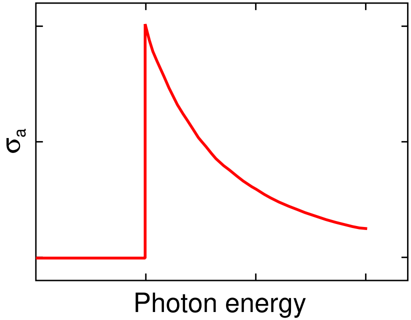

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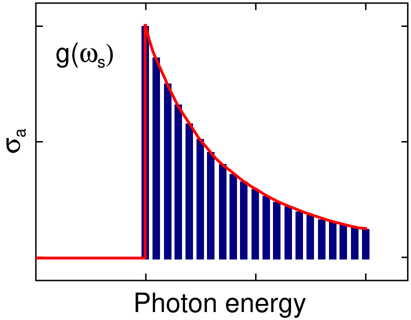

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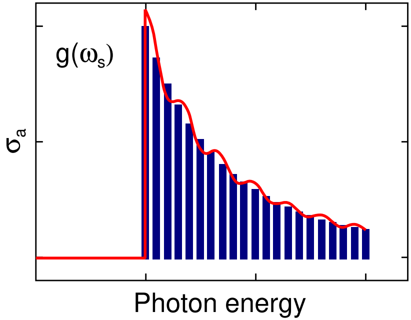

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This will produce the resonant scattering term but not the XANES and EXAFS, which are purely quantum effects.

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The amplitude of the response has a resonance and dissipation

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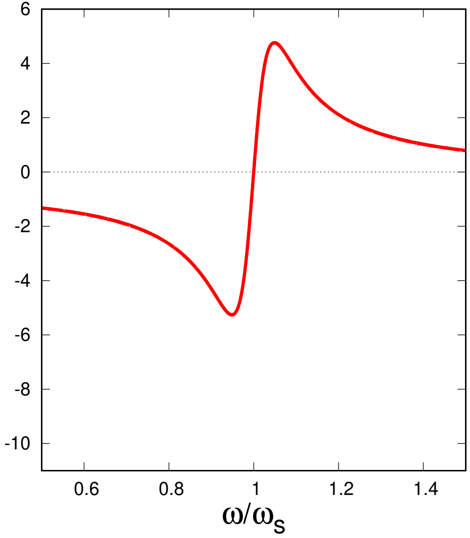

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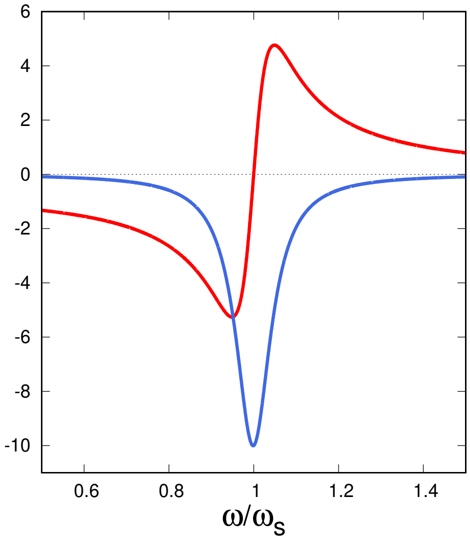

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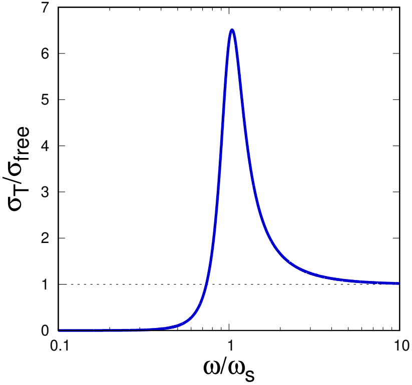

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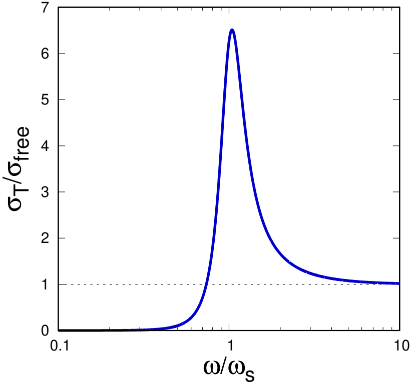

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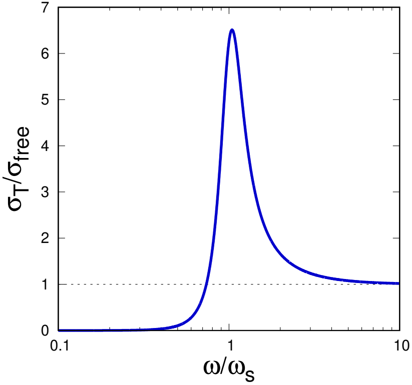

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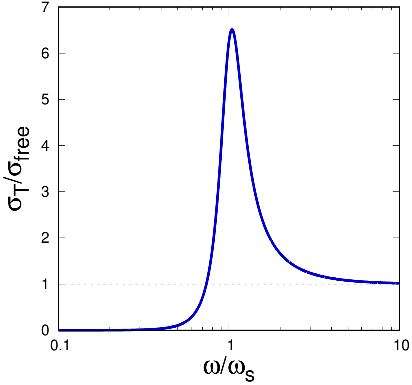

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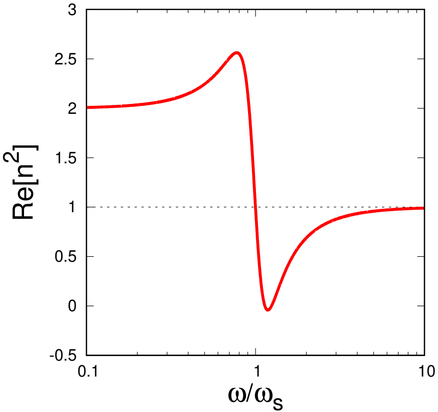

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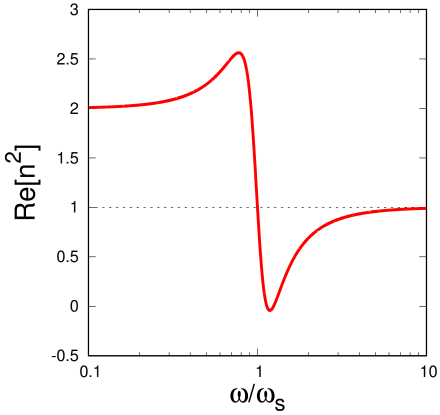

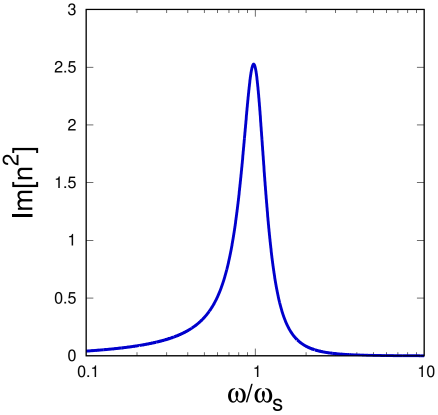

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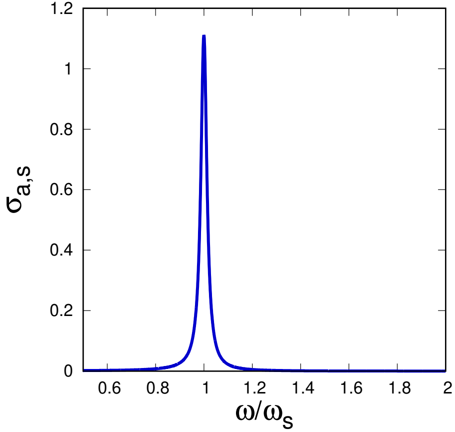

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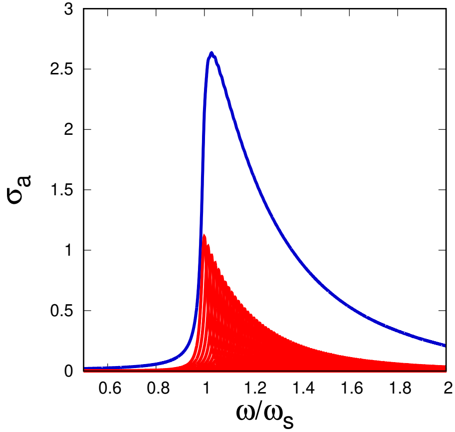

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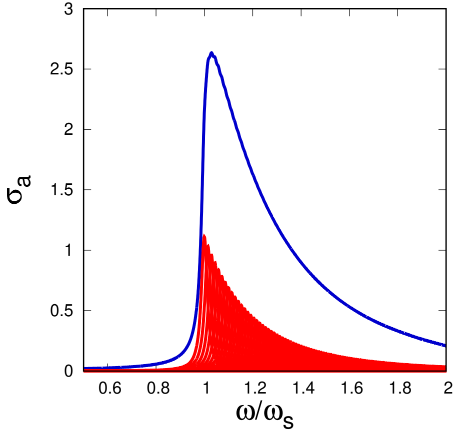

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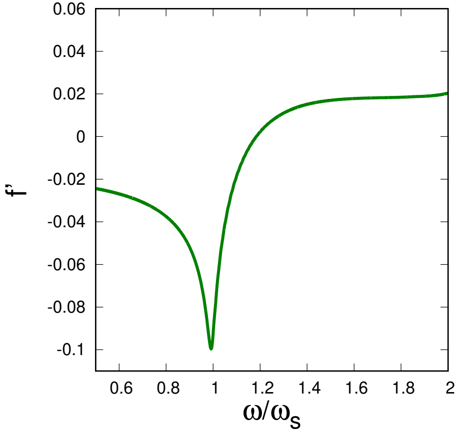

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The Kramers-Kronig relations are derived using Cauchy's theorem to integrate a function with a pole

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Starting with the Kramers-Kronig relation for f'

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if ω_K is the frequency of the K absorption edge and a substitution is made with $x = \omega'/\omega_K$ and $x_K = \omega/\omega_K$, f' becomes

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$$f'(\omega) = \frac{2}{\pi}\mathcal{P}\int_0^\infty \frac{\omega' f''(\omega')}{(\omega'^2 - \omega^2)}d\omega' = -\frac{2}{\pi}\frac{1}{4\pi r_0 c}\mathcal{P}\int_0^\infty \frac{\omega'^2 \sigma_a(\omega')}{(\omega'^2 - \omega^2)}d\omega'$$

if ω_K is the frequency of the K absorption edge and a substitution is made with $x = \omega'/\omega_K$ and $x_K = \omega/\omega_K$, f' becomes

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this can be evaluated for two $1s$ electrons

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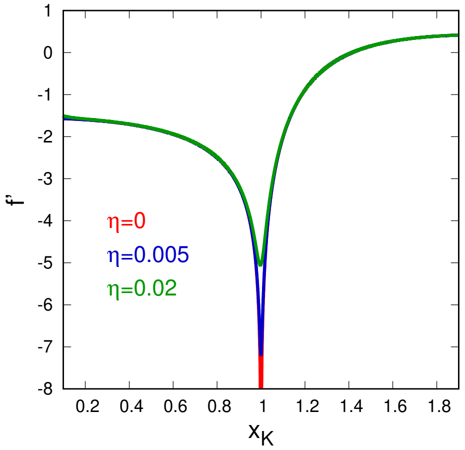

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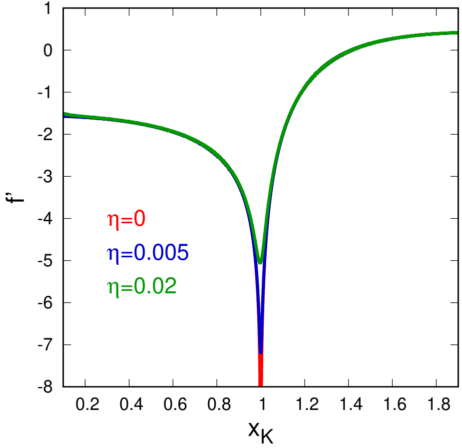
at high energies ($x_K \to \infty$) this dispersion correction vanishes as expected and at low energies ($x_K, q \to 0$) the correction is -1.565, thereby partially quenching the scattering from the two 1s electrons



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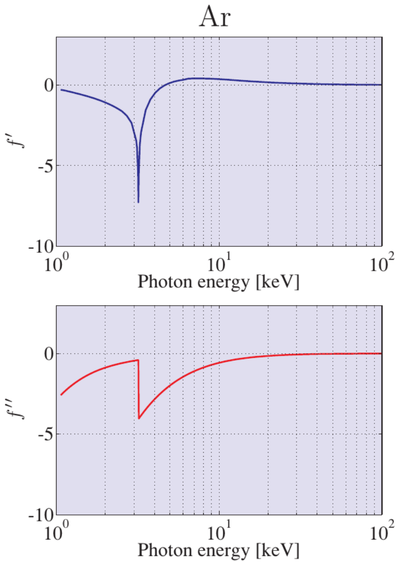

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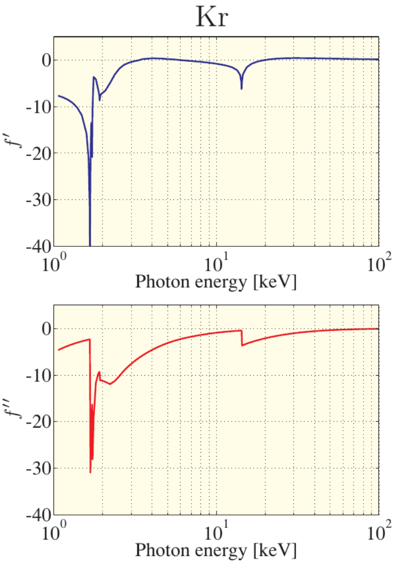

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What is lacking, even in the more sophisticated calcuations, are the resonances near the absorption edges due to XANES, EXAFS and other localized resonance phenomena