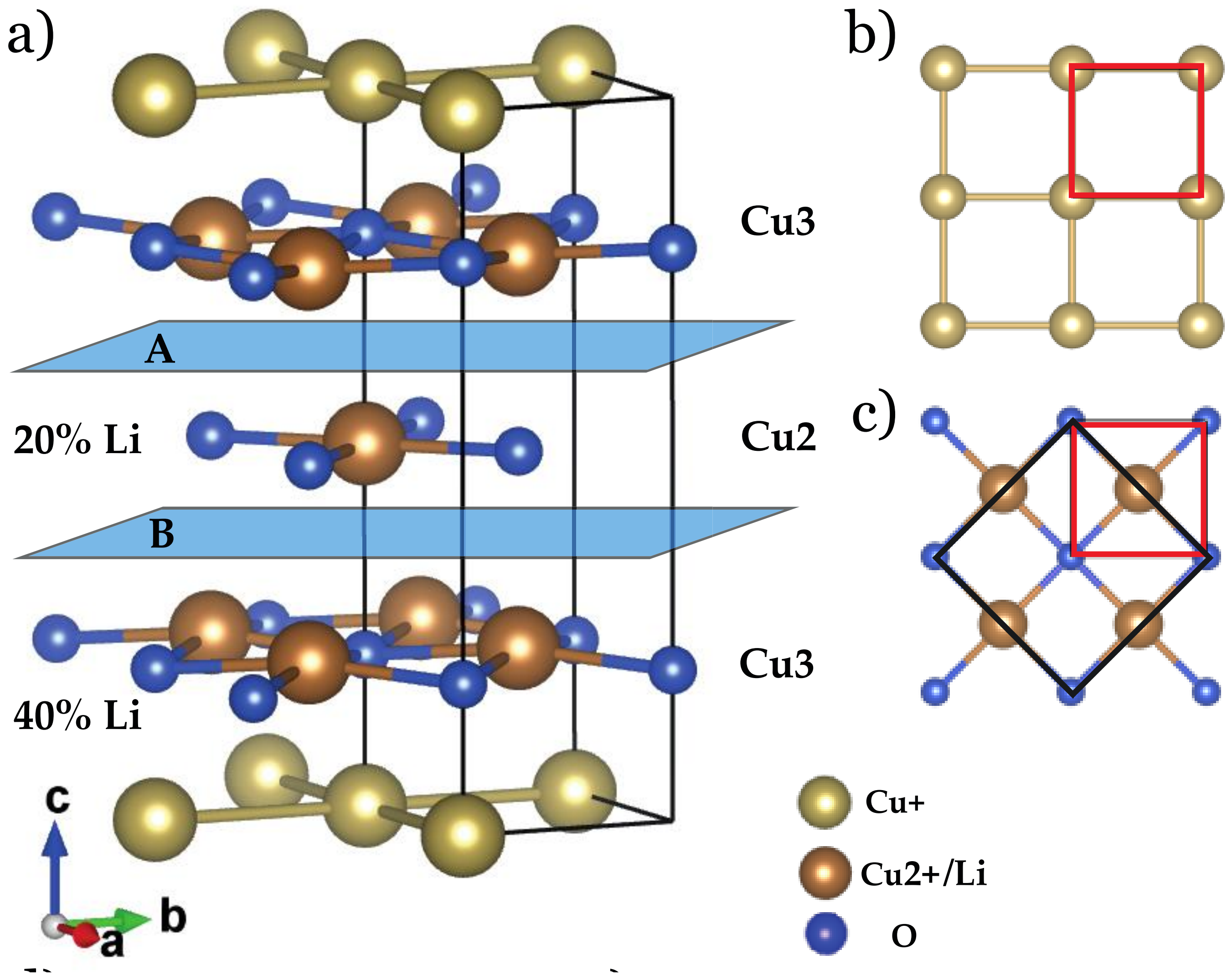
RESONANT SOFT X-RAY SPECTROSCOPY ON $LiCu_3O_3$

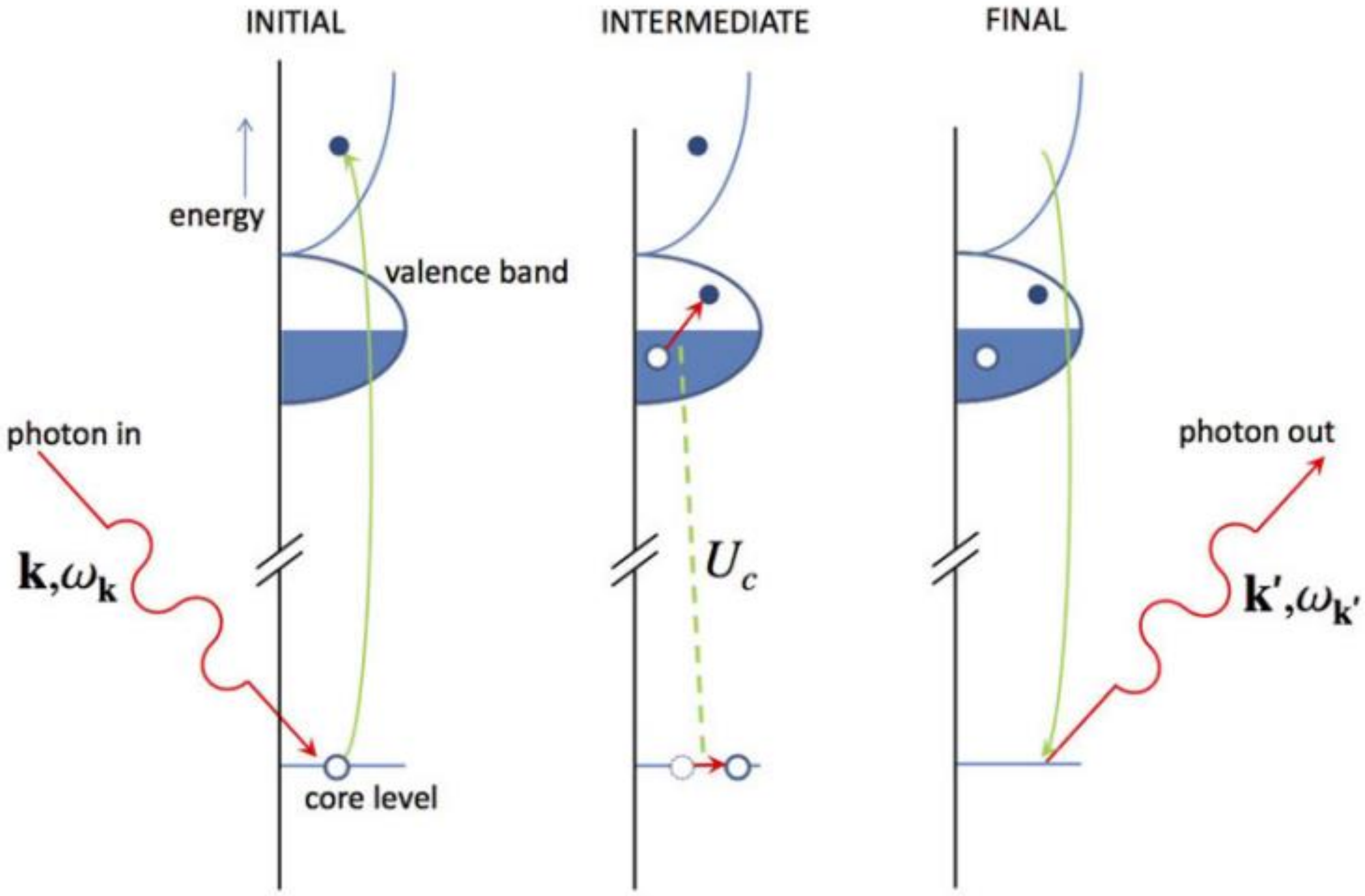
LICU$_3$O$_3$

- Trilayers of rocksalt Cu(II)O are sandwiched between planes of Cu(I)
- The Lithium randomly substitutes the Cu(II) ions
- Lattice: tetragonal crystal structure (P4/mmm, a = 2.81 A˚, c = 8.90 A˚)

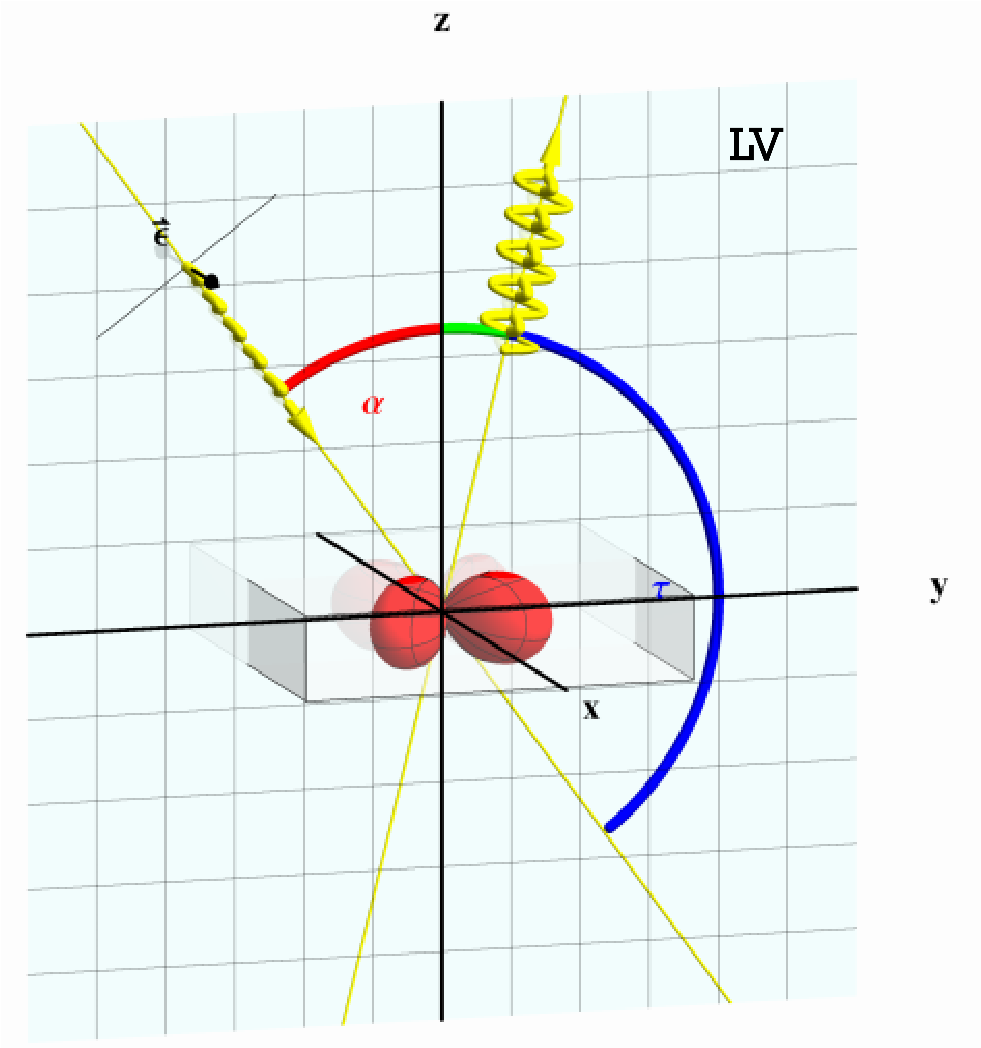


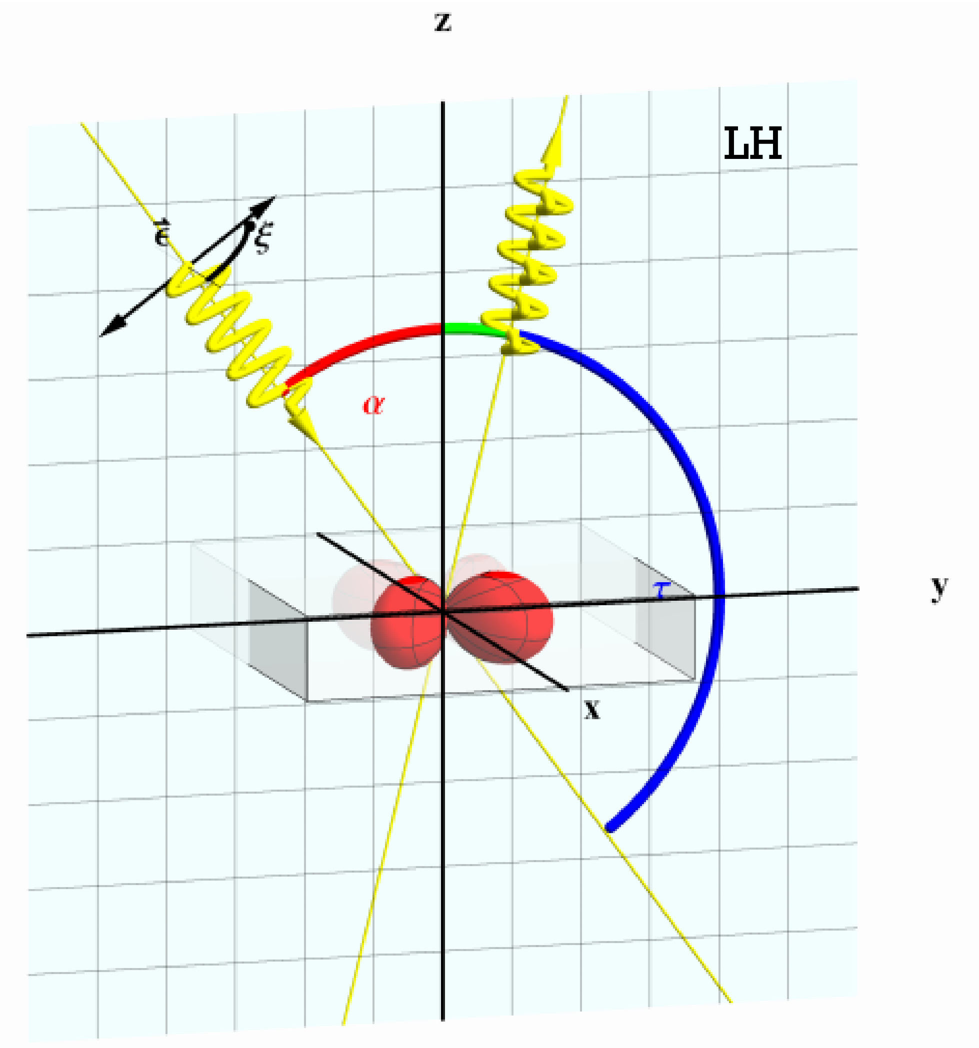
RIXS

Strong core hole – electron coulomb interaction, causes exciton generation (dd exciation)

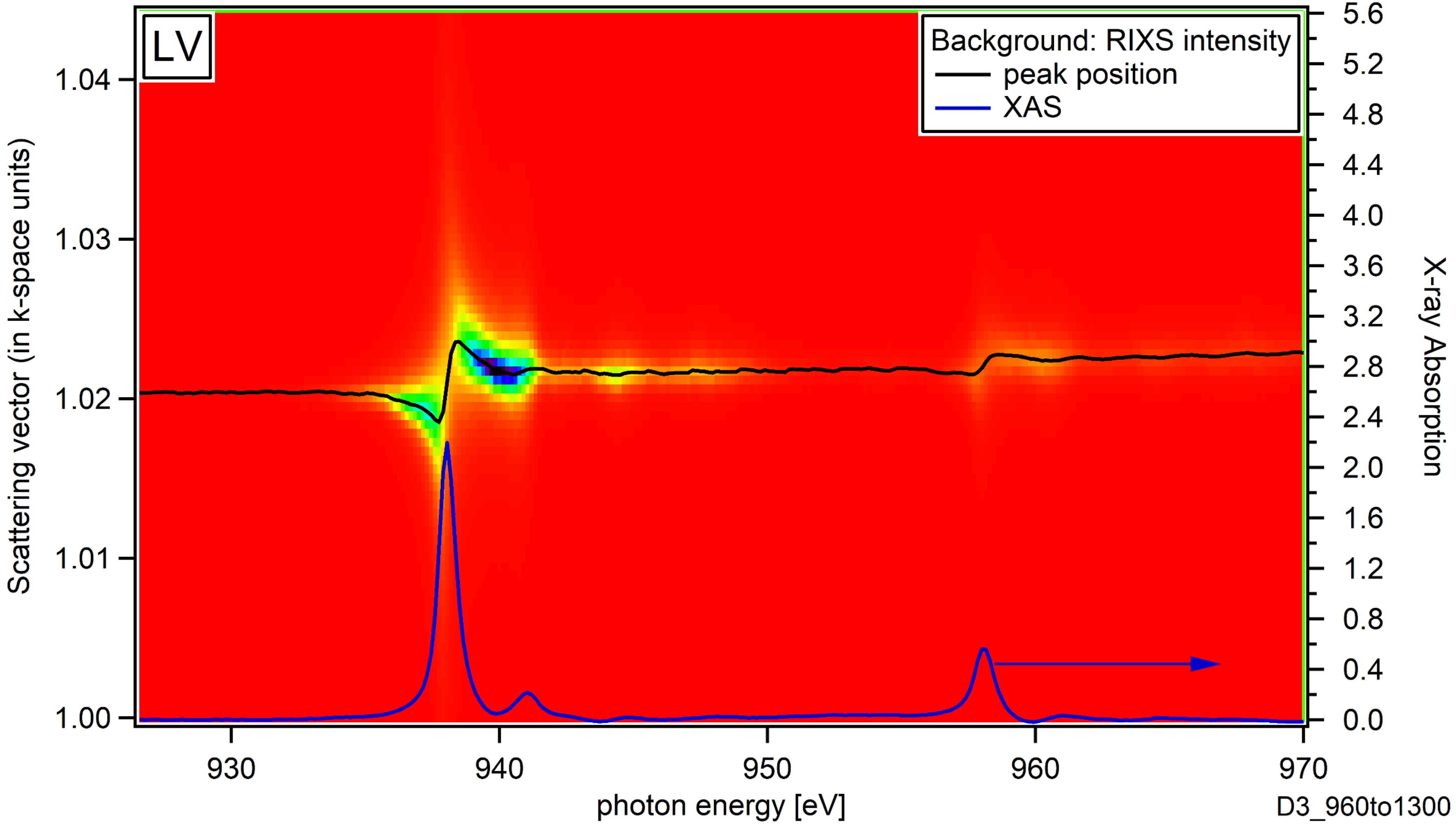


WAVE POLARISATION

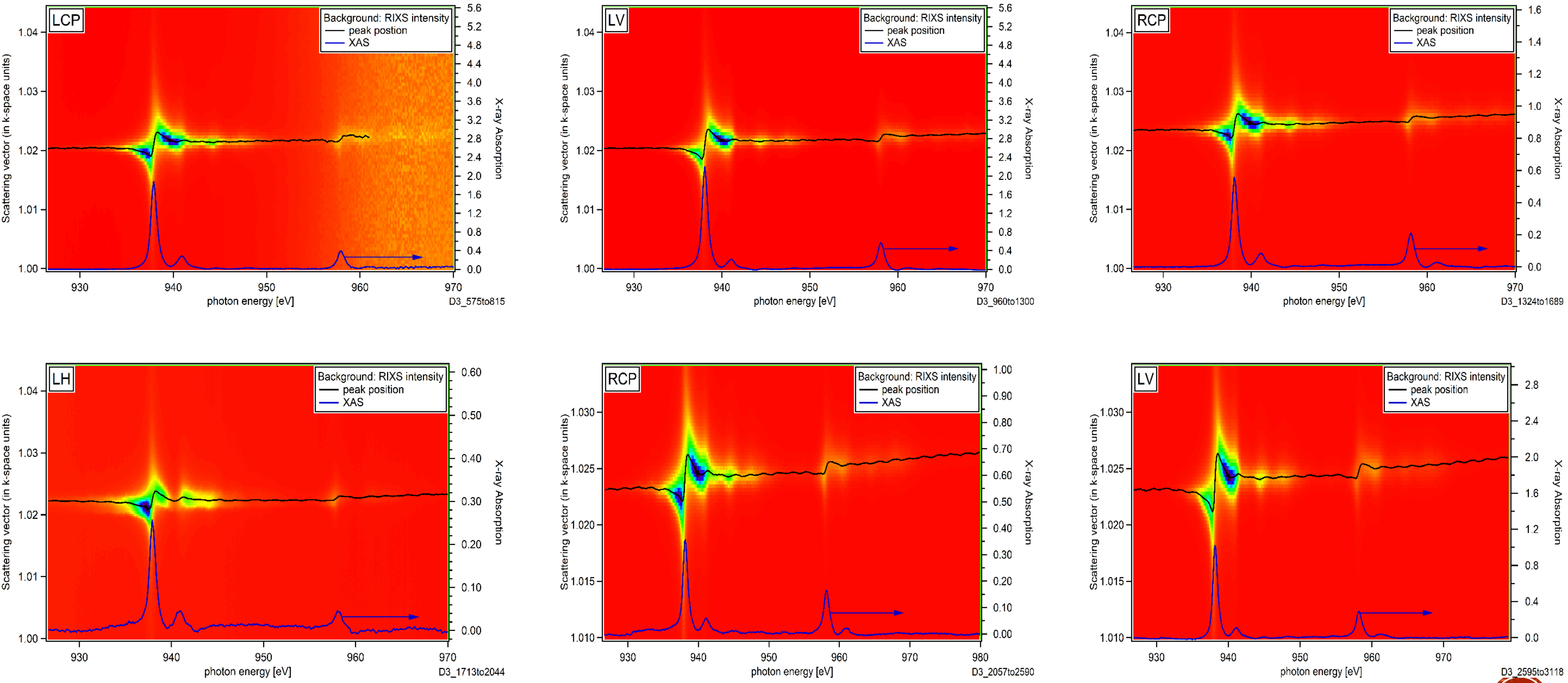




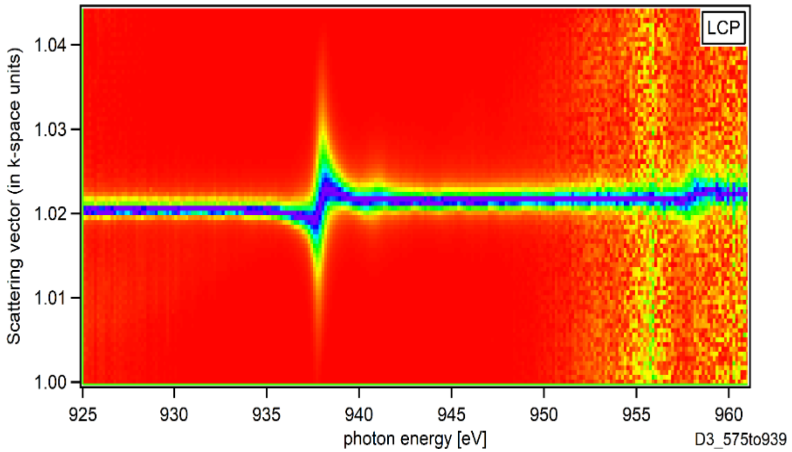
RIXS RESULTS

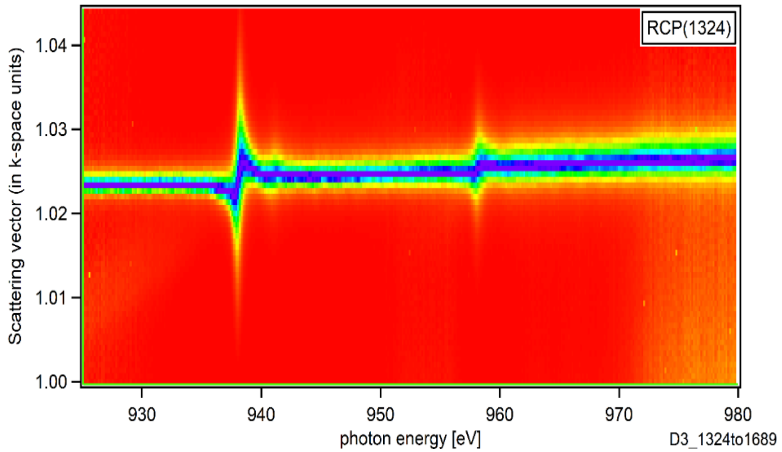


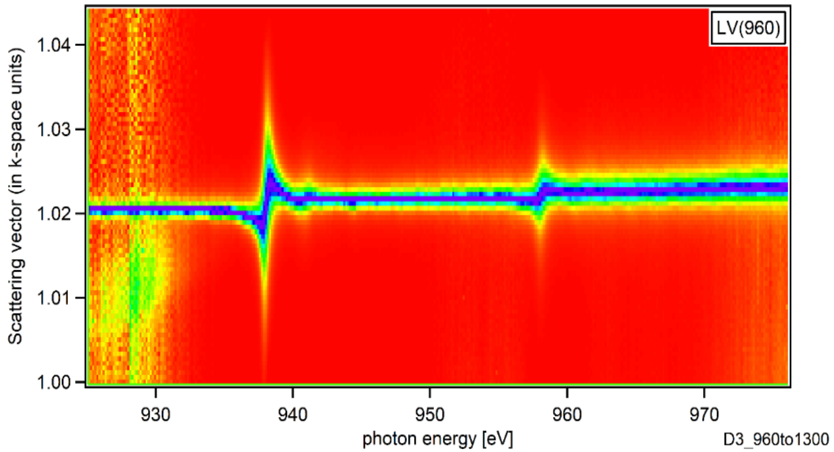
RSXS RESULT

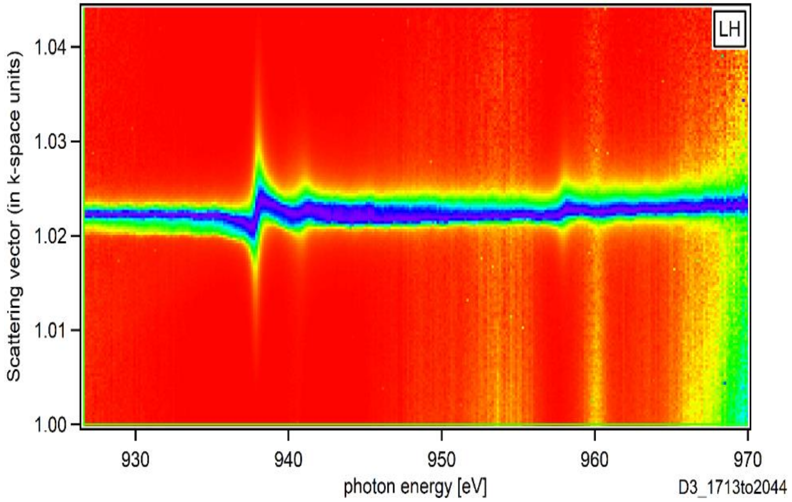

LCP
Background: RIXS intensity
peak postion
XAS
Scattering vector (in k-space units)
X-ray Absorption
photon energy [eV]
D3_575to815
LV
Background: RIXS intensity
peak position
XAS
D3_960to1300
RCP
Background: RIXS intensity
peak position
XAS
D3_1324to1689
LH
Background: RIXS intensity
peak position
XAS
D3_1713to2044
RCP
Background: RIXS intensity
peak position
XAS
D3_2057to2590
LV
Background: RIXS intensity
peak position
XAS
D3_2595to3118

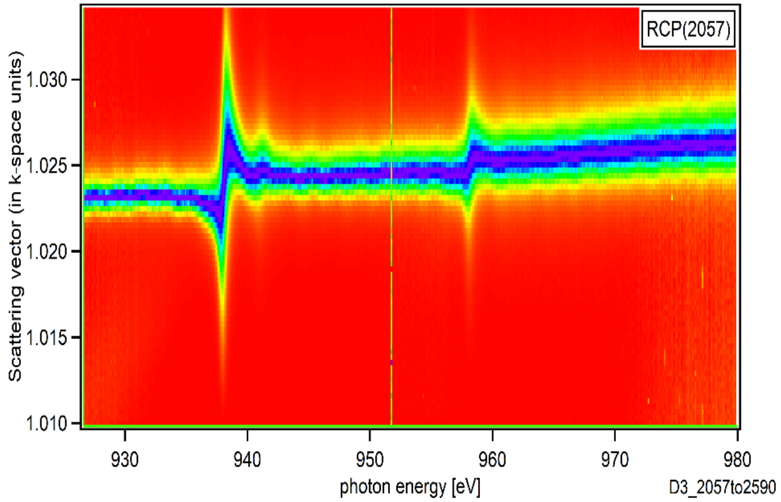
RIXS RESULTS – NORMALIZED ALONG THE PEAK

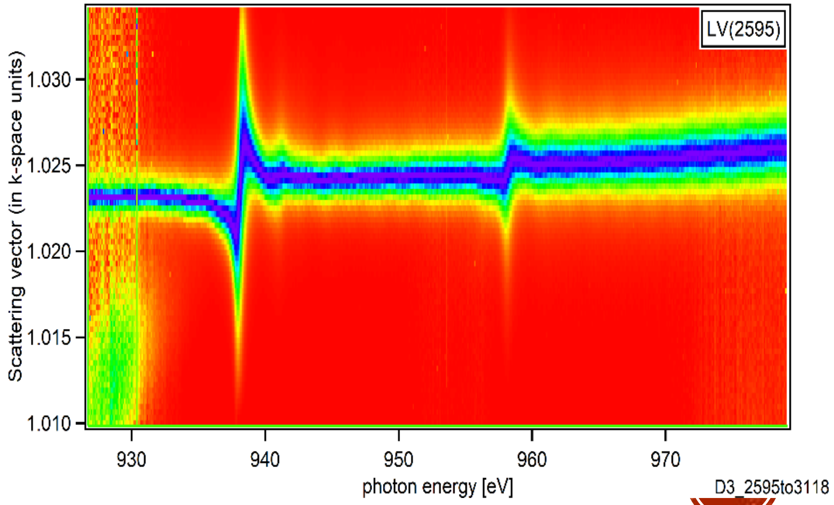




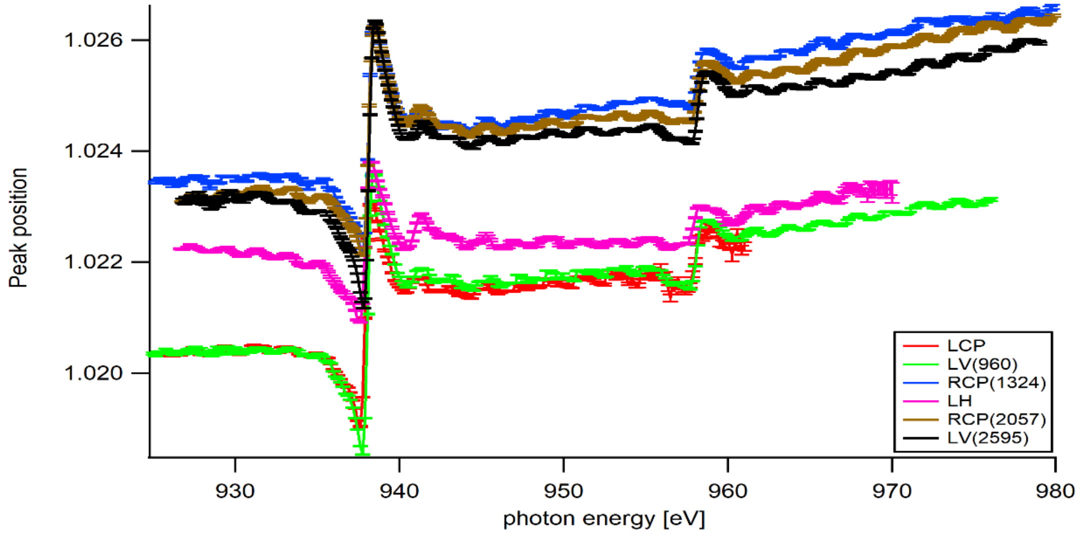








FITTING SPECTRUM WITH LORENTZIAN CURVE



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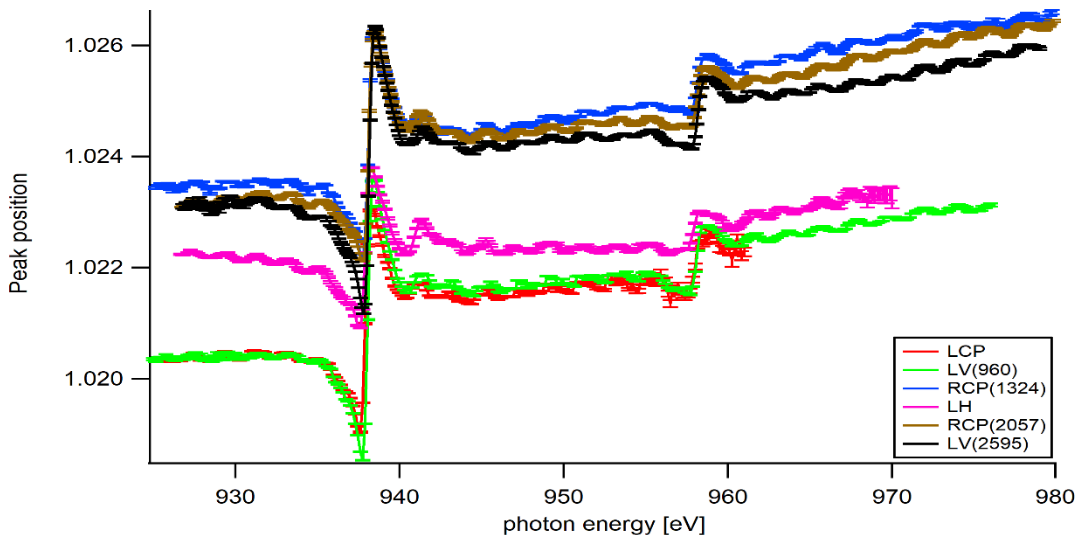

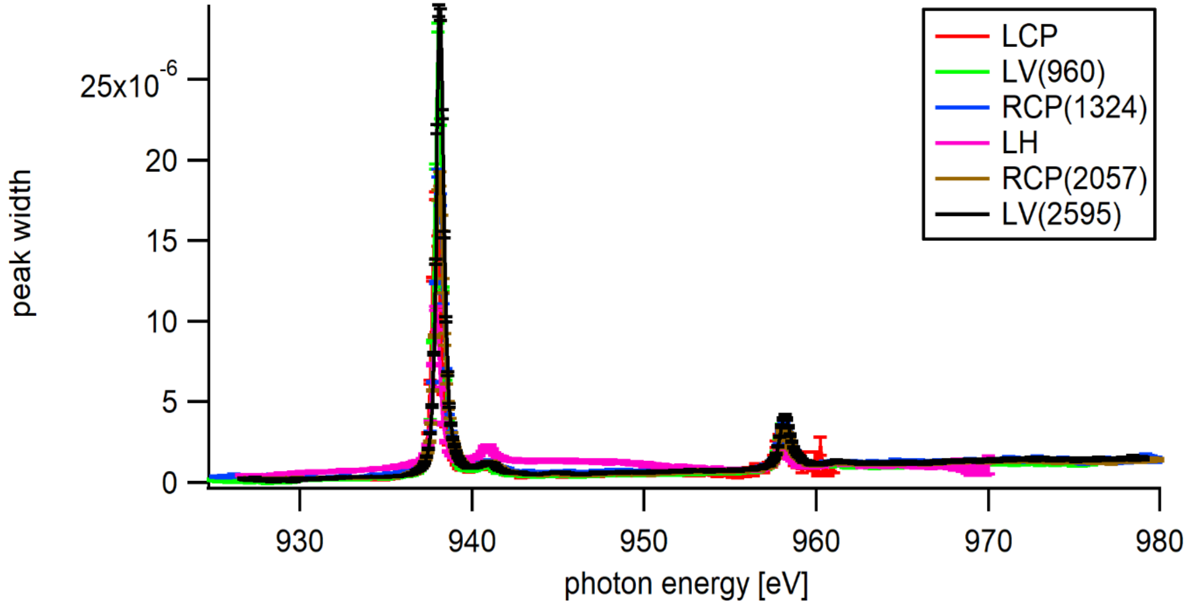

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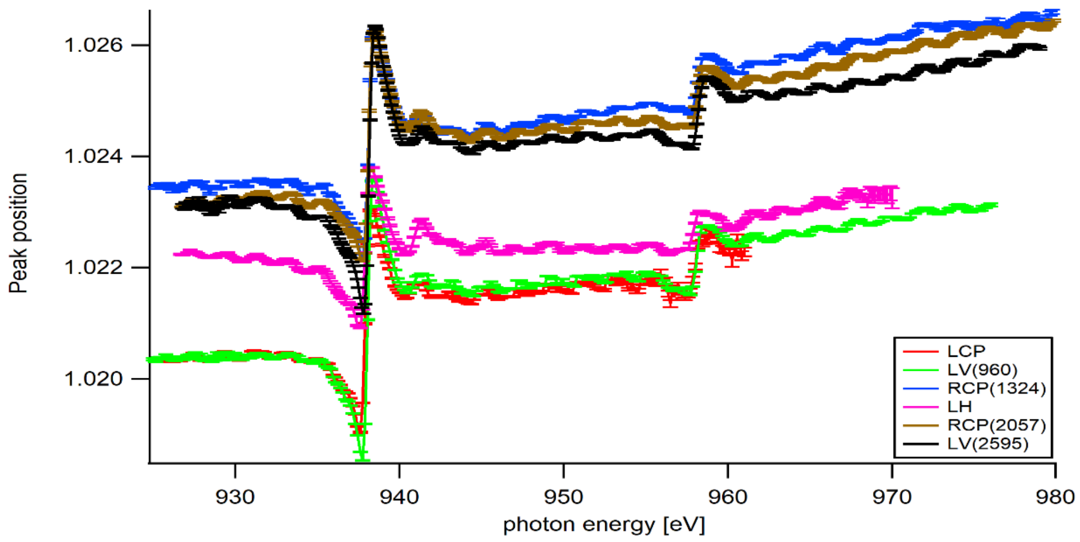

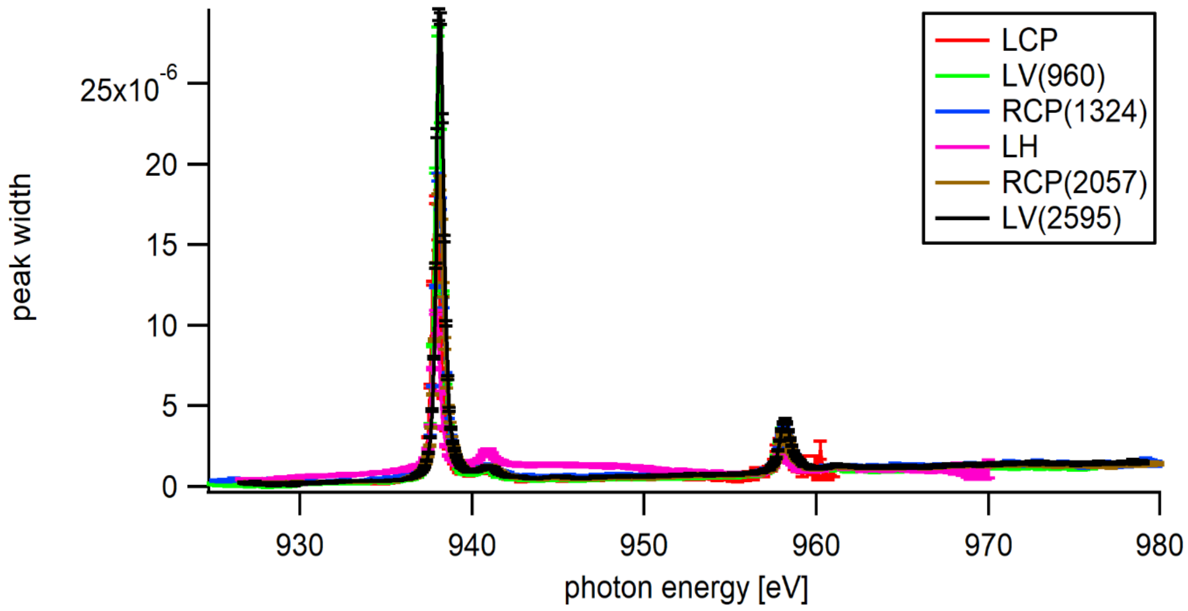

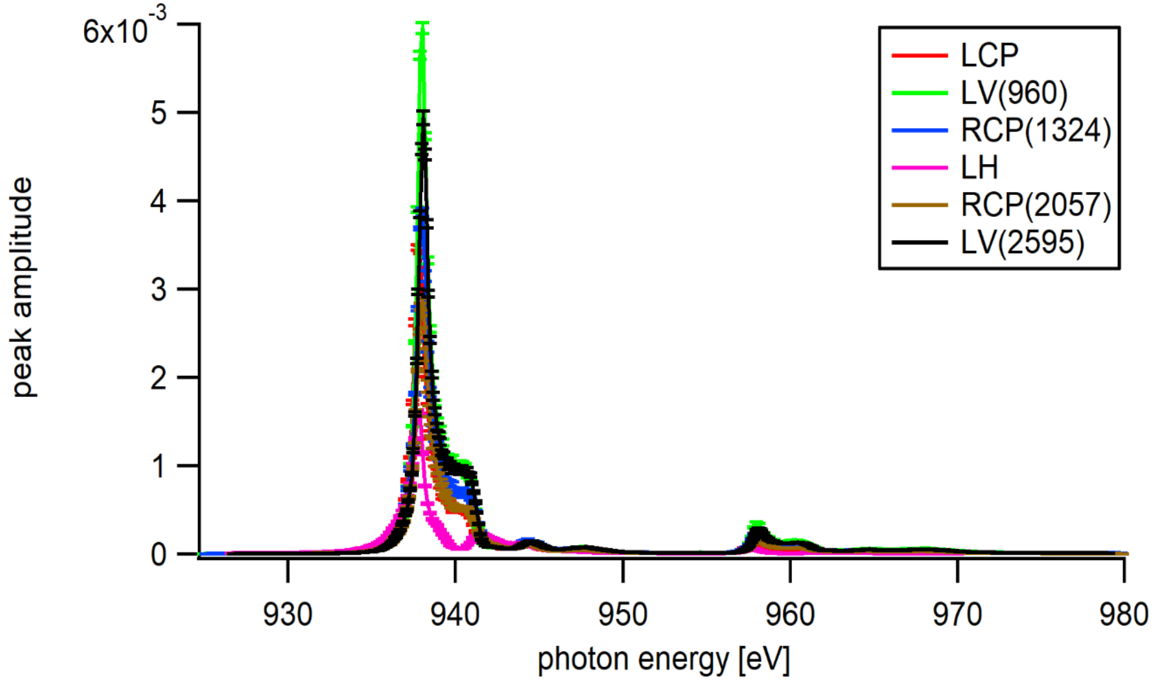

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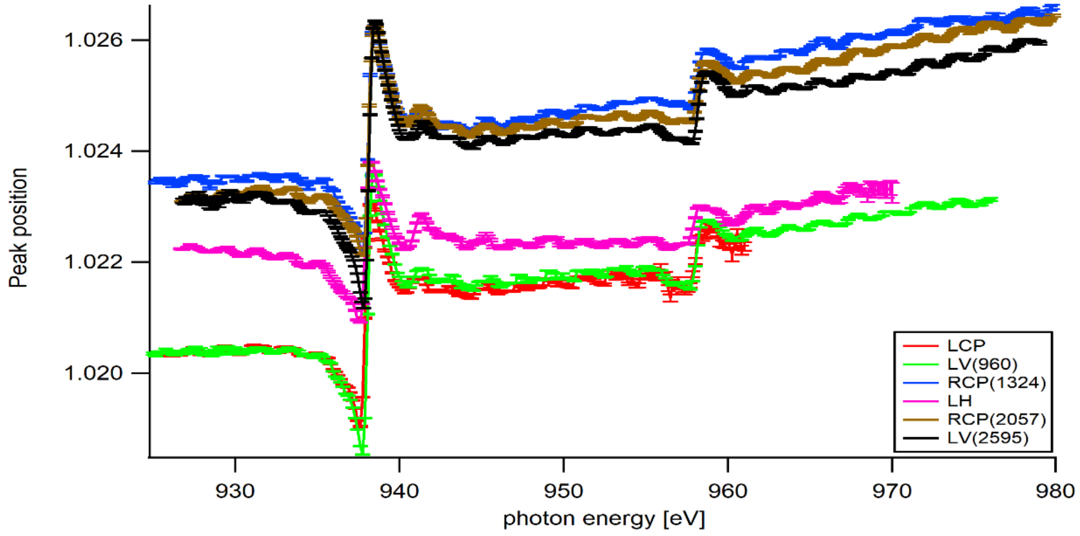
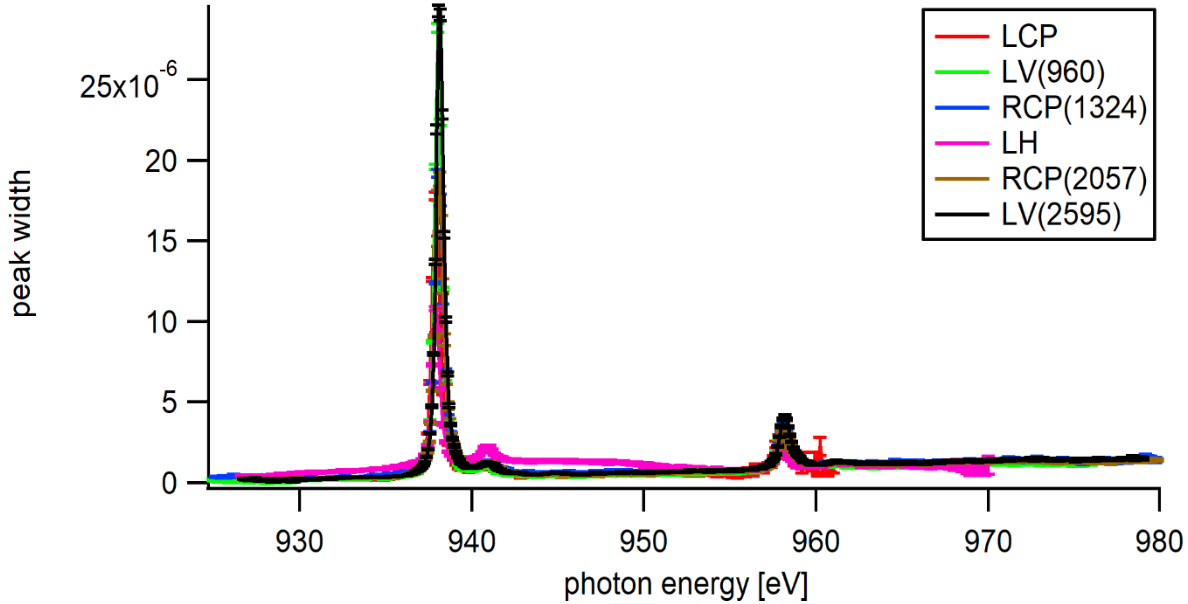
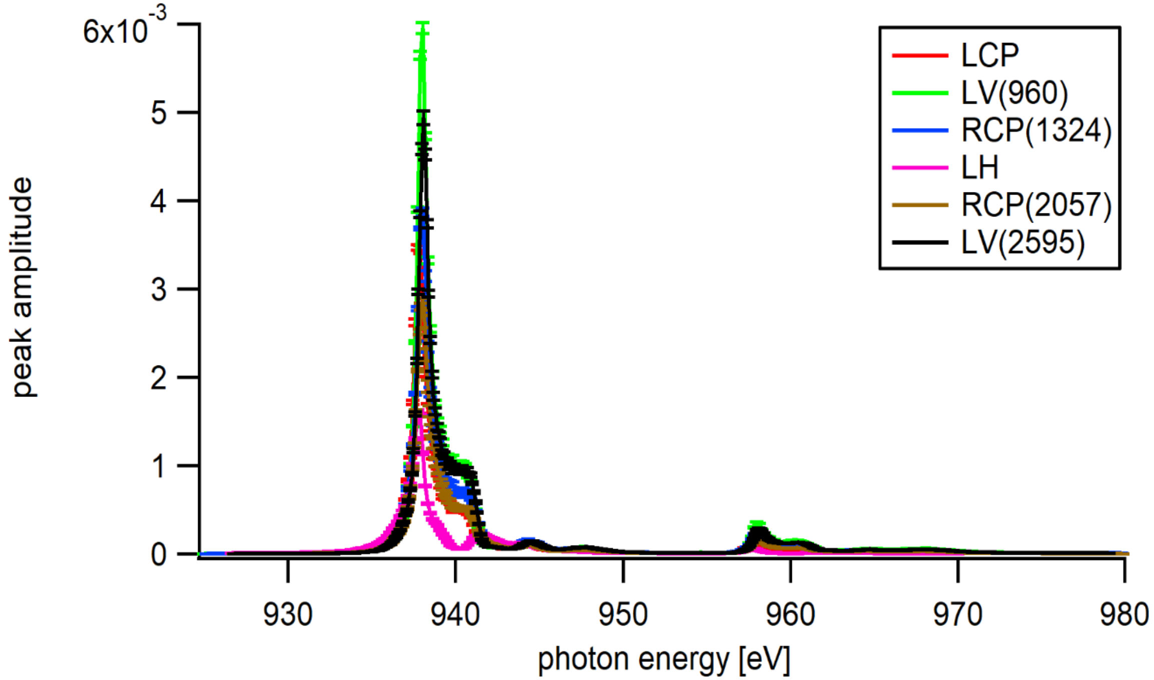


Bragg condition

$\lambda = 2d\sin\theta$





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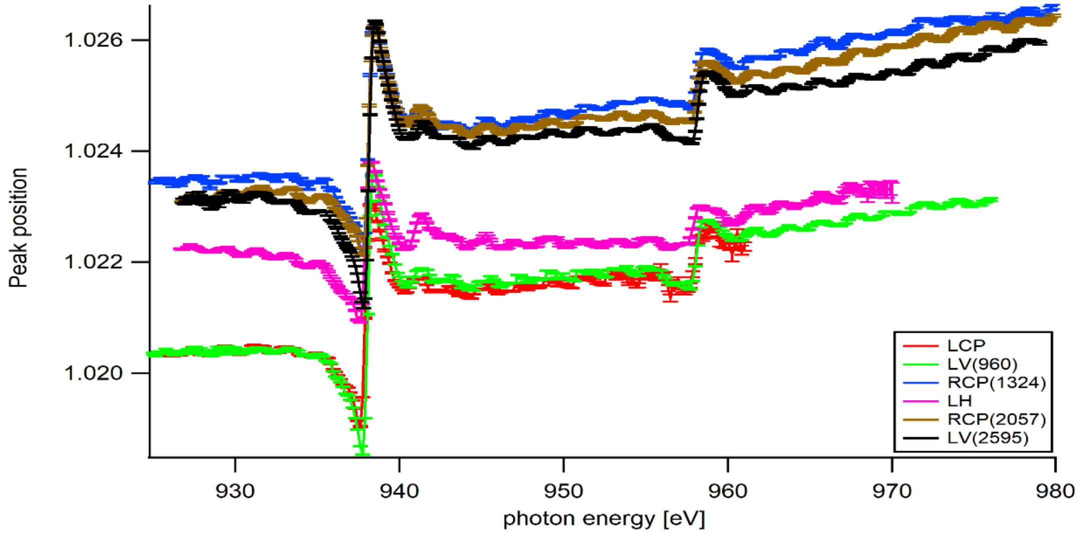

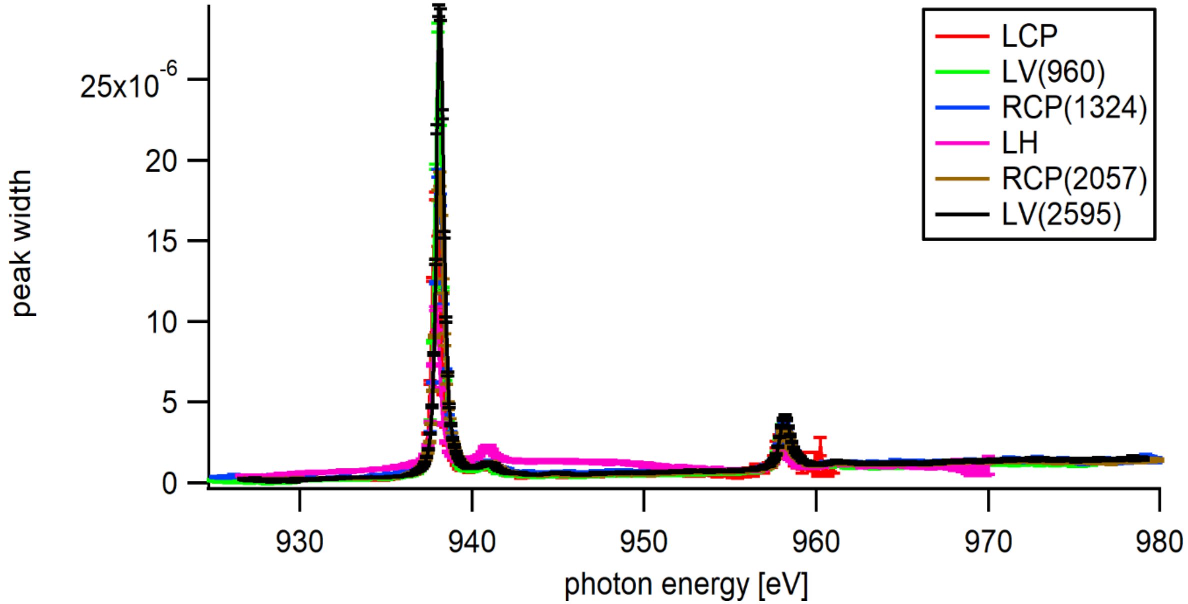

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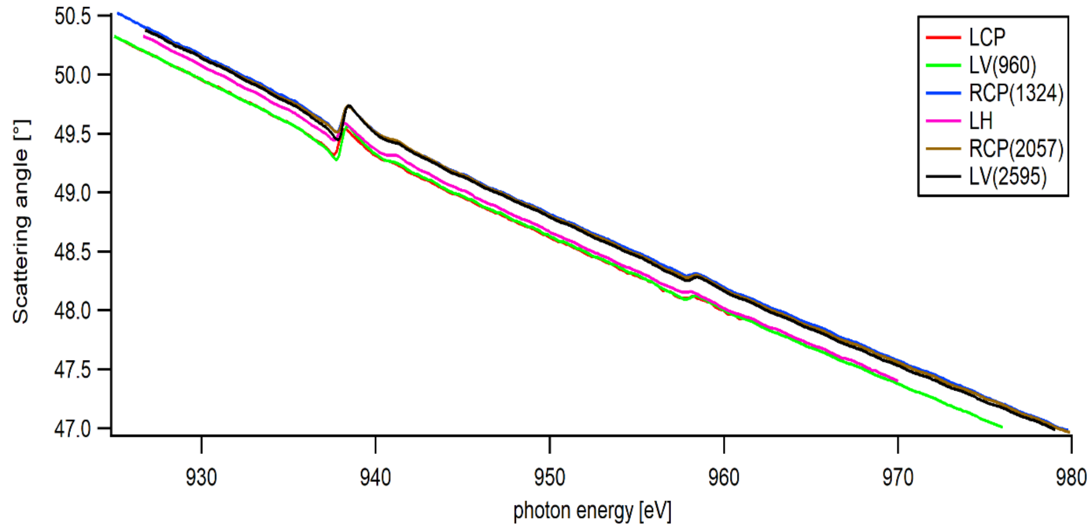

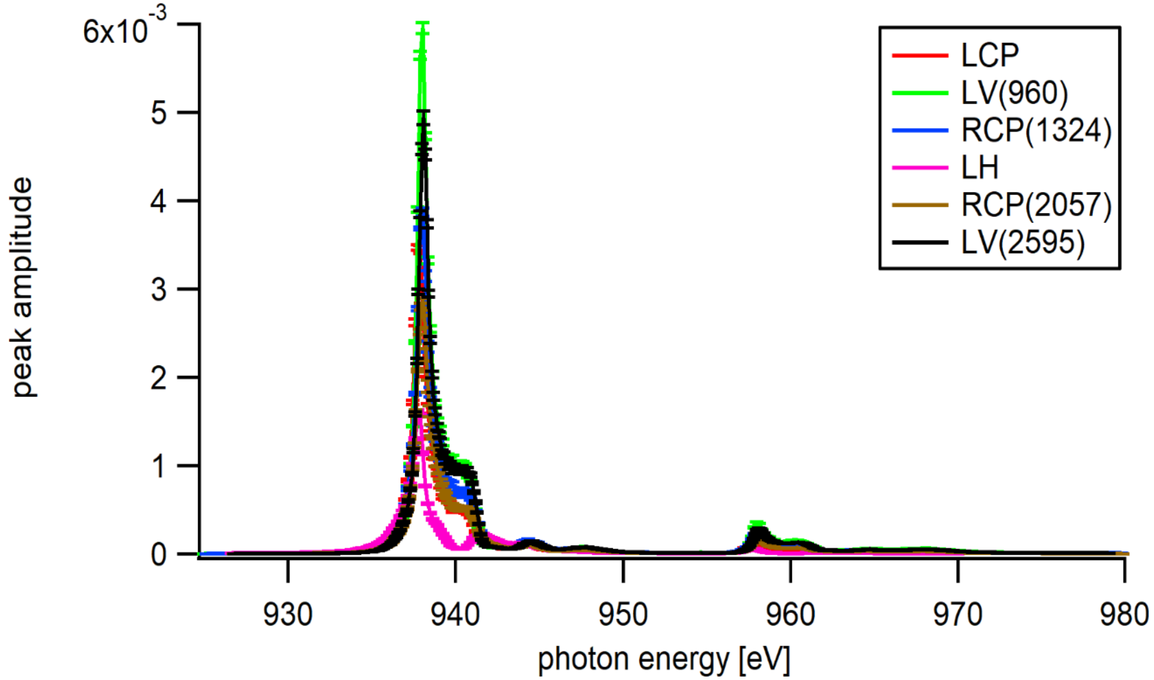

RESONANCE FREQUENCIES

Polarization	L3 edge		L2 edge	
	Cu^{2+}	Cu^{1+}	Cu^{2+}	Cu^{1+}
LCP	937.9	940.9	958	961.15
LV(960)	938.05	941.05	958.15	961
RCP(1324)	938.05	941.05	958.15	961.15
LH	937.9	940.9	958.3	961.3
RCP(2057)	938.15	941.05	958.15	961.15
LV(2595)	938.2	941.2	958.2	961.3

- Differences due to not sufficiently small enough Energy steps??
- Difference from theory – about 6eV ??

EXTRACTING PHYSICAL QUANTITIES FROM FIT DATA

Lorentzian curve: $y = y_0 + \frac{A}{(x-x_0)^2+B}$

$$FWHM = 2\sqrt{B}\,.$$

$$n_c(E) = n(E) + i\kappa(E)$$

According to [Seve,2]:

$$n(E) = 1 + \frac{1}{8}\left(\frac{hc}{2dE}\right)^2 - \frac{1}{2}\sin^2\theta_B$$

With d being the lattice constant in the [001] direction.

FWHM~$\frac{2\mu}{\sin\theta_B}$

$$\mu = \frac{2\omega\kappa}{c}$$

Thus:

$$\kappa(E) = \left(\frac{hc}{2dE}\right)^2 \cdot \sqrt{B} \cdot x_0(E)$$

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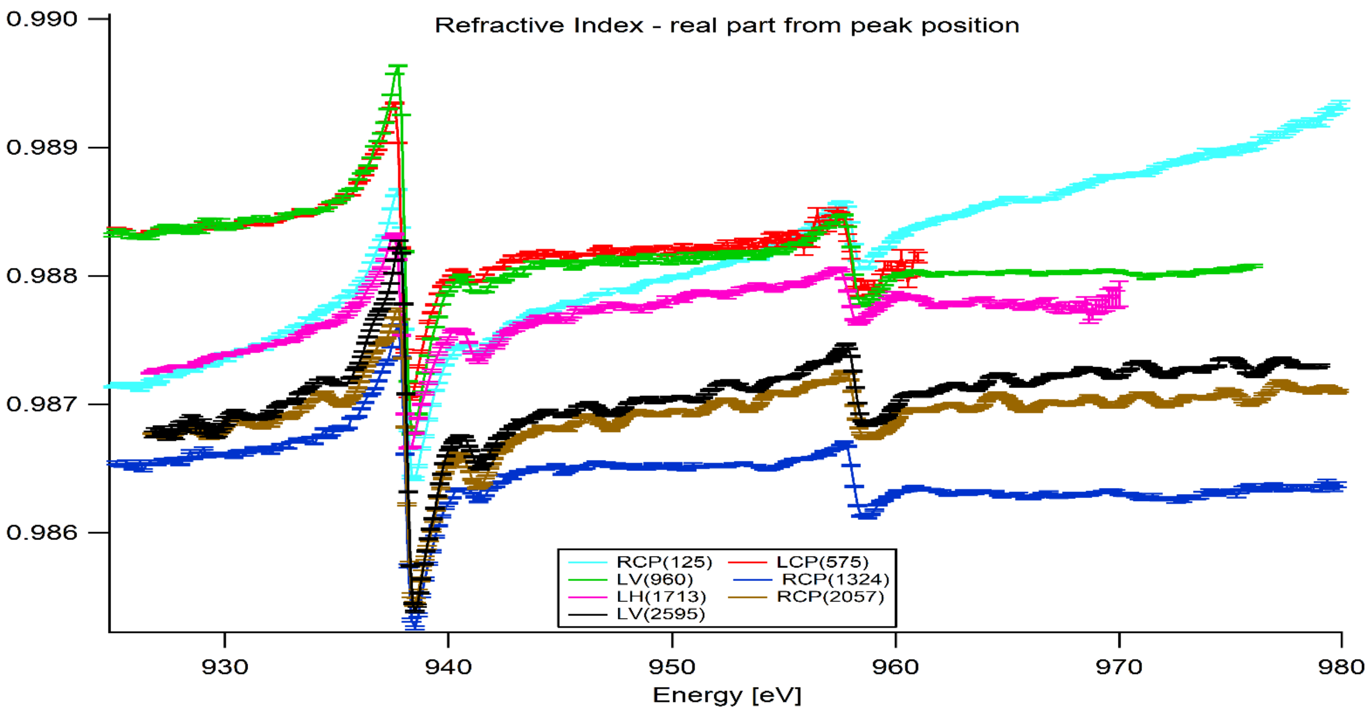

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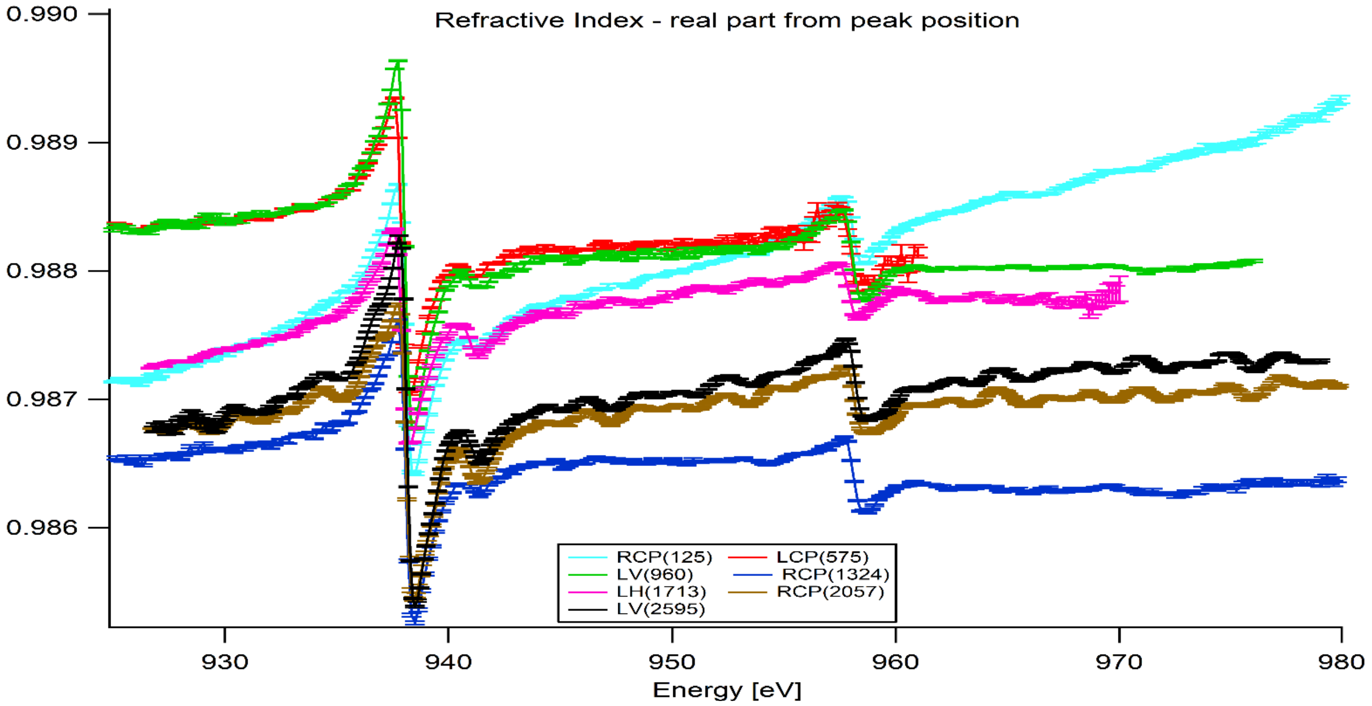
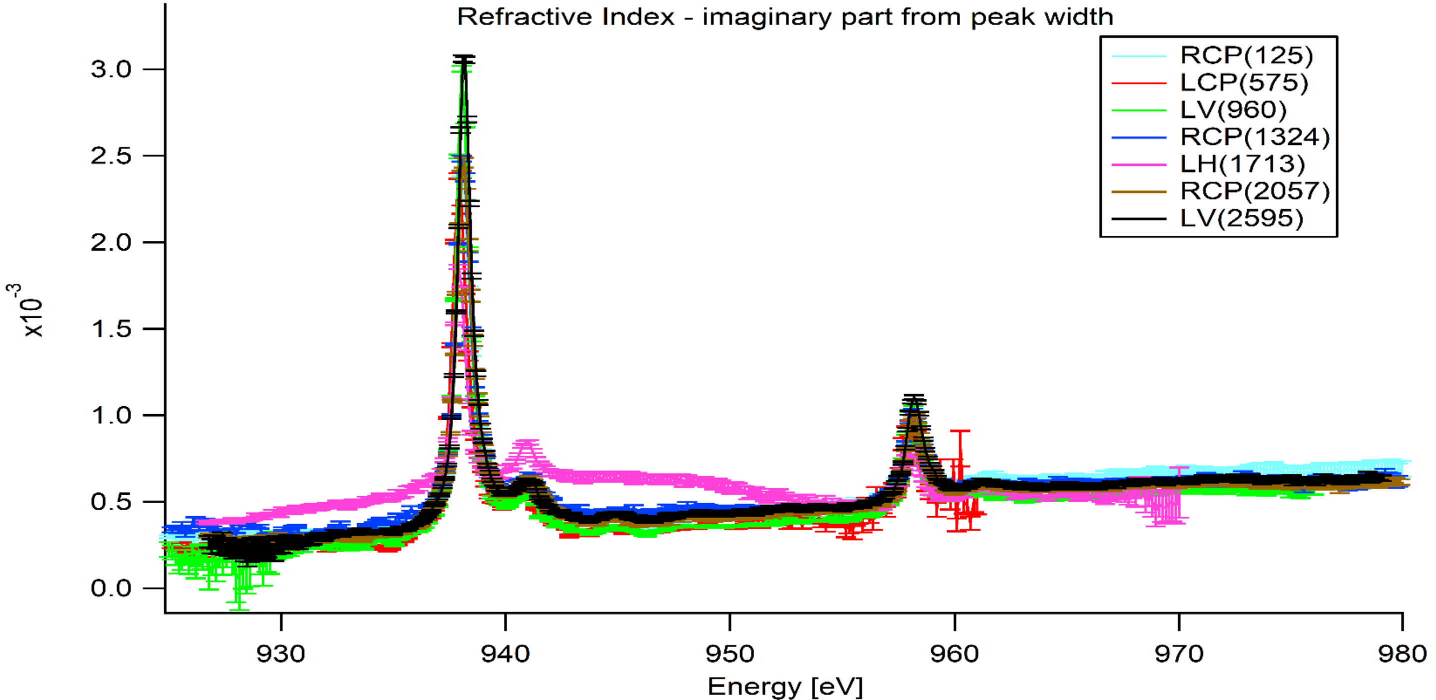
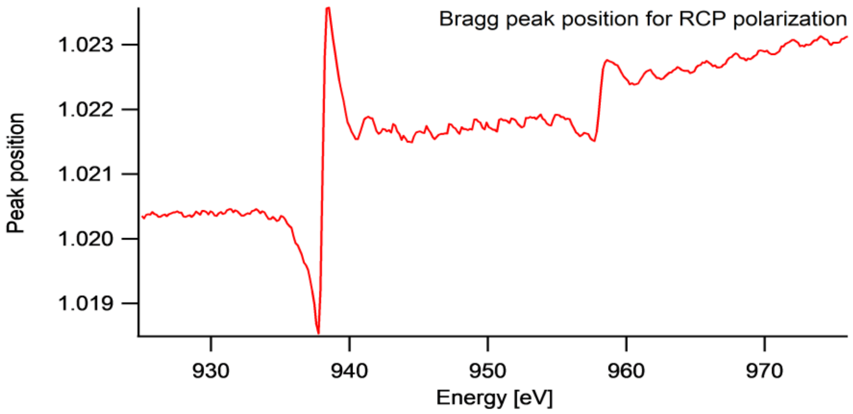
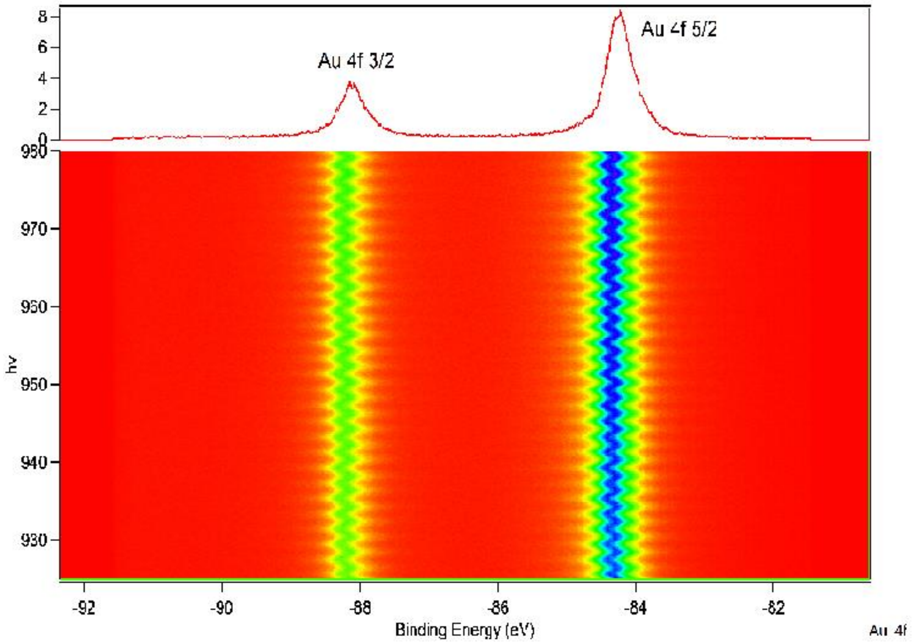
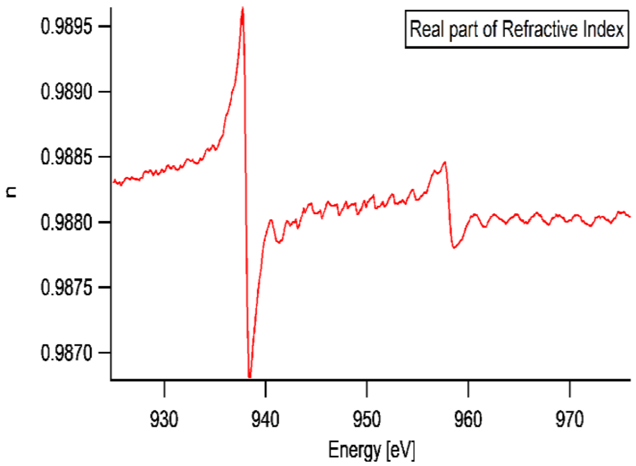




UNREALISTIC OSCILATIONS

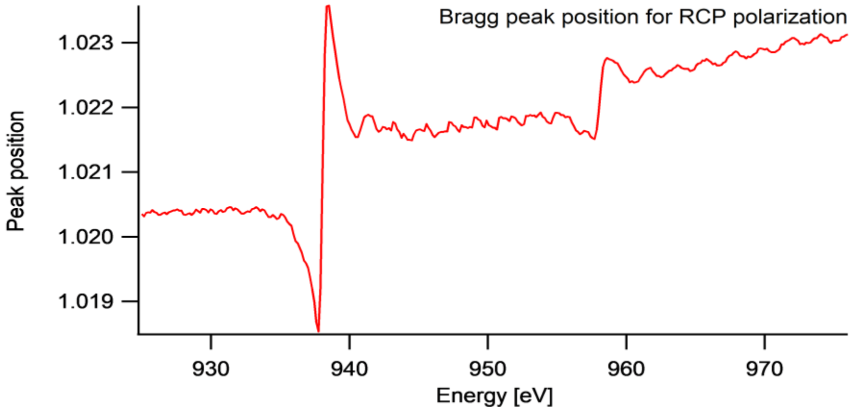


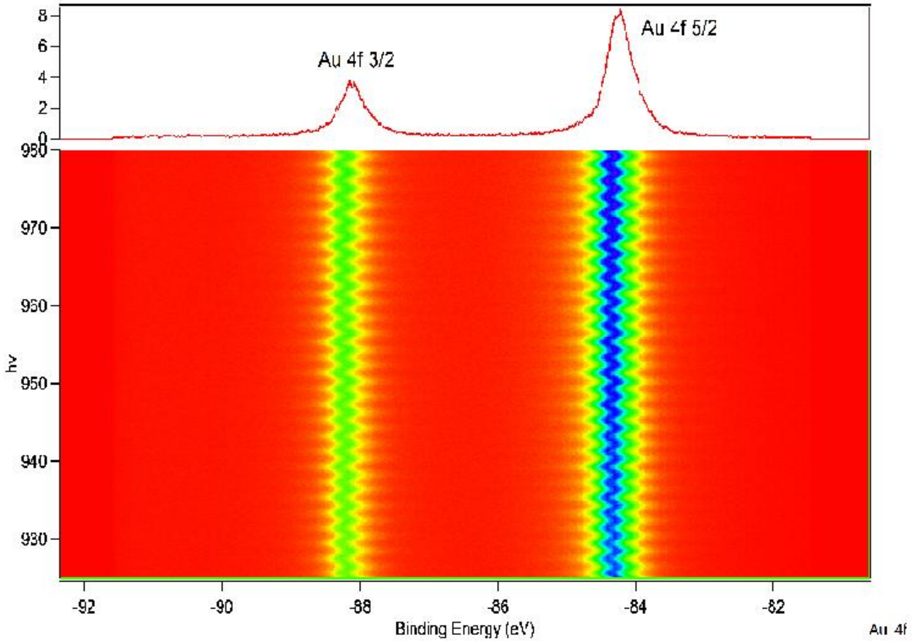


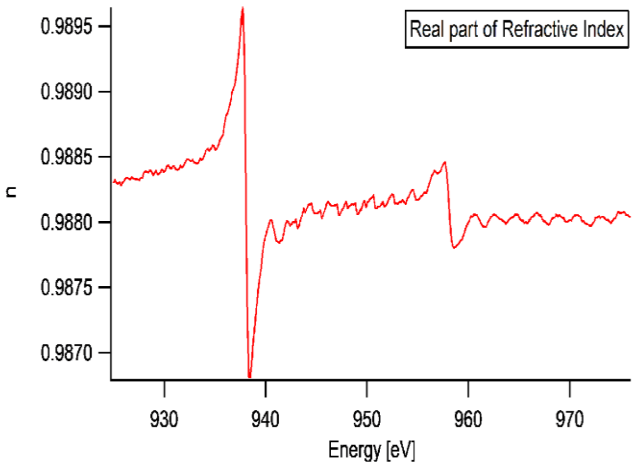


UNREALISTIC OSCILATIONS

1. Fitting gold 4f edge for obtaining reference oscilations







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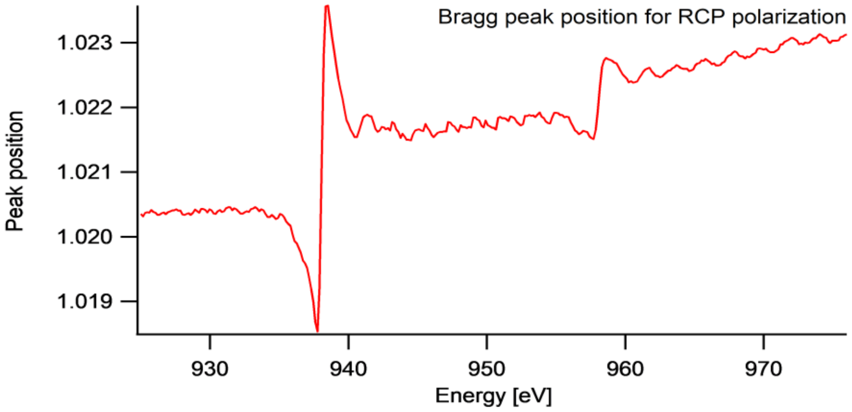

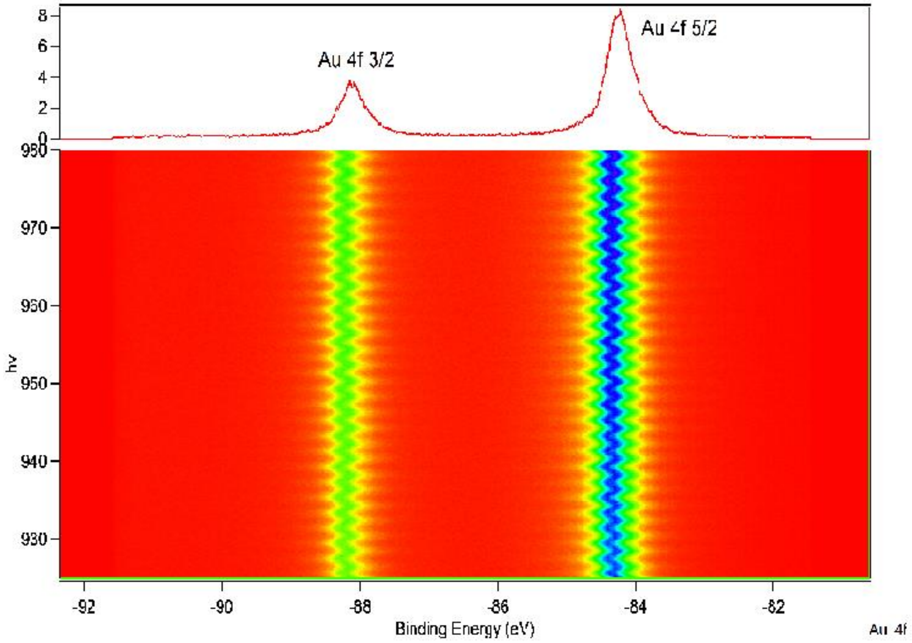

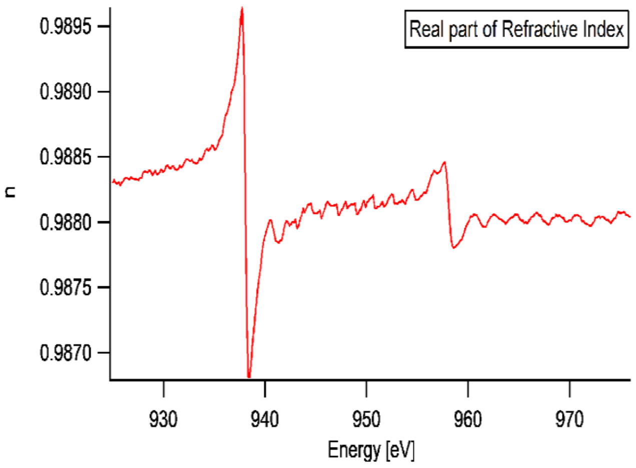

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2. Transforming data from fit to relative scattering angle as:

$$\Delta\theta_B = \frac{\partial\theta_B}{\partial E}\Delta E = \frac{2d}{hc}\frac{\sin^2\theta_B}{\cos\theta_B}\cdot\Delta E$$

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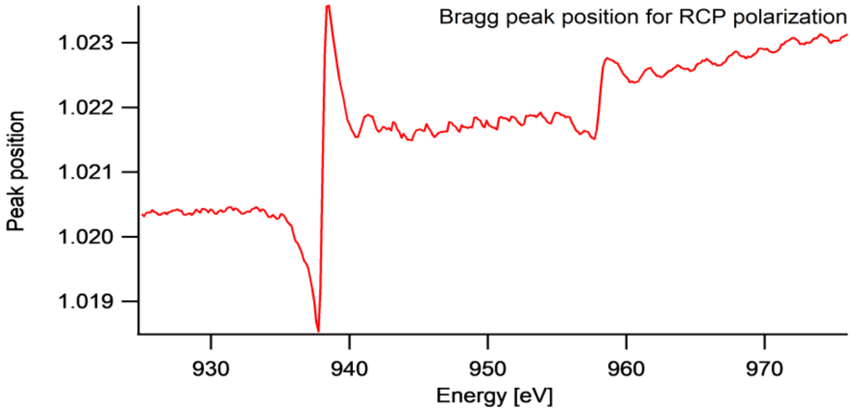

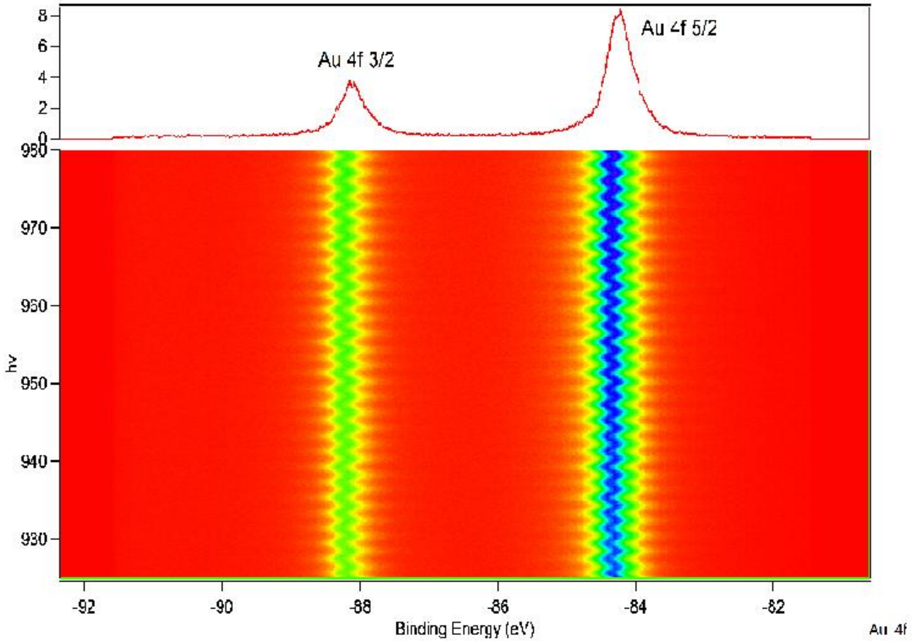

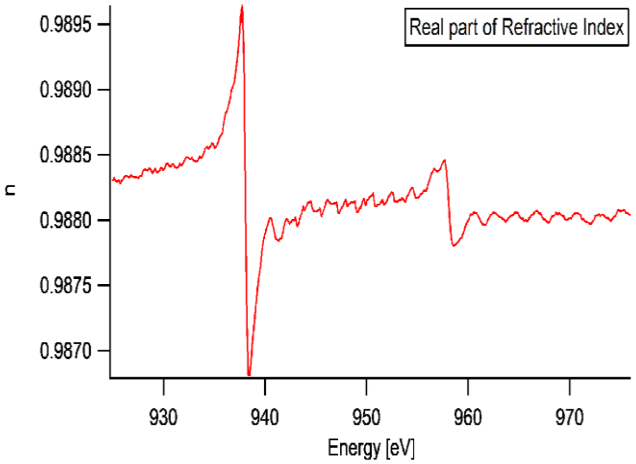

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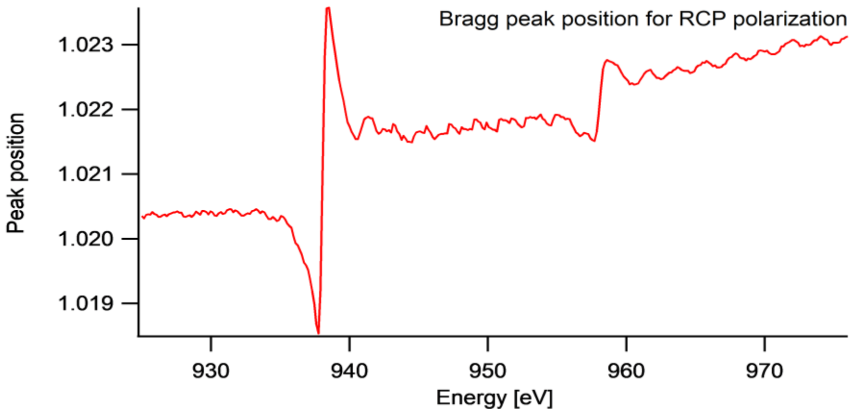

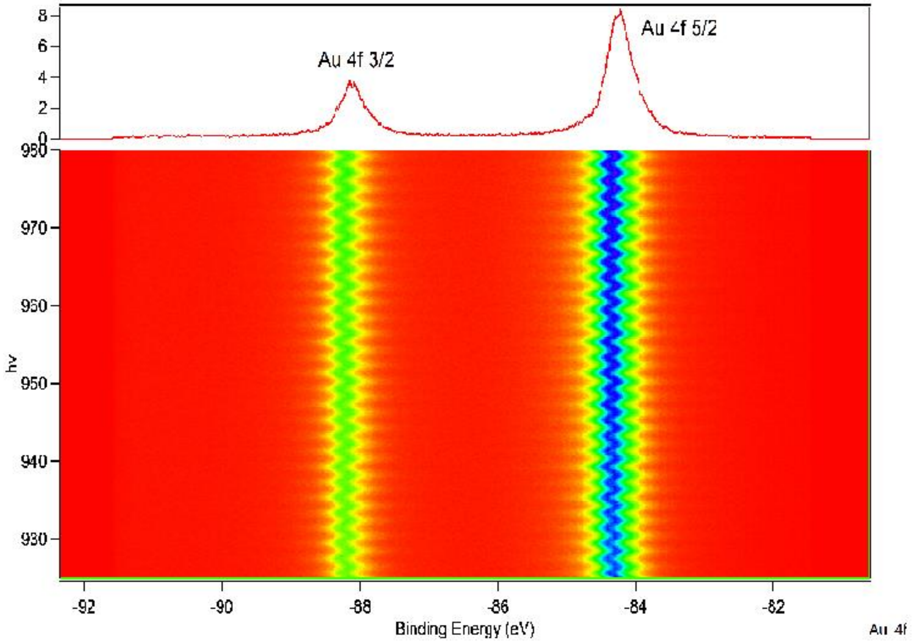

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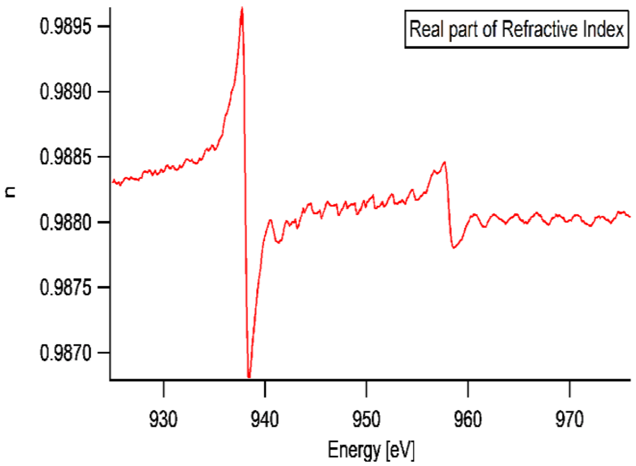

unwiggling

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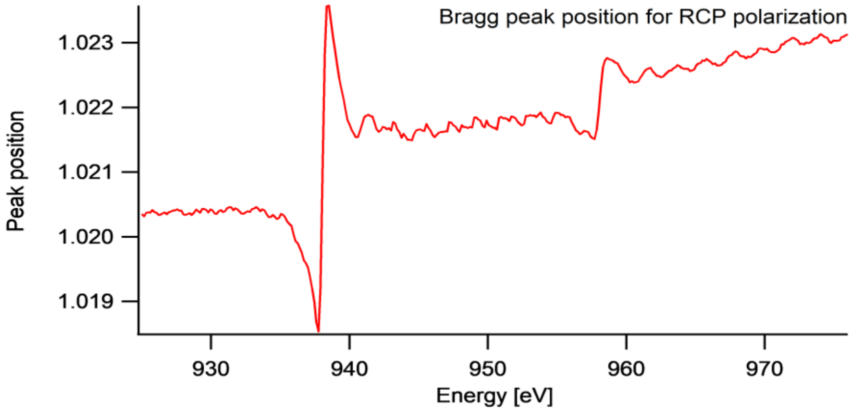
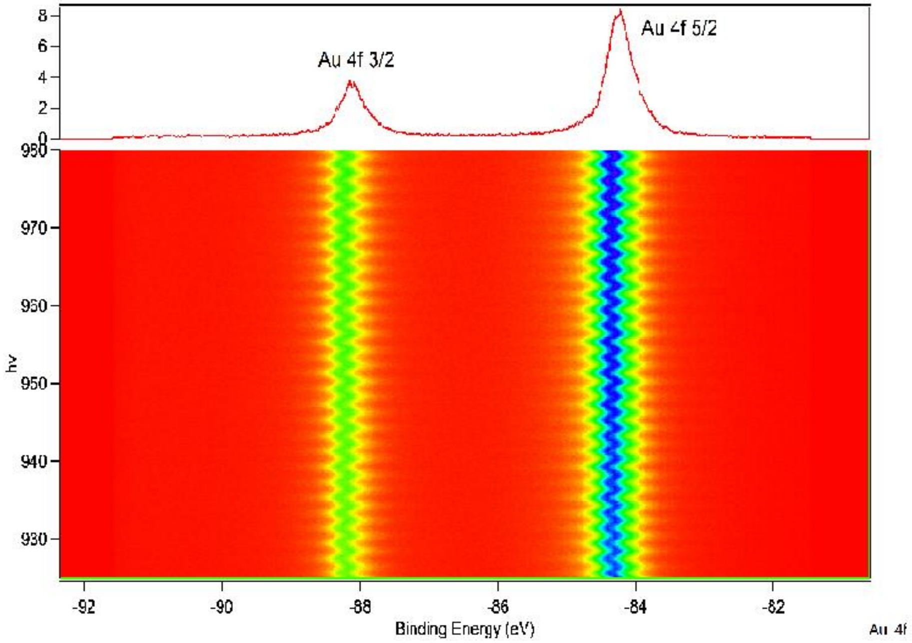
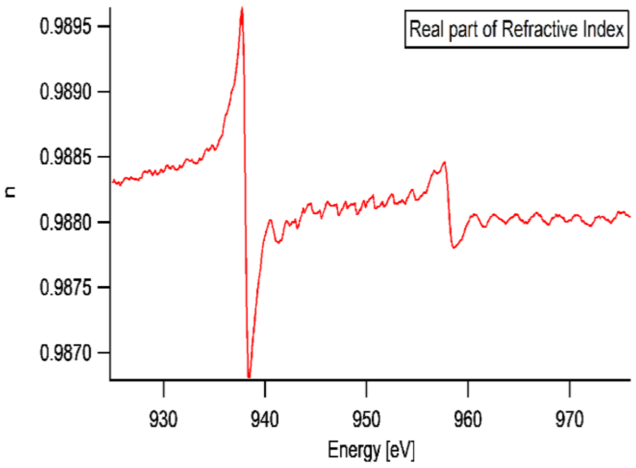
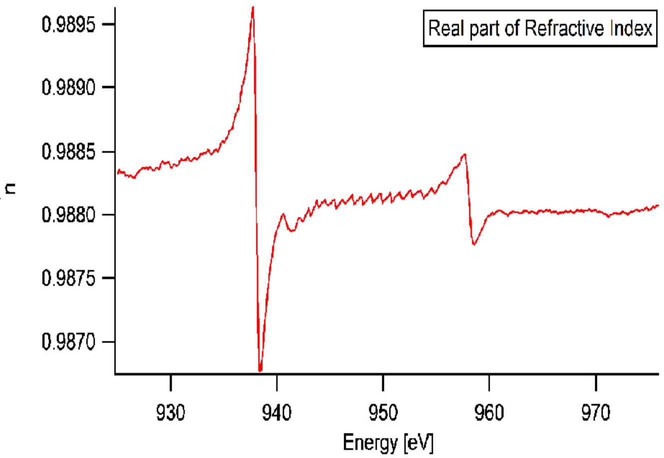






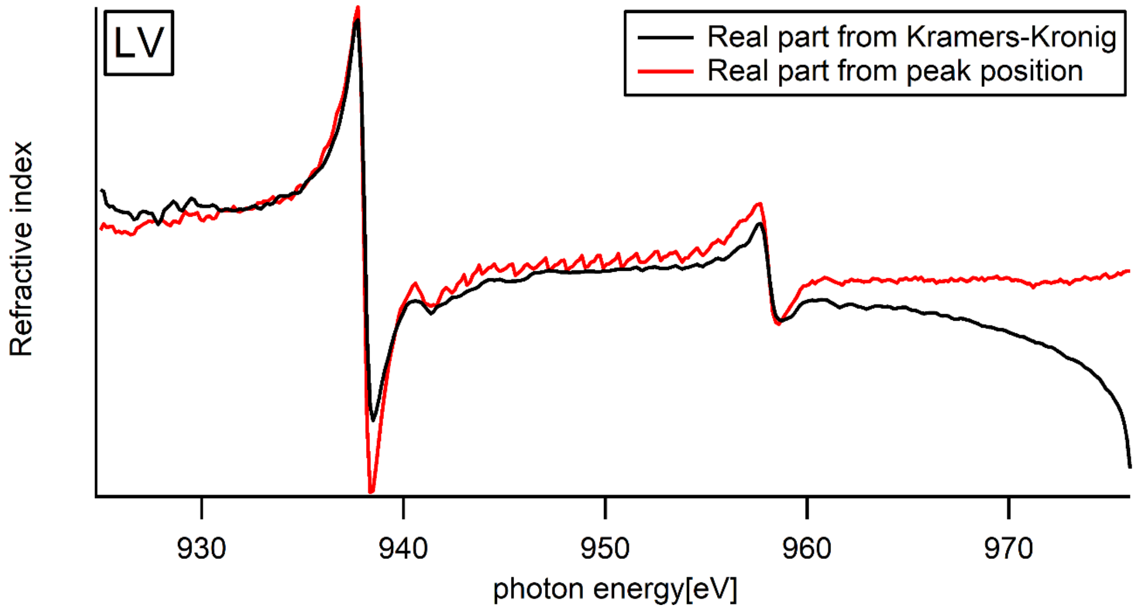
unwiggling

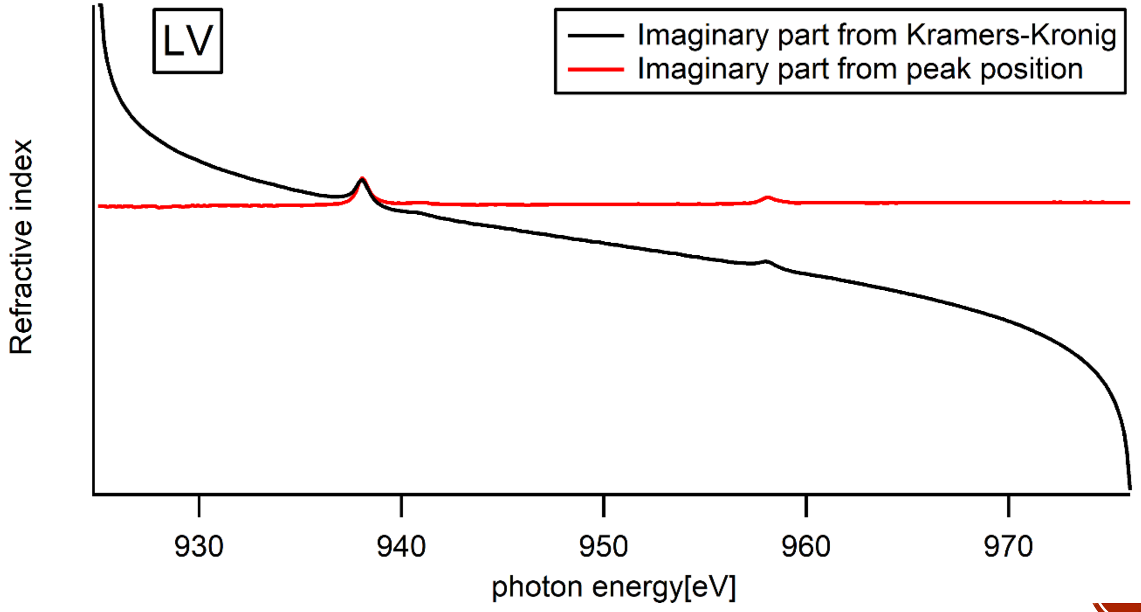


KRAMERS KRONIG ANALYSIS

$$n(E) = 1 + \frac{2E}{\pi}\int_0^{\infty}\frac{\kappa(E')dE'}{E^2 - E'^2}$$

$$\kappa(E) = -\frac{2E}{\pi}\int_0^{\infty}\frac{n(E') - 1}{E^2 - E'^2}dE'$$

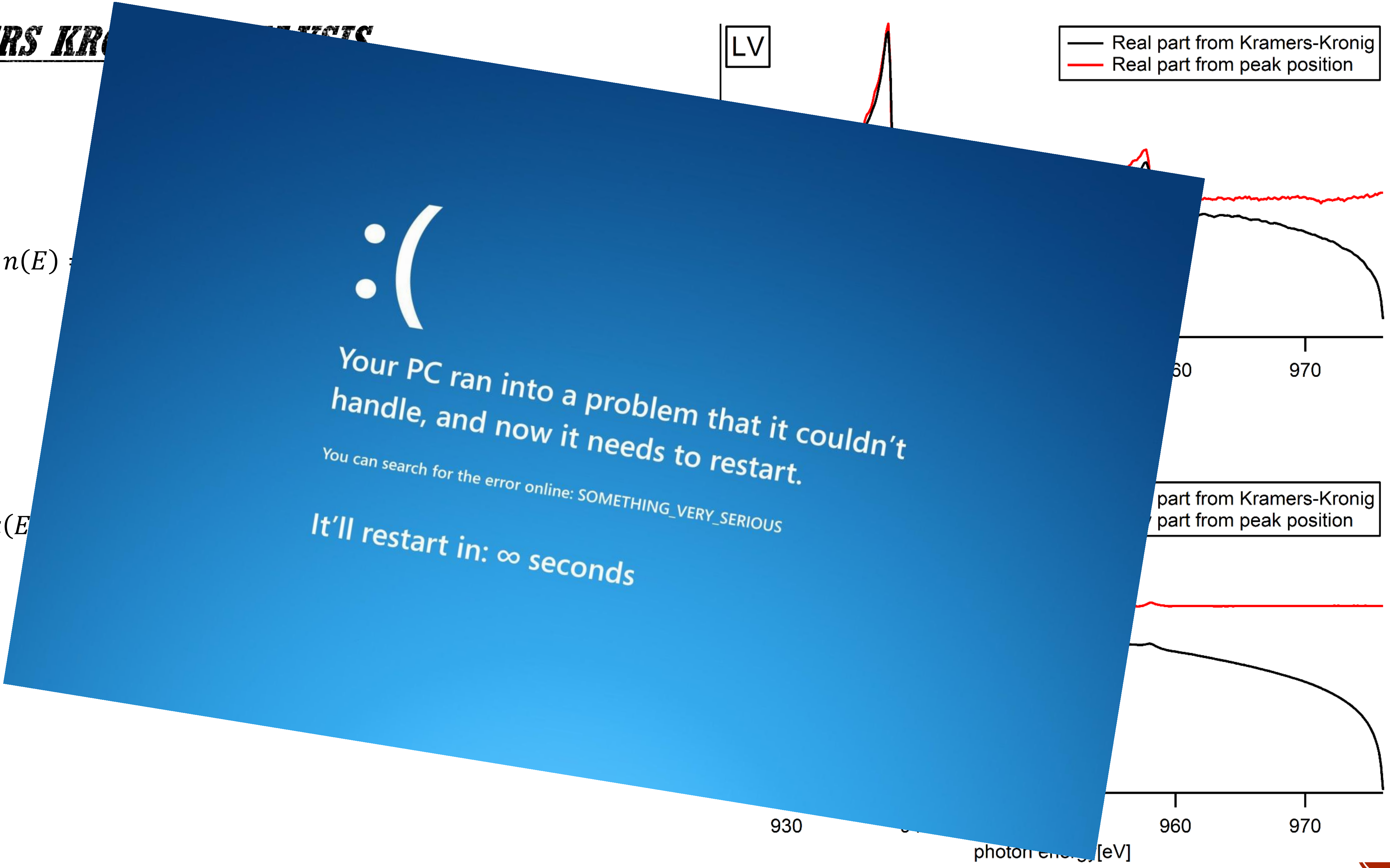




KRAMERS KR

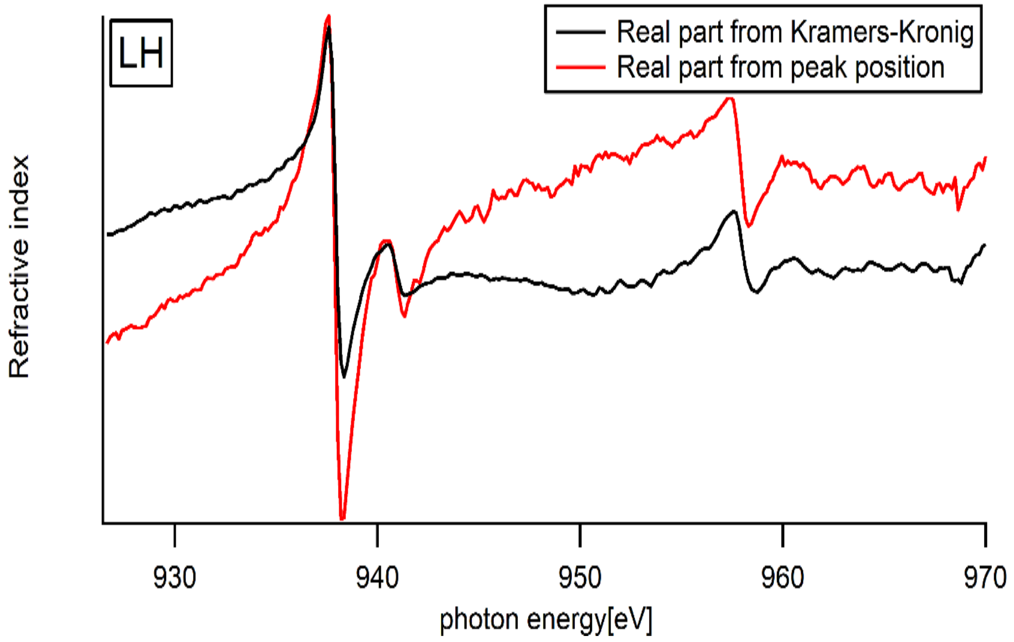
$n(E) =$

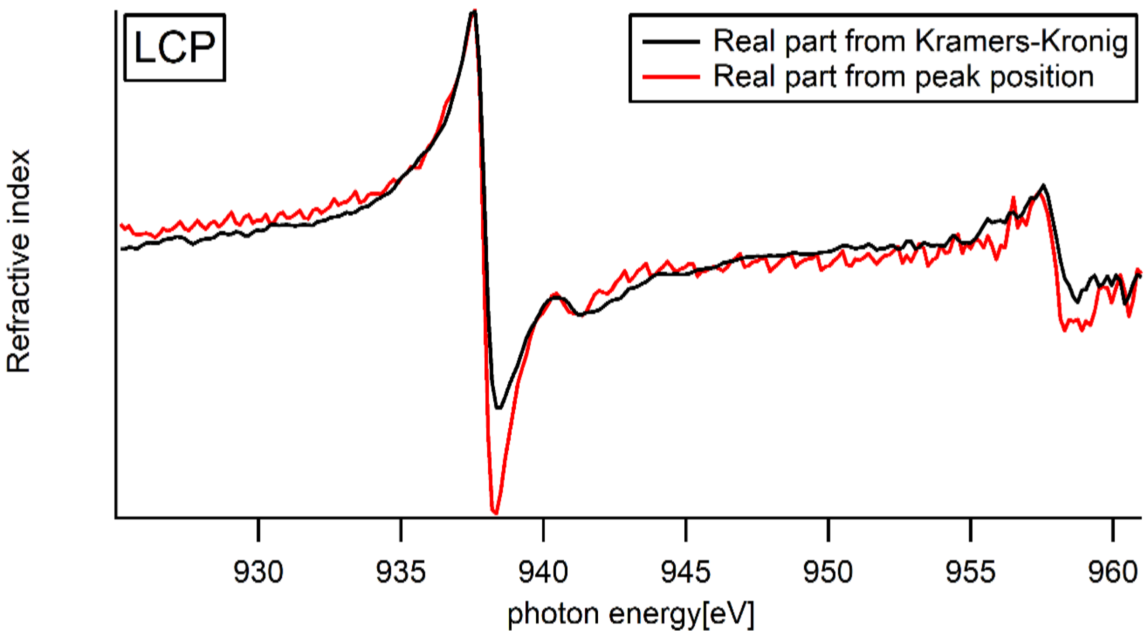
$\kappa(E$

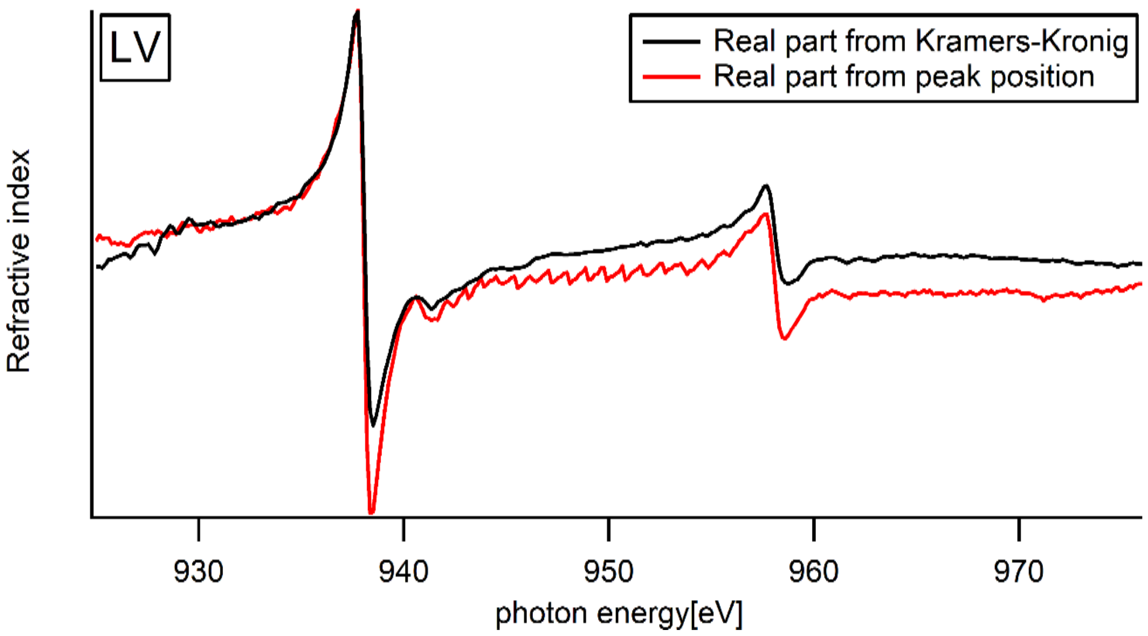


KRAMERS KRONIG ANALYSIS

SOLUTION?







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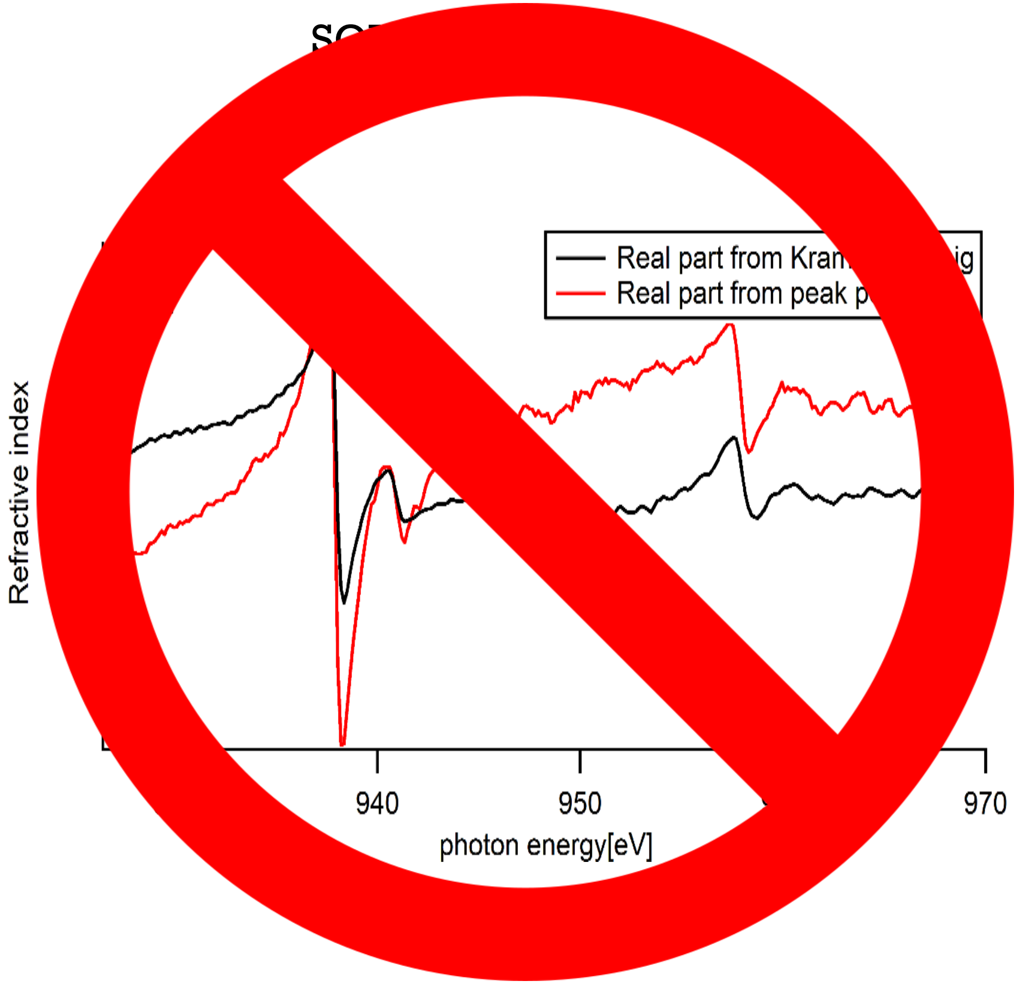
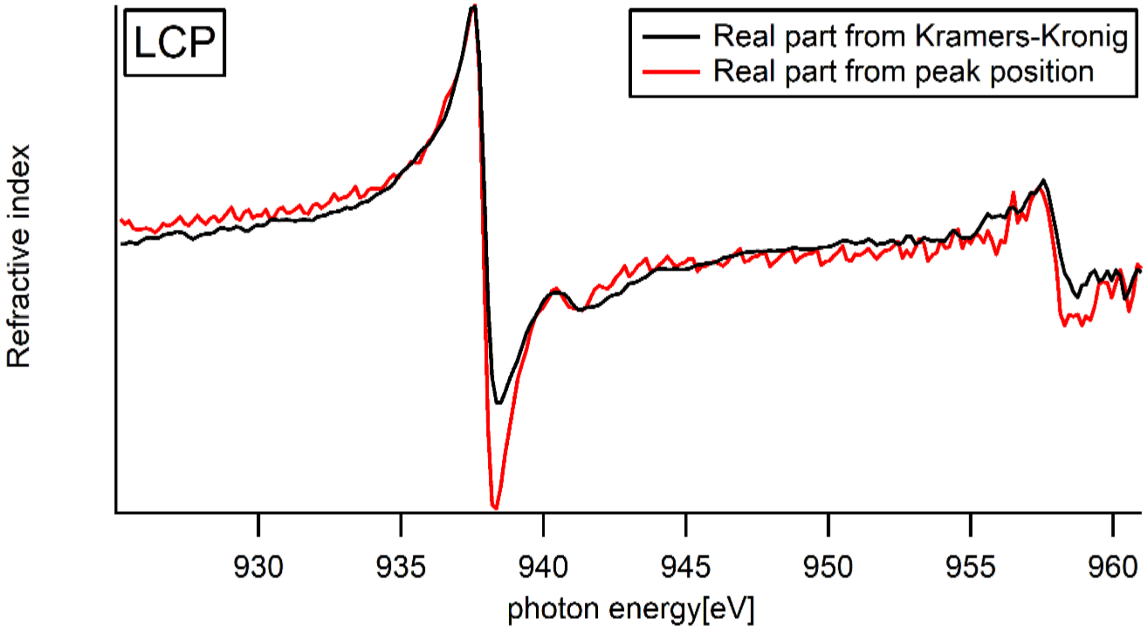
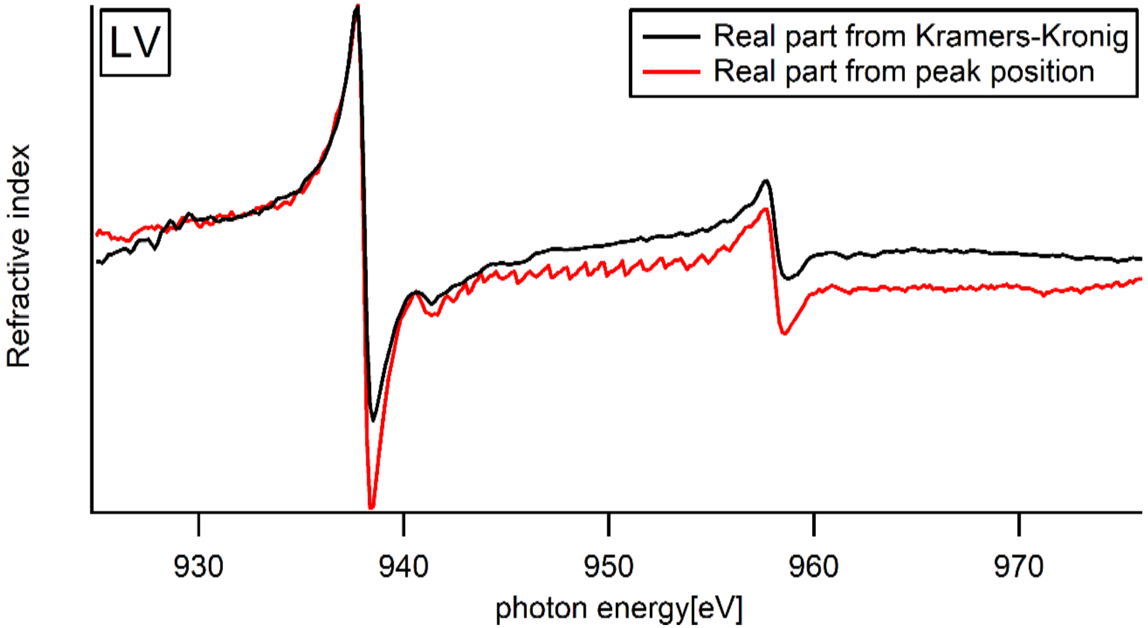
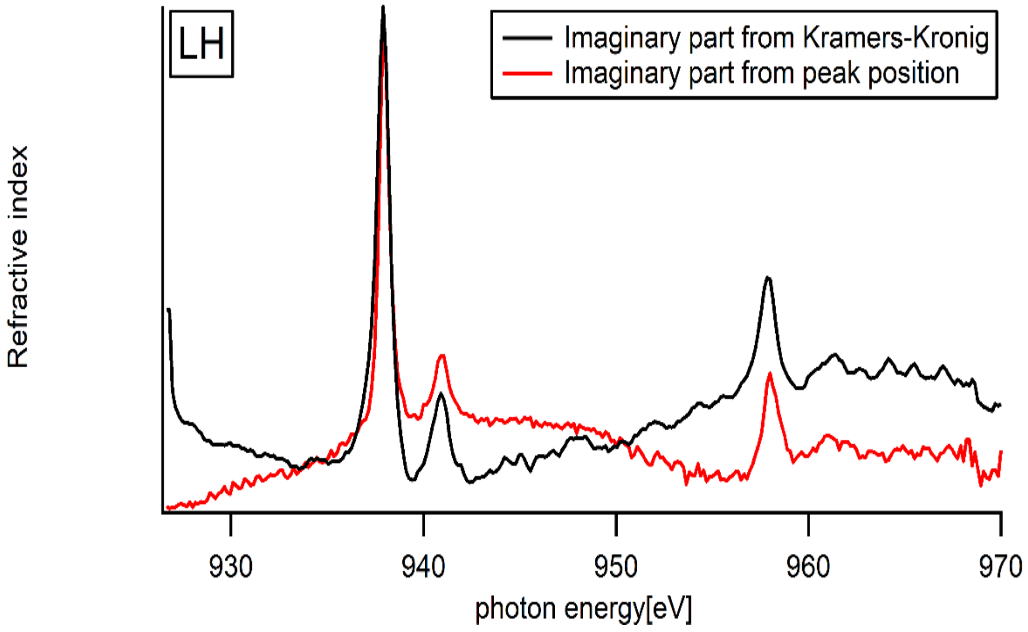
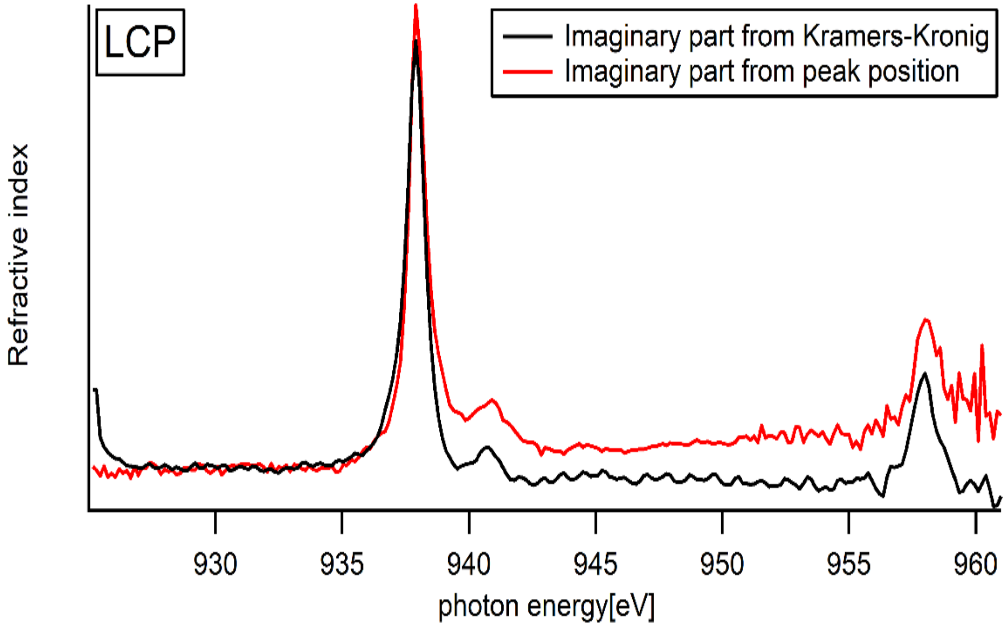


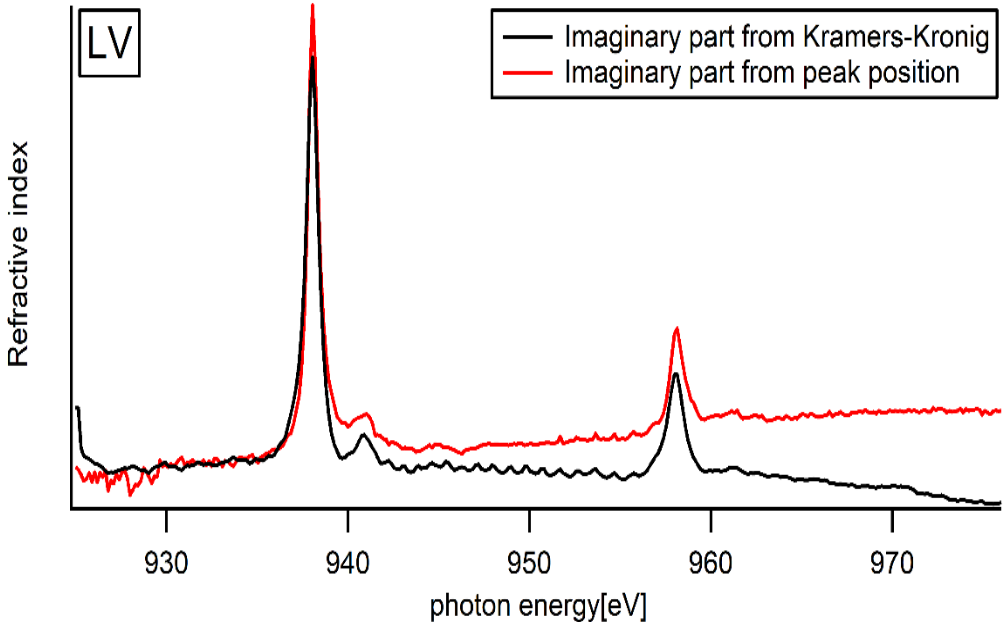




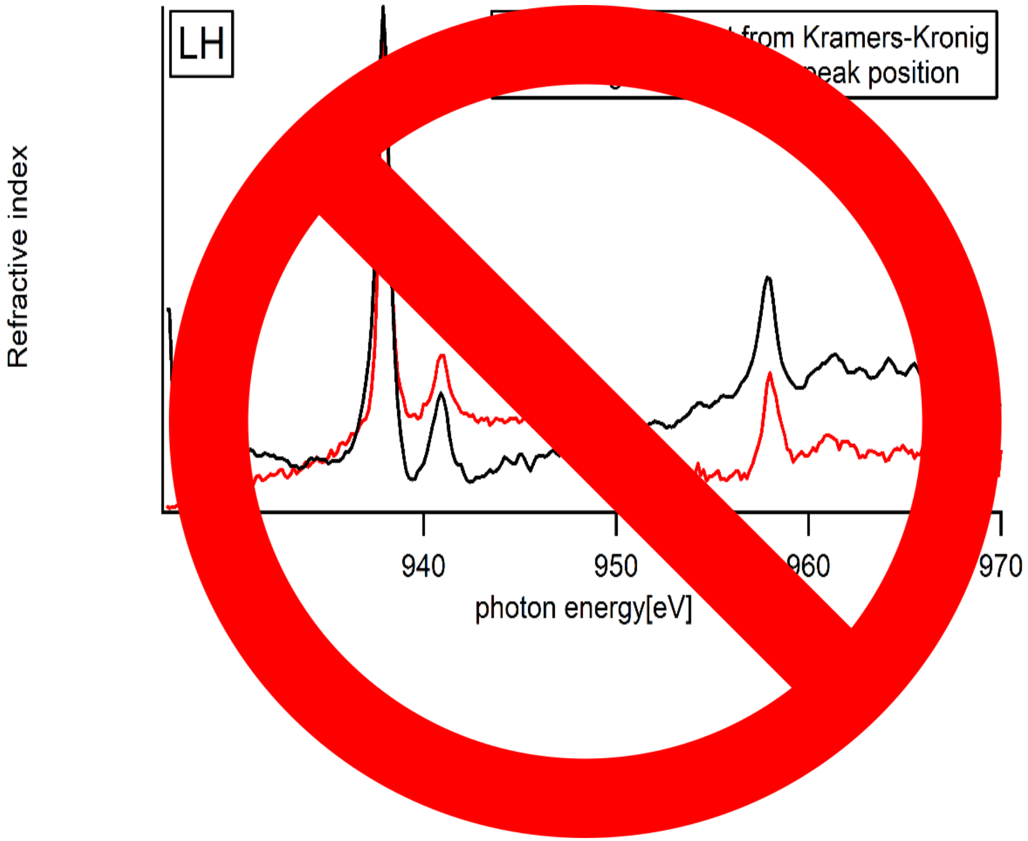
KRAMERS KRONIG ANALYSIS FOR IMAGINARY PART

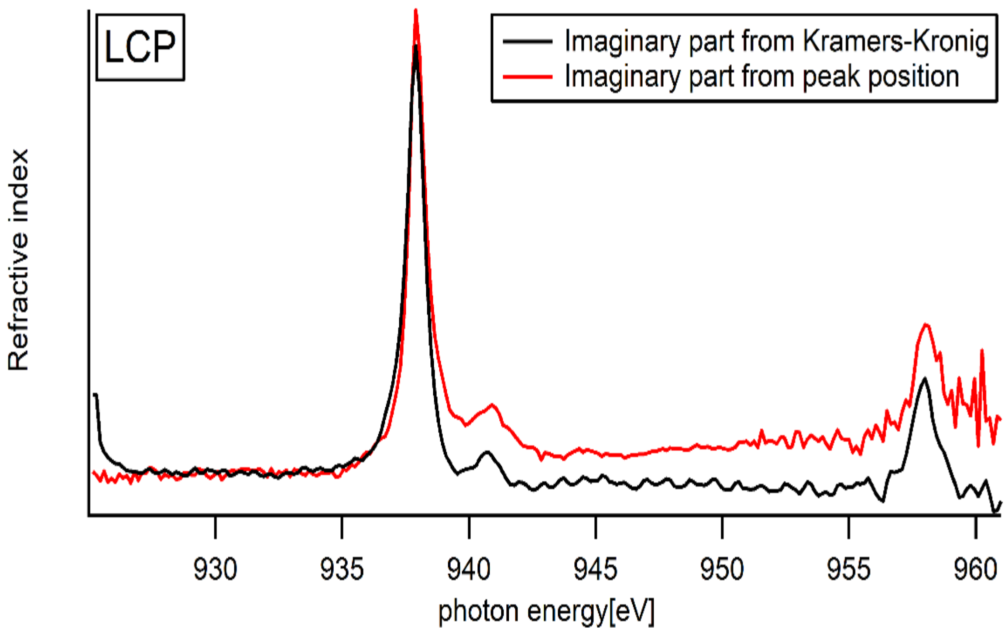


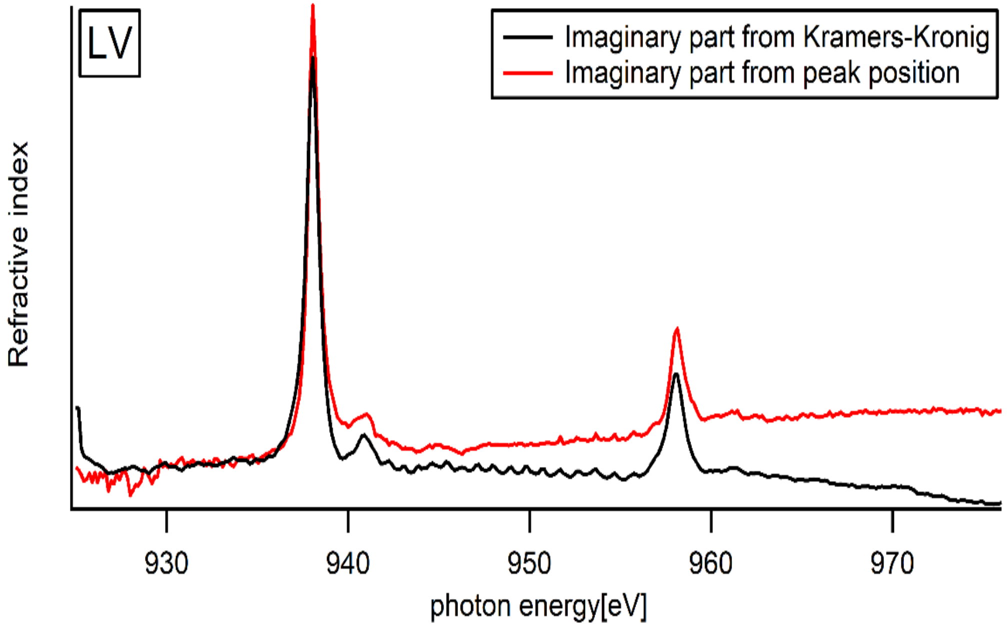




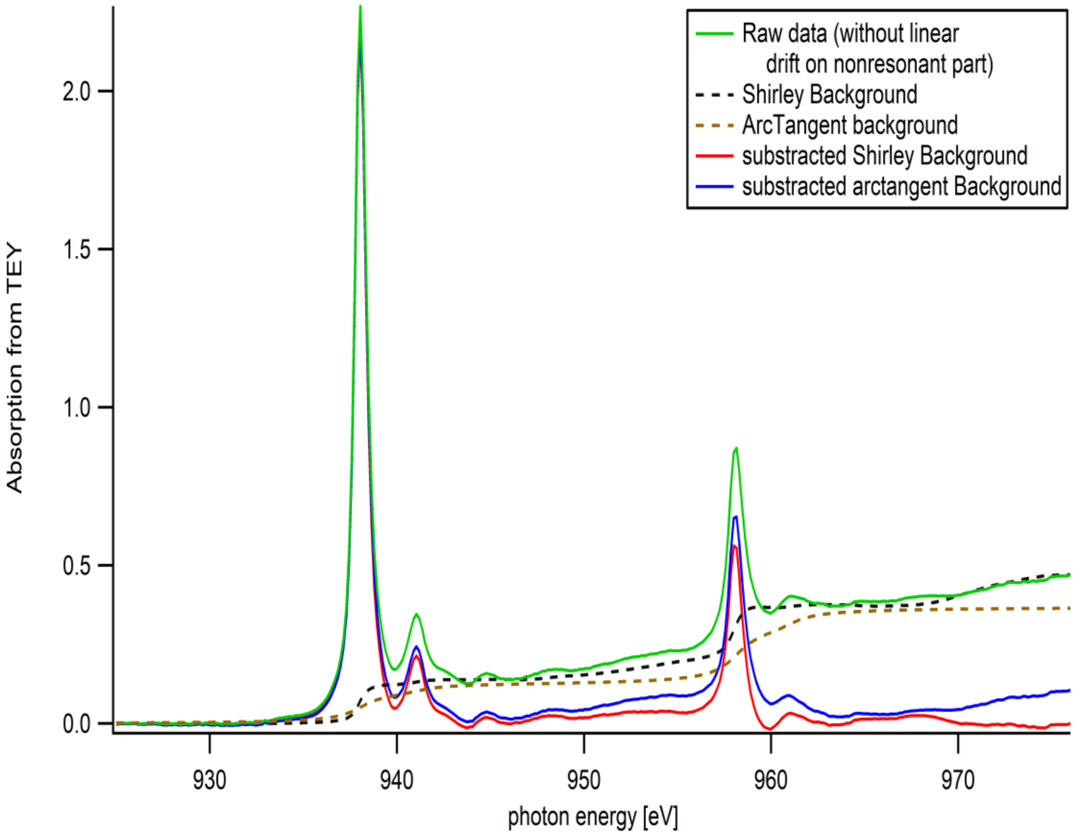
KRAMERS KRONIG ANALYSIS FOR IMAGINARY PART

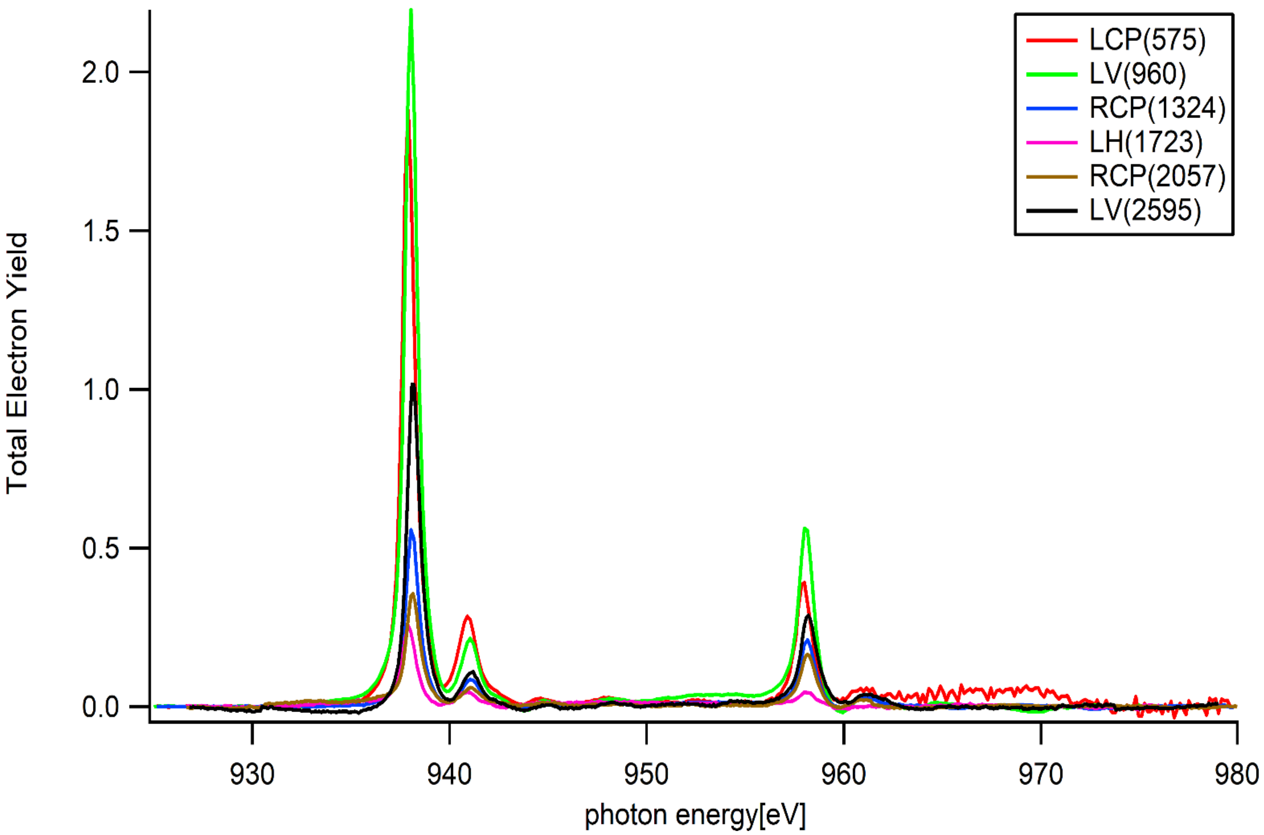




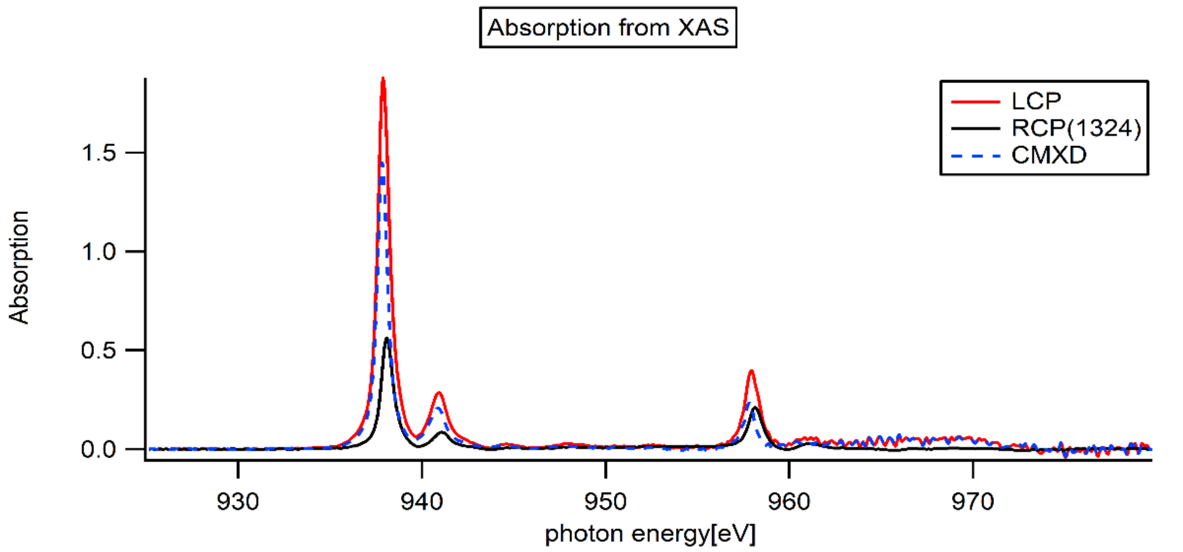


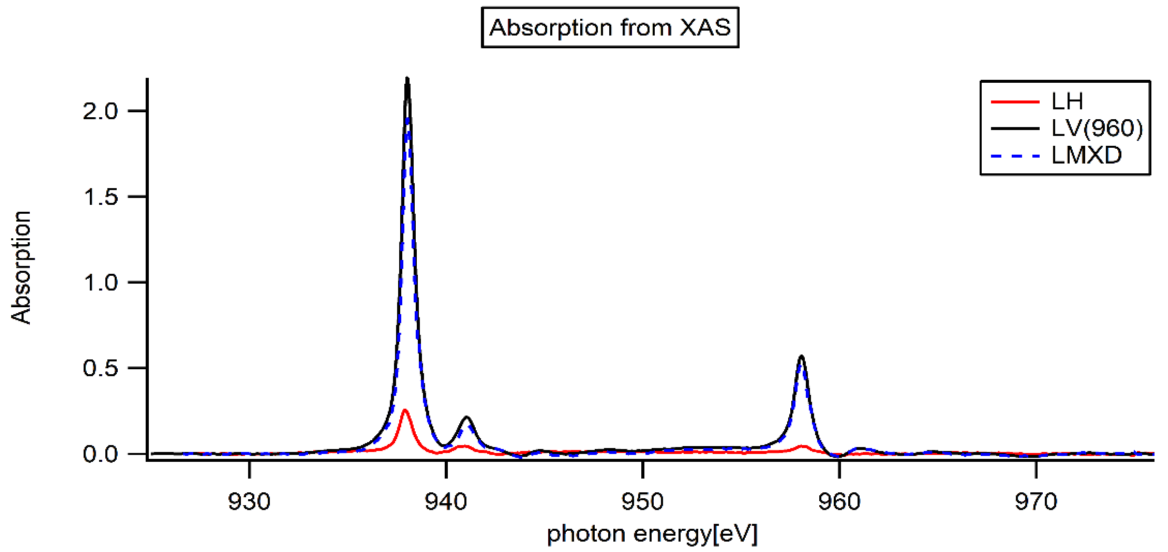
TOTAL ELECTRON YIELD

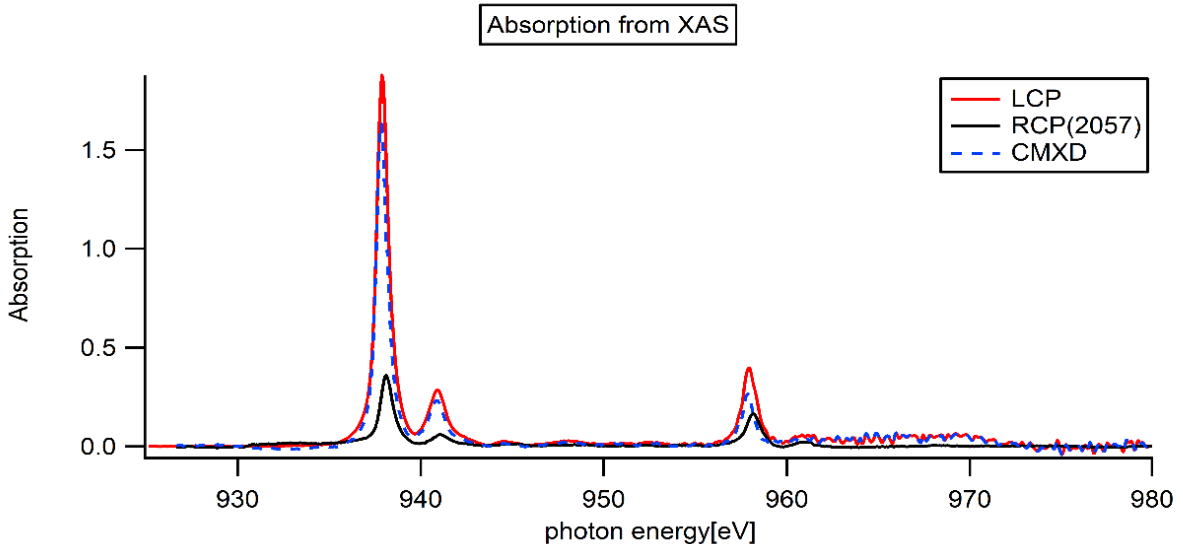


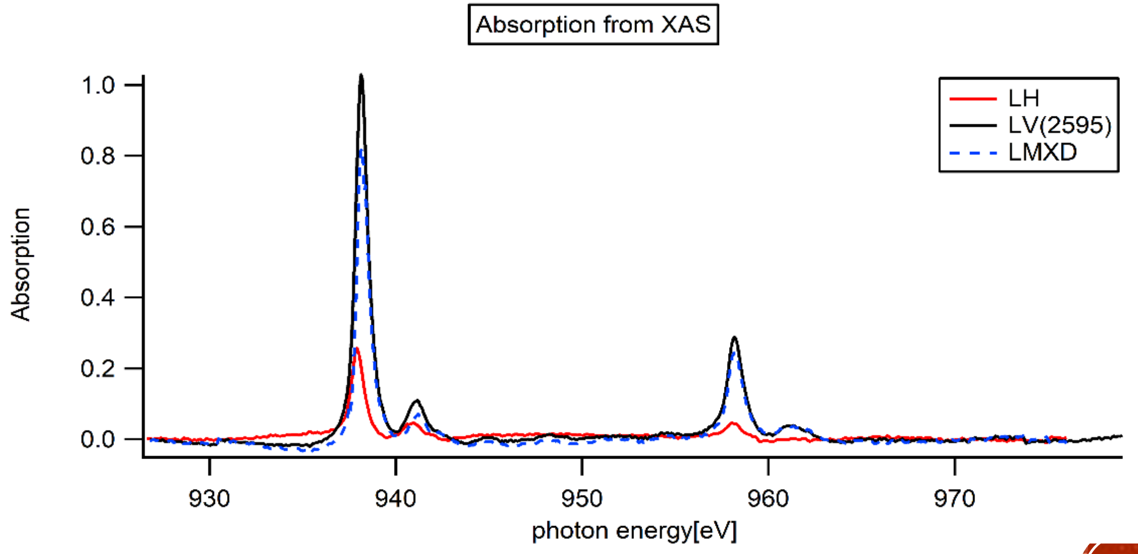


CIRCULAR MAGNETIC X-RAY DICHROISM (CMXD)







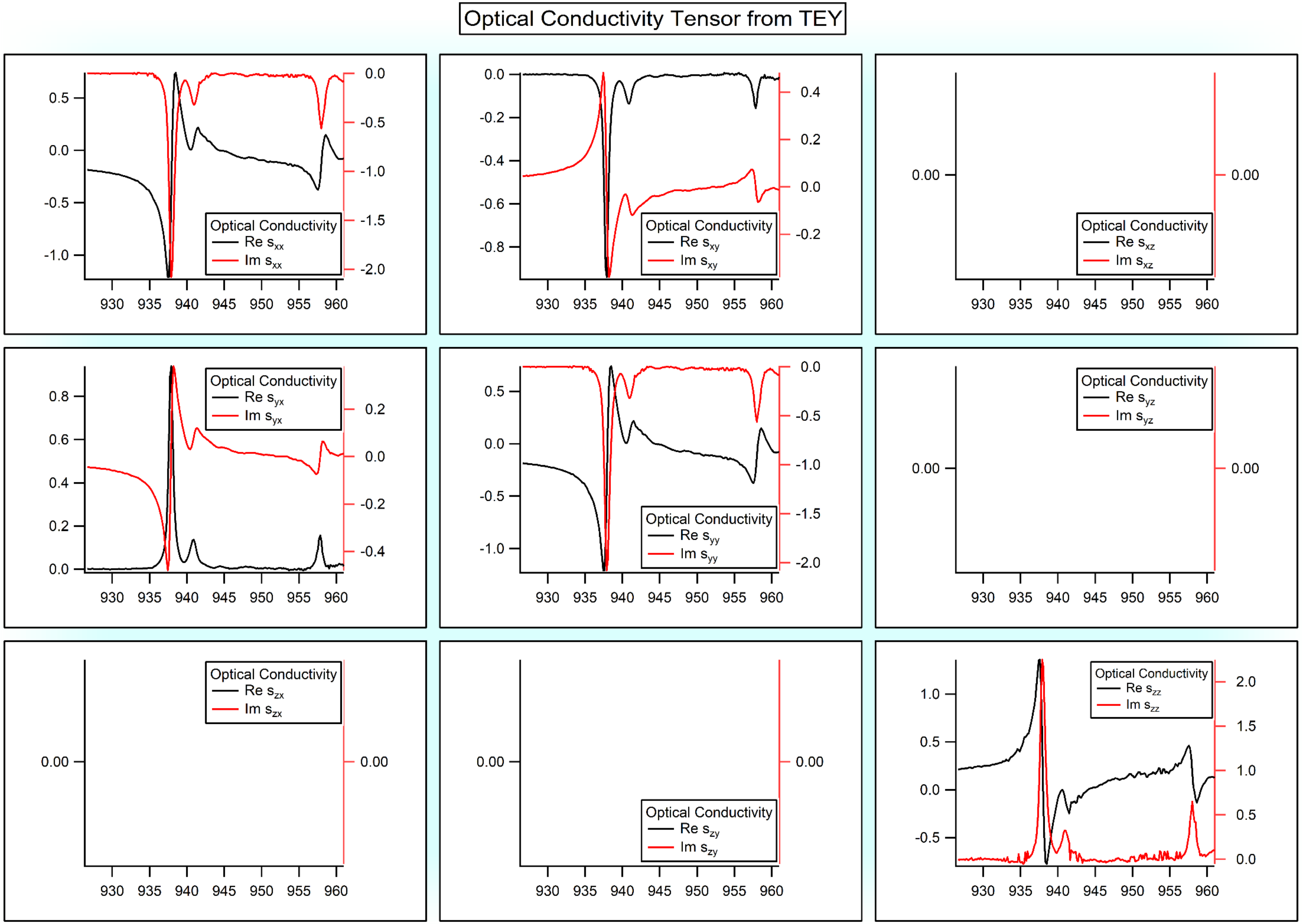


OPTICAL CONDUCTIVITY

$$\overleftrightarrow{\sigma} = \begin{pmatrix} \sigma^{(0)}_{a^B_{1g}} & 2S_z\sigma^{(1)}_{a_{2u}} & -2S_y\sigma^{(1)}_{e_u} \\ -2S_z\sigma^{(1)}_{a_{2u}} & \sigma^{(0)}_{a^B_{1g}} & 2S_x\sigma^{(1)}_{e_u} \\ 2S_y\sigma^{(1)}_{e_u} & -2S_x\sigma^{(1)}_{e_u} & \sigma^{(0)}_{a^A_{1g}} \end{pmatrix}$$

$$I_{TEY} = -\mathcal{Im}(\boldsymbol{\epsilon}^* \cdot \overleftrightarrow{\sigma} \cdot \boldsymbol{\epsilon})$$

OPTICAL CONDUCTIVITY



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