Today's outline - November 06, 2024

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- Photoelectric absorption

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- Reversibility in tin-based anode materials

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Reading Assignment: Chapter 8.1–8.3

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

Homework Assignment #07:
Chapter 7: 2,3,9,10,11
due Monday, November 25, 2024

Dirac bra-ket notation

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$$\mathcal{H}_I = \frac{e\vec{p}\cdot\vec{A}}{m} + \frac{e^2A^2}{2m}$$

The first term gives absorption while the second produces Thomson scattering so we take only the first into consideration now.

$$\vec{A} = \hat{\varepsilon}\sqrt{\frac{\hbar}{2\epsilon_0 V\omega}}\left[a_k e^{i\vec{k}\cdot\vec{r}} + a_k^\dagger e^{-i\vec{k}\cdot\vec{r}}\right]$$

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$$M_{if} = \frac{e}{m}\sqrt{\frac{\hbar}{2\epsilon_0 V\omega}}\left[{}_e\langle 1|_\gamma\langle 0|(\vec{p}\cdot\hat{\varepsilon})ae^{i\vec{k}\cdot\vec{r}} + (\vec{p}\cdot\hat{\varepsilon})a^\dagger e^{-i\vec{k}\cdot\vec{r}}|1\rangle_\gamma|0\rangle_e\right]$$

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The calculation is simplified if the interaction Hamiltonian is applied to the left since the final state has only a free electron and no photon

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Photoelectron integral

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$$\psi_i = \psi_{1s}(\vec{r}) \qquad \psi_f = \sqrt{\frac{1}{V}}e^{i\vec{q}\cdot\vec{r}}$$

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which is the Fourier transform of the initial state 1s electron wave function

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$$\sigma_a = \frac{2\pi}{\hbar c}\frac{V^2}{4\pi^3}\left(\frac{e\hbar}{m}\right)^2 \frac{\hbar}{2\epsilon_0 V^2 \omega} I_3$$

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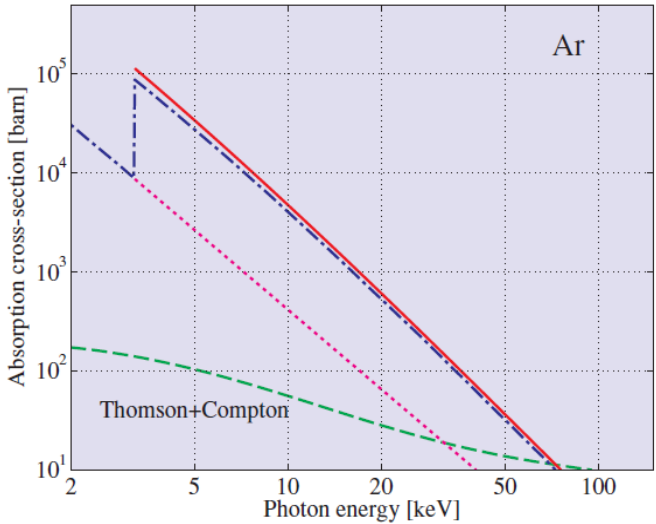
Calculated cross sections



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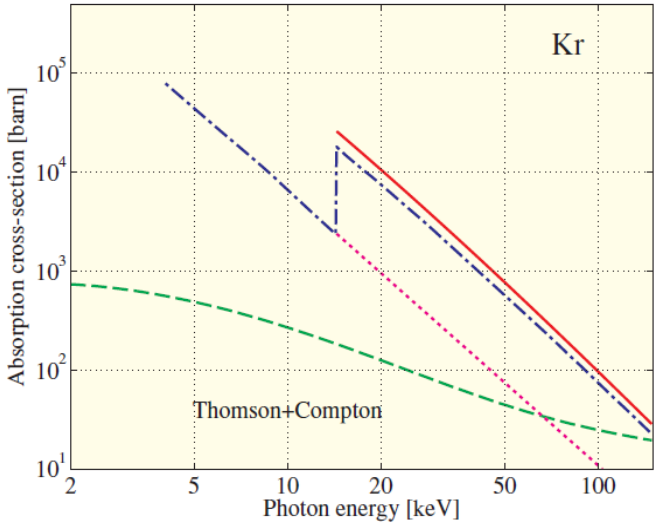

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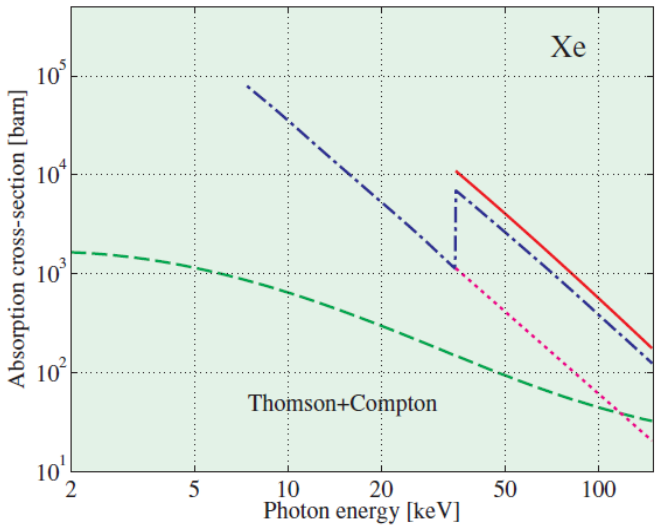

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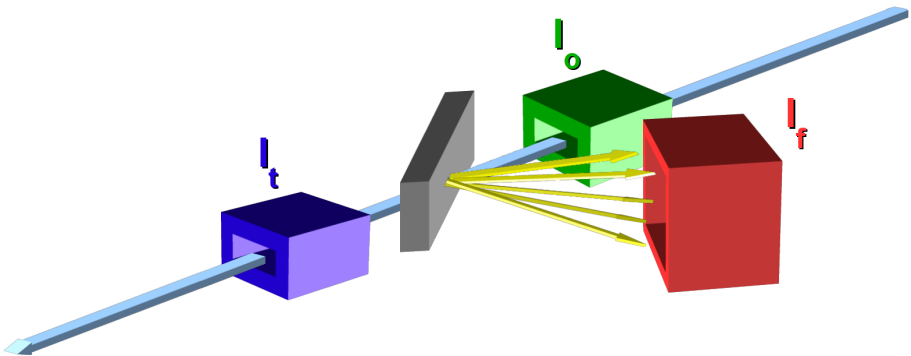
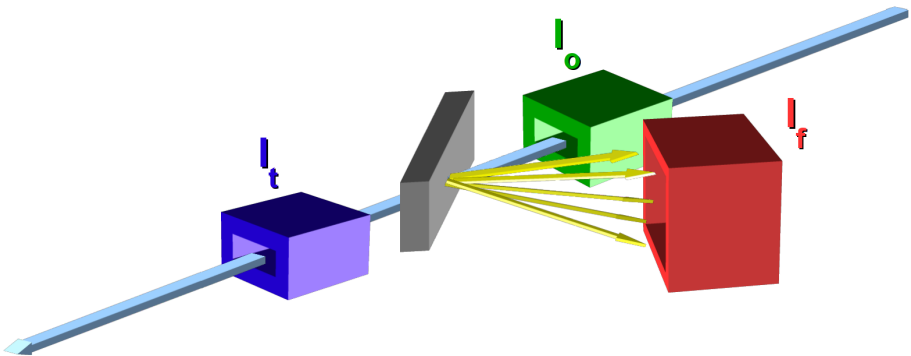
The EXAFS experiment



The EXAFS experiment

I_o = incident intensity



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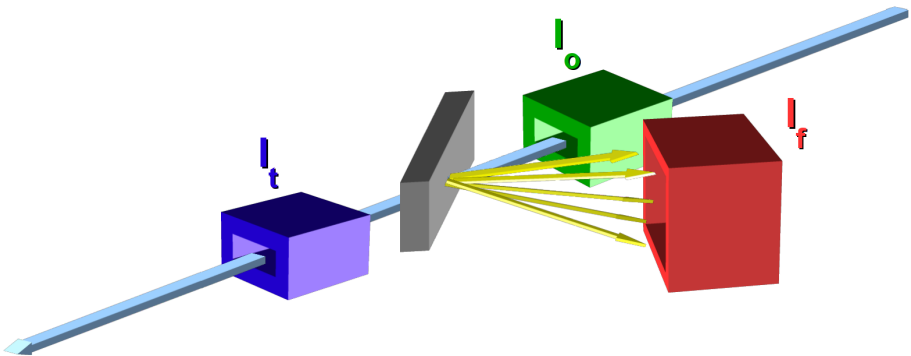

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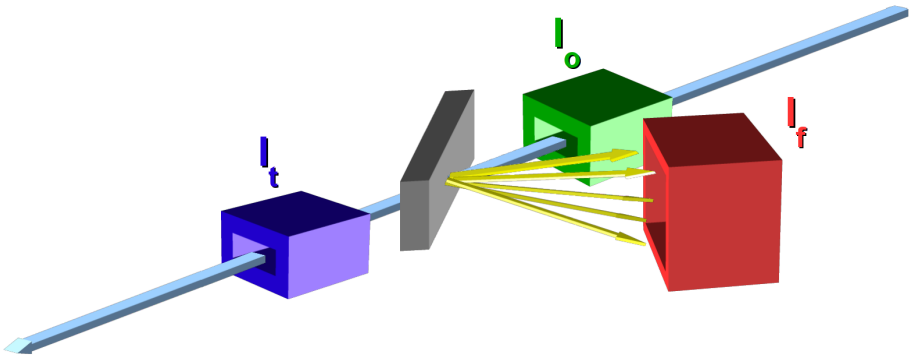

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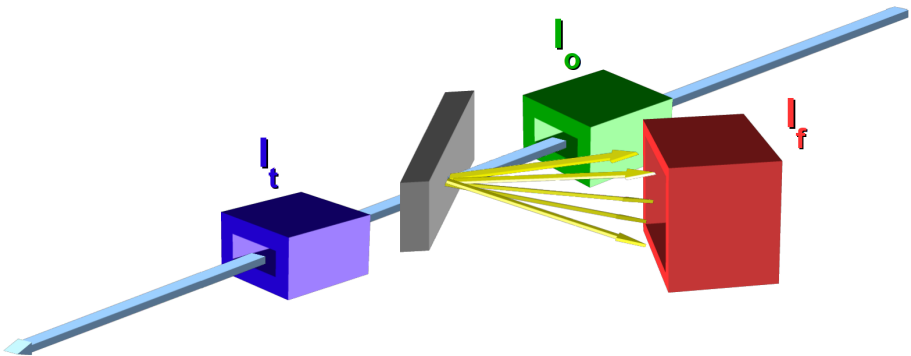

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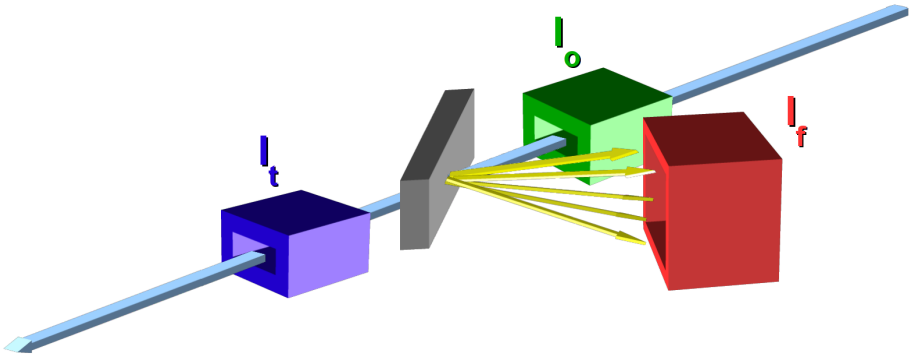

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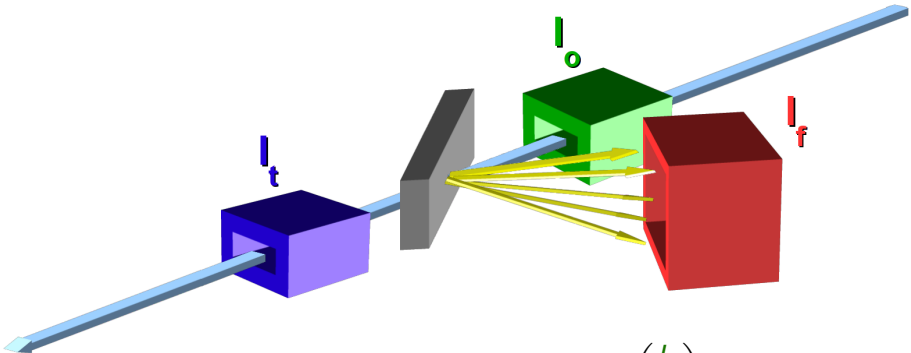

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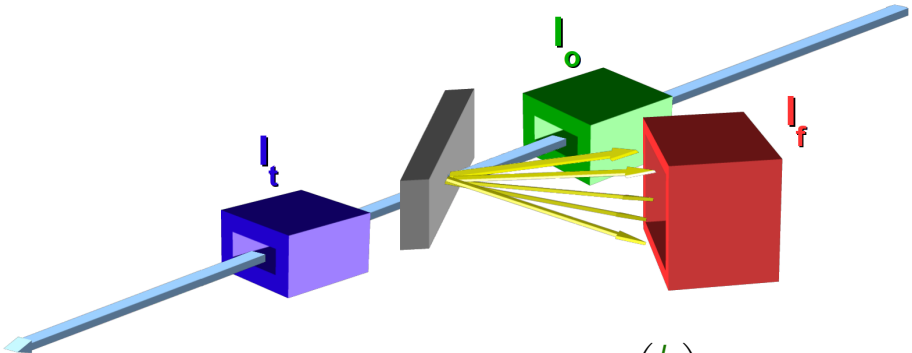

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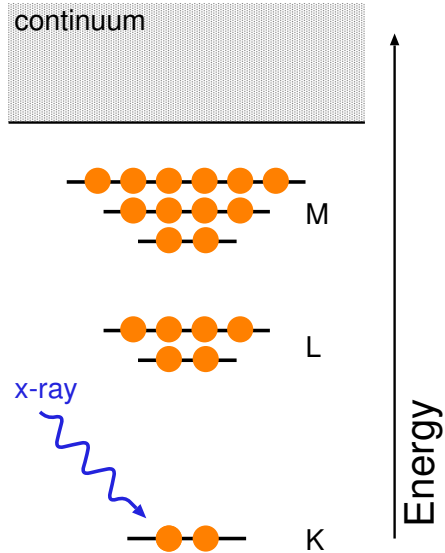

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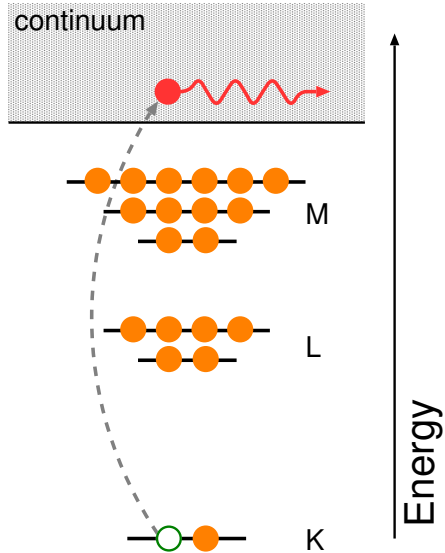

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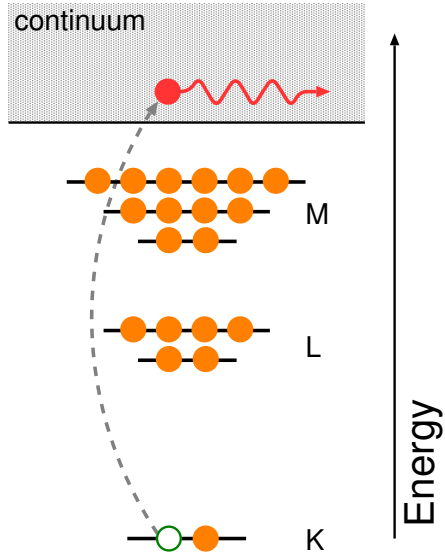

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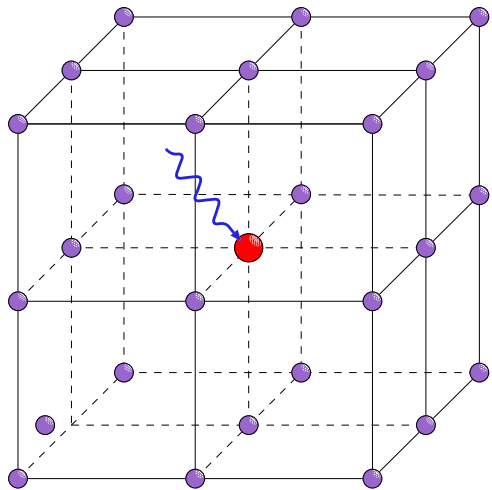

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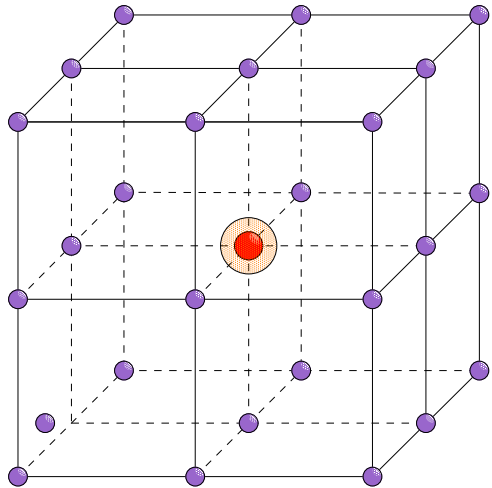

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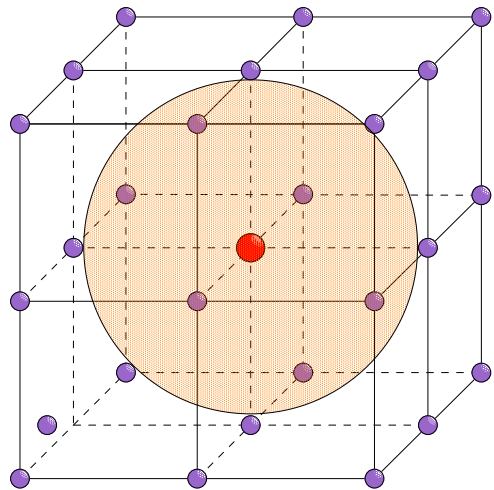

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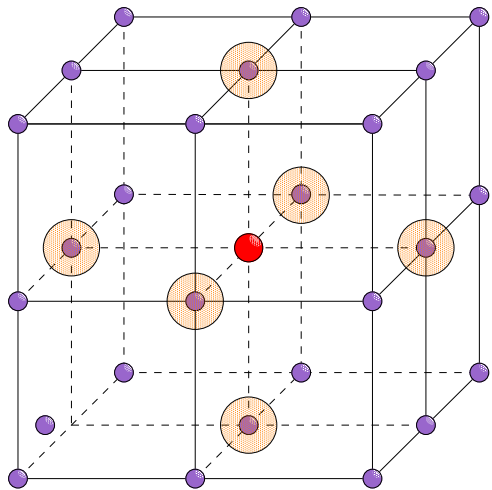

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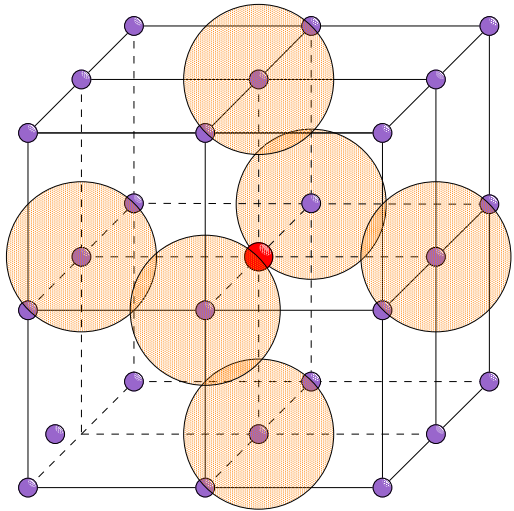

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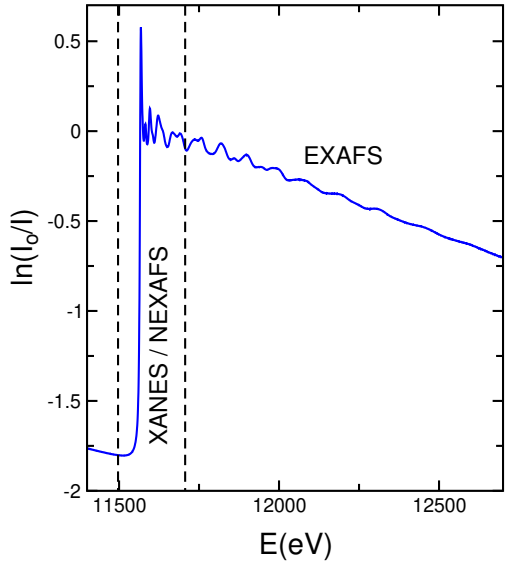
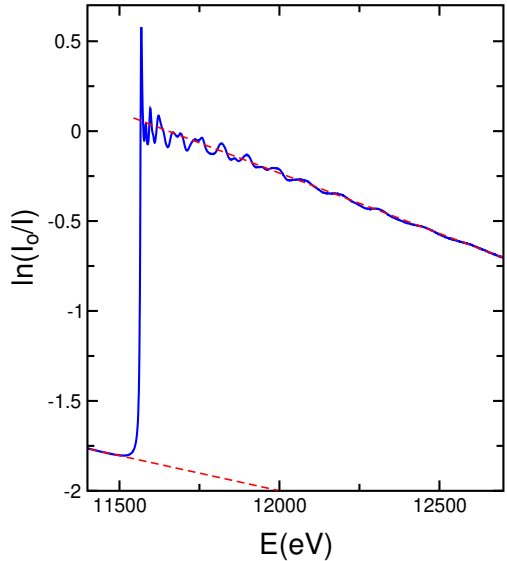


EXAFS data extraction

normalize by fitting pre-edge and post-edge trends



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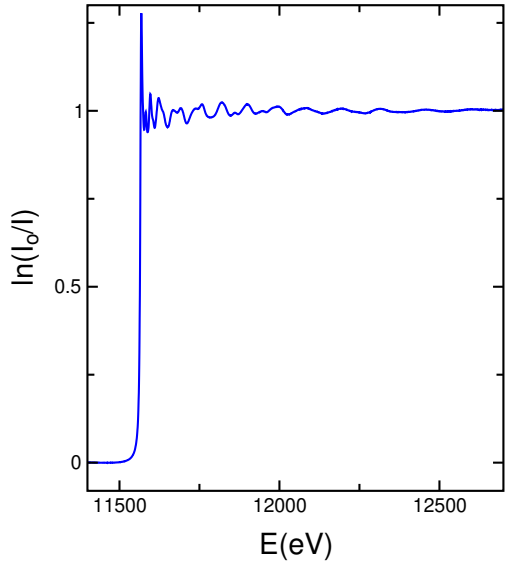

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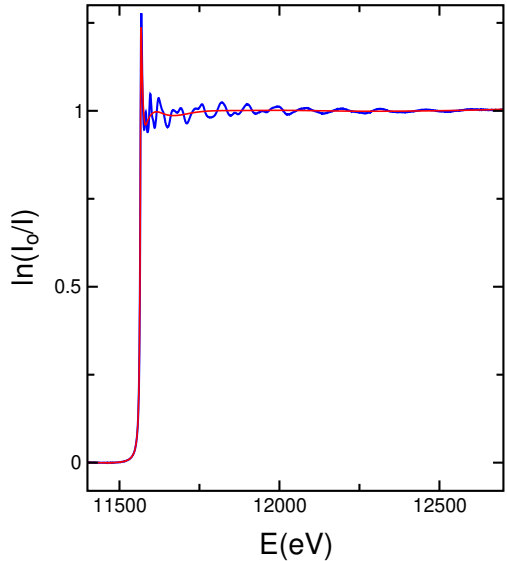

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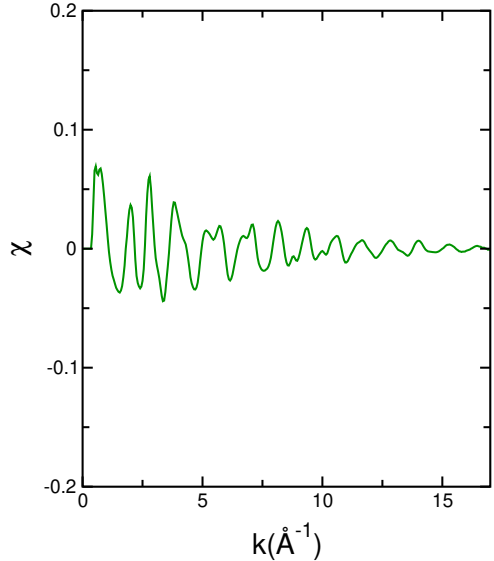

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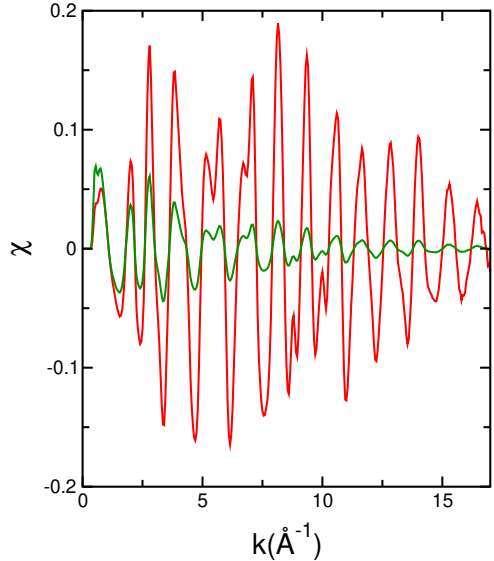

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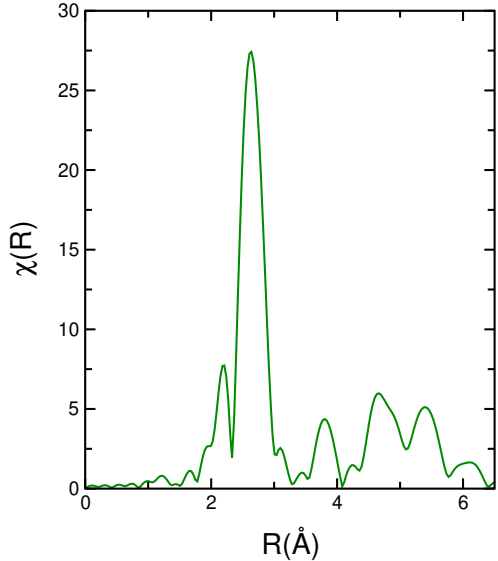
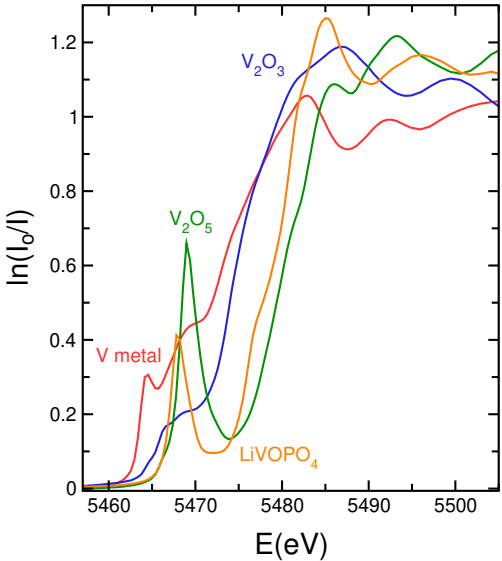
Fourier transform to get real space EXAFS



XANES edge shifts and pre-edge peaks



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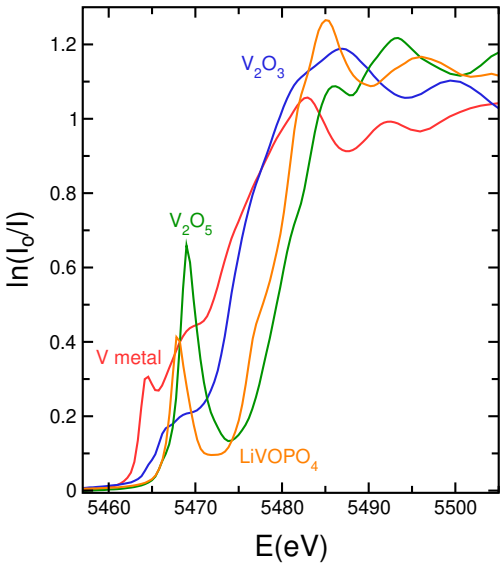

The shift of the edge position can be used to determine the valence state.

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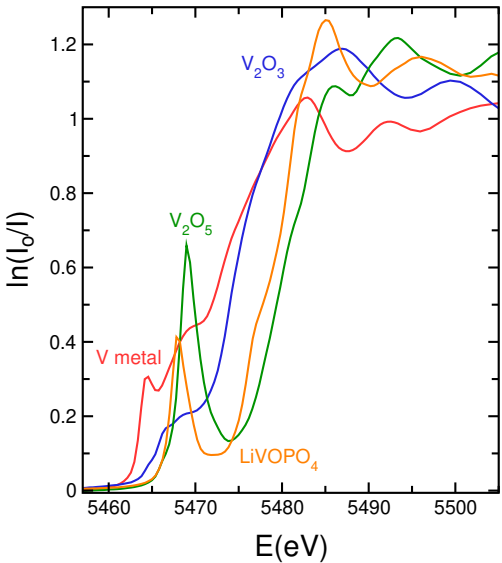

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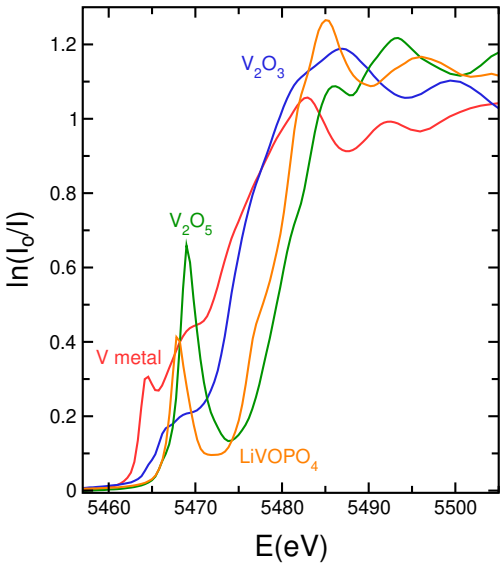

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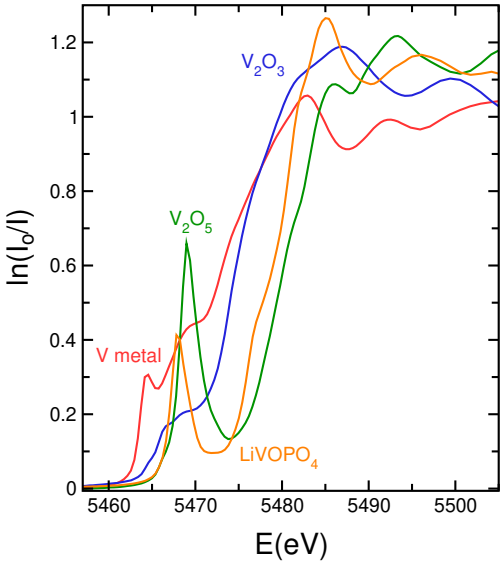

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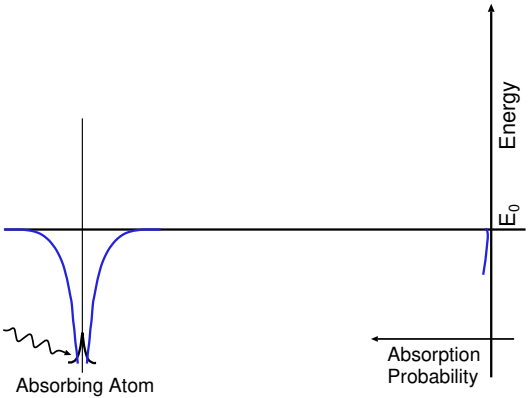
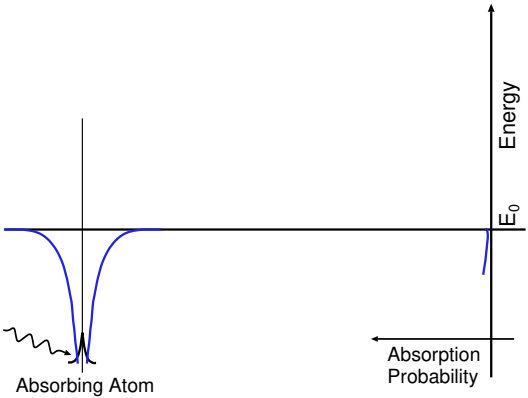
Modern codes, such as FEFF9, are able to accurately compute XANES features.

X-ray absorption by a free atom



X-ray absorption needs an available state for the photoelectron to go into

X-ray absorption by a free atom



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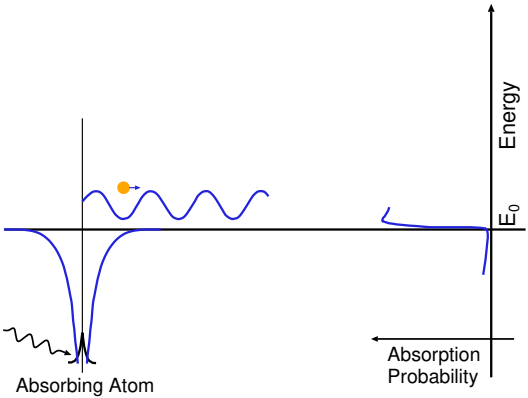

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Once the x-ray energy is large enough to promote a core-level to the continuum, there is a sharp increase in absorption.

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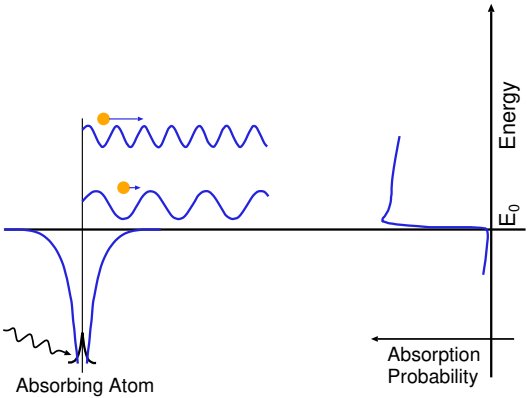

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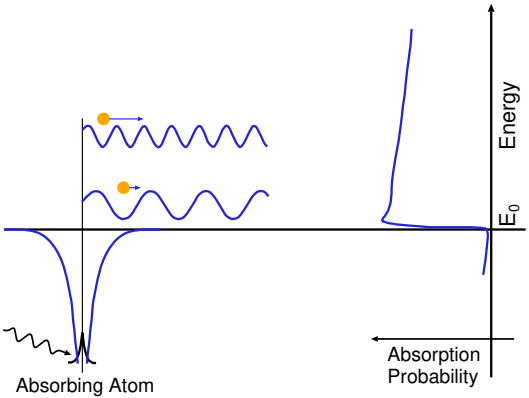
$\mu(E)$ has a sharp step at the core-level binding energy, and is a smooth function of energy above this absorption edge.

X-ray absorption by a free atom



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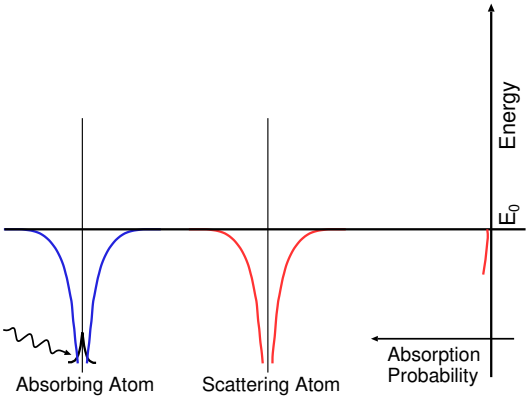
An atom absorbs an x-ray of energy E, destroying a core electron with energy E_0 and creating a photoelectron with energy $(E - E_0)$. The core hole is eventually filled, and a fluorescence x-ray or Auger electron is ejected from the atom.

X-ray absorption with photoelectron scattering



With another atom nearby, the ejected photoelectron can scatter from a neighboring atom and return back to the absorbing atom

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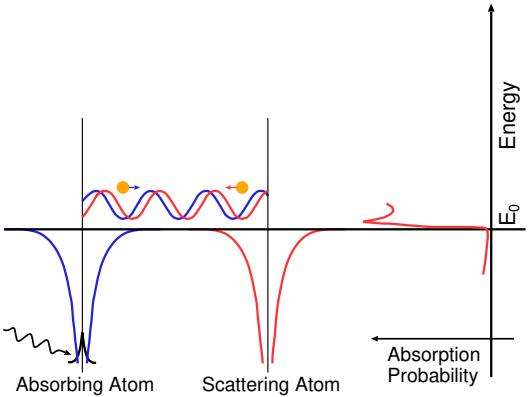

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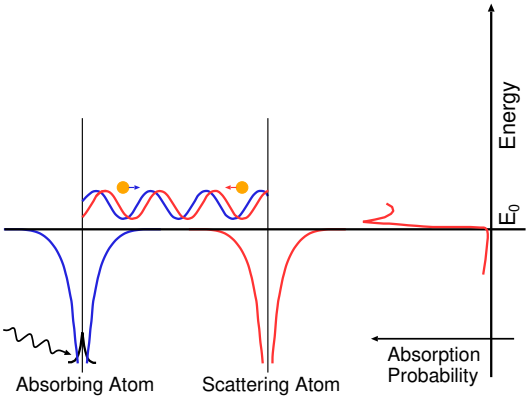
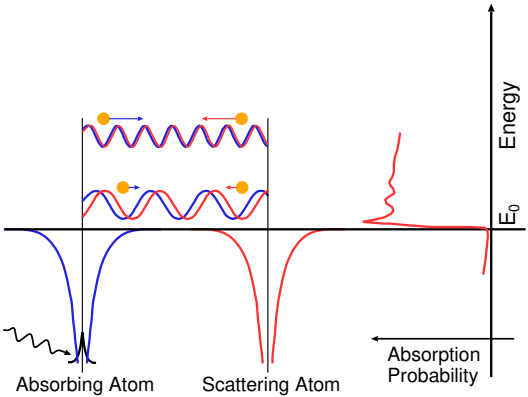


With another atom nearby, the ejected photoelectron can scatter from a neighboring atom and return back to the absorbing atom

In the XANES region $\mu(E)$ depends on the density of electron states with energy $(E - E_0)$, at the absorbing atom with the appropriate symmetry ($\Delta l = \pm 1$, $\Delta m = 0, \pm 1$)

X-ray absorption with photoelectron scattering



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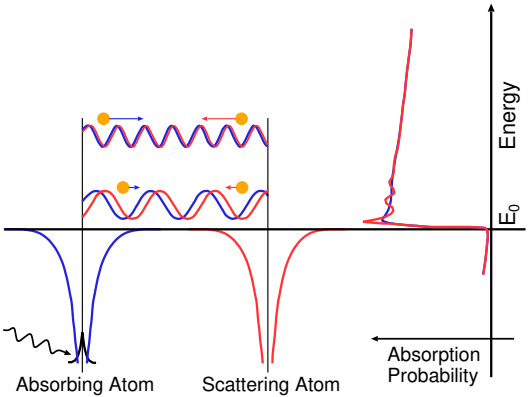
X-ray absorption with photoelectron scattering



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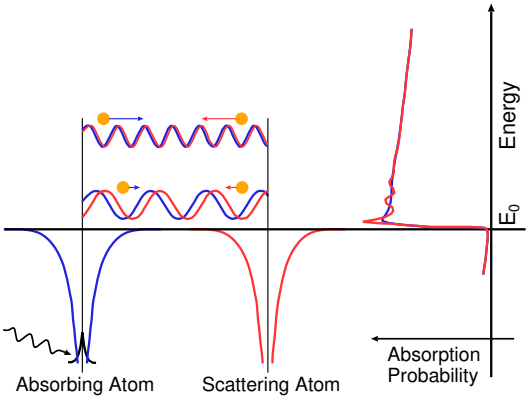
The amplitude and phase of the back-scattered photoelectron at the absorbing atom will vary with energy, causing the oscillations in $\mu(E)$

X-ray absorption: Fermi's golden rule



$$\mu(E) = \mu_0(E) + \Delta\mu(E)$$

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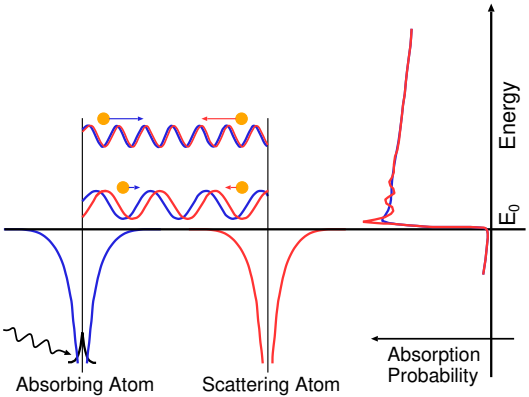

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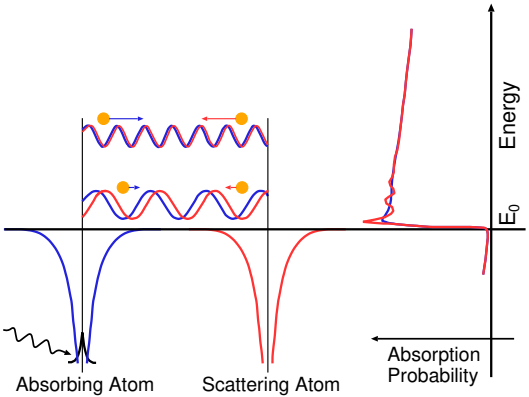

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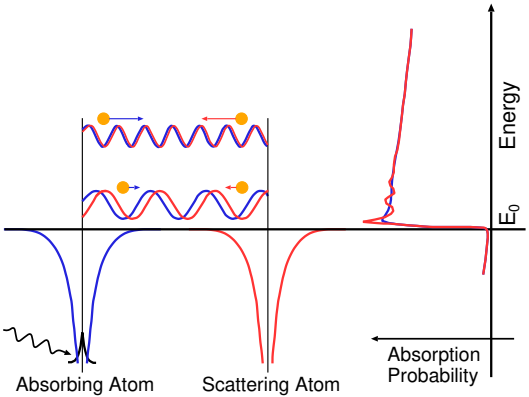

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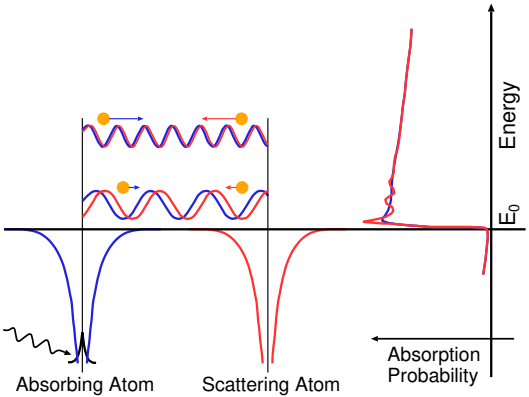

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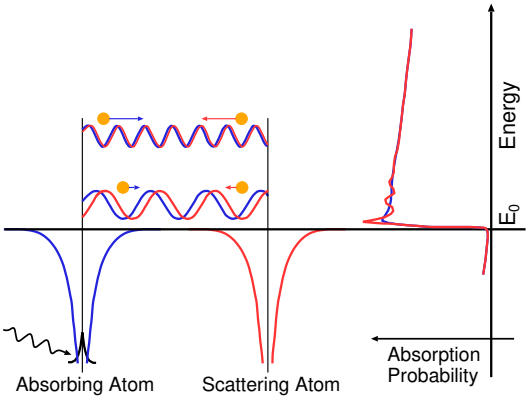

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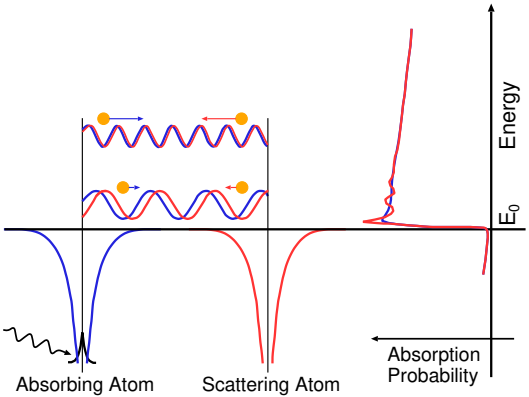

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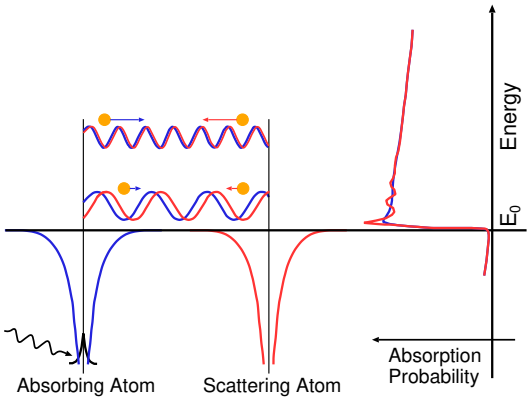

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$\mathcal{H}$ is the interaction. In the dipole approximation, $\mathcal{H} = e^{ikr} \approx 1$.

$|f\rangle$ is the final state which has a photoelectron, a hole in the core, and no photon. This is altered by the neighboring atom: the photoelectron scatters.