Theory of Resonant x-ray spectroscopy

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Spectroscopy: interaction of photons with matter

Photons: x-rays

Matter: Transition metal compounds

Group	1	2		3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
Period																			
1	1 H																		2 He
2	3 Li	4 Be												5 B	6 C	7 N	8 O	9 F	10 Ne
3	11 Na	12 Mg												13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4	19 K	20 Ca		21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5	37 Rb	38 Sr		39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba	*	71 Lu	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra	**	103 Lr	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Uub	113 Uut	114 Uuq	115 Uup	116 Uuh	117 Uus	118 Uuo
*Lanthanoids			*	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb		
**Actinoids			**	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No		

Spectroscopy: interaction of photons with matter

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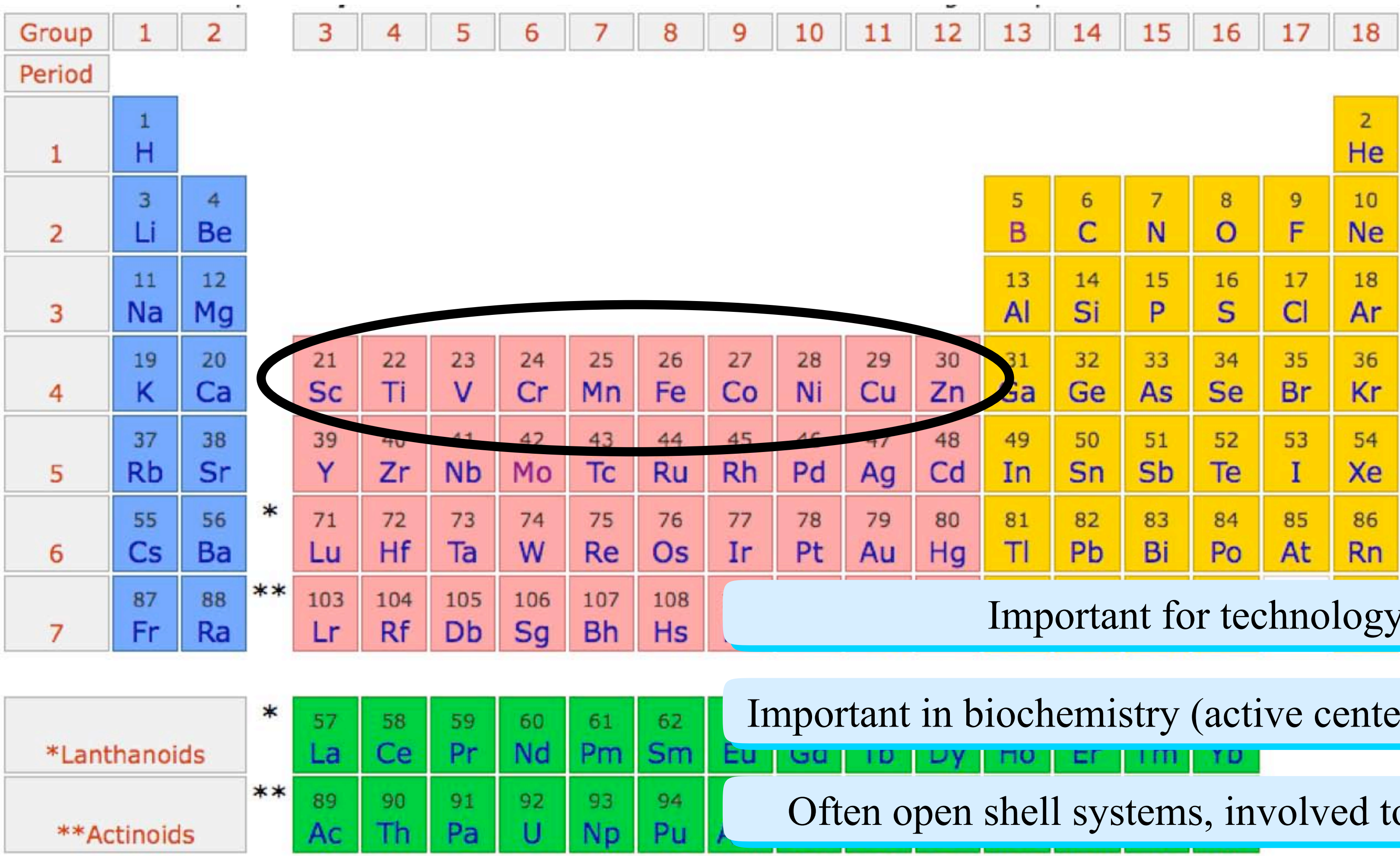
Matter: Transition metal compounds



Important for technology

Important in biochemistry (active centers of enzymes)

Often open shell systems, involved to understand

Transition metal compounds show a large variety of properties

Exchange bias

PHYSICAL REVIEW VOLUME 102, NUMBER 5 JUNE 1, 1956

Letters to the Editor

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New Magnetic Anisotropy

W. H. Meiklejohn and C. P. Bean
General Electric Research Laboratory, Schenectady, New York
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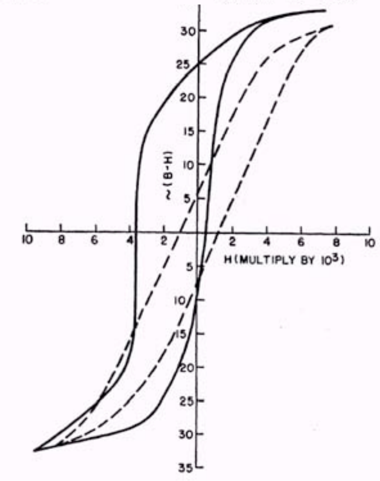
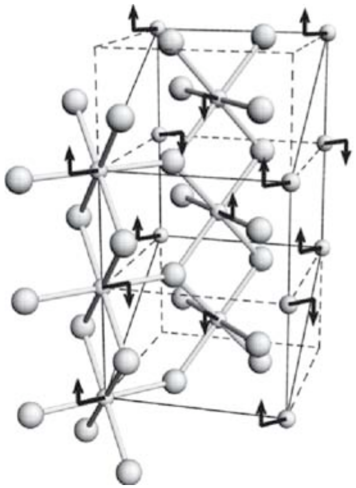
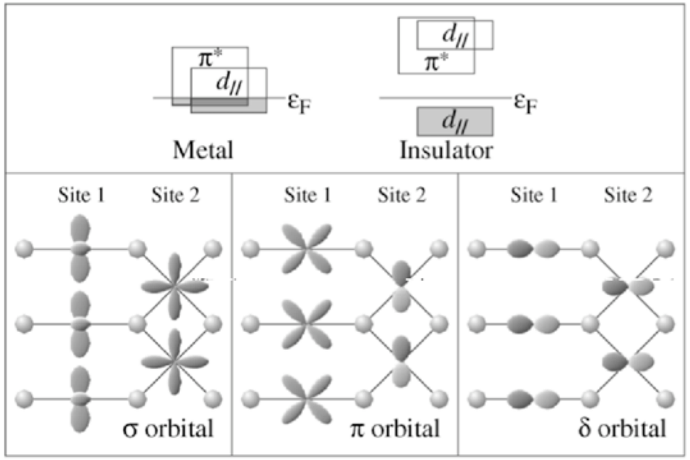


Transition metal compounds show a large variety of properties

Metal Insulator transitions



Phys. Rev. Lett. 95, 196404 (2005)



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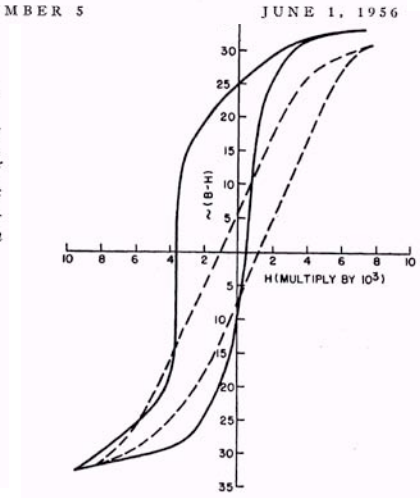

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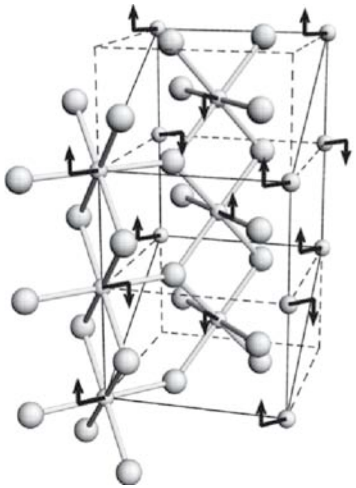

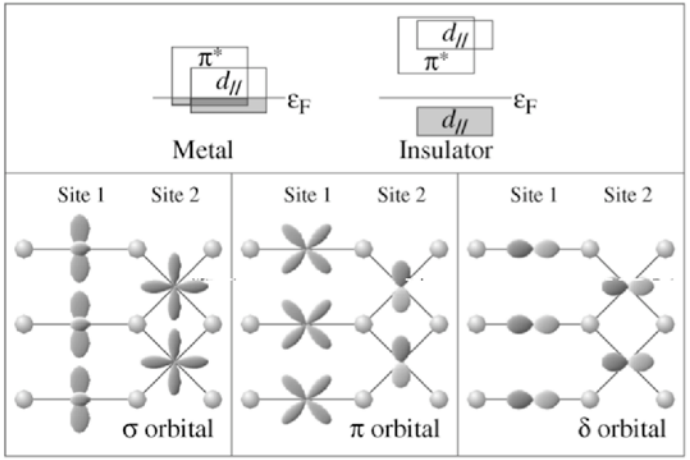

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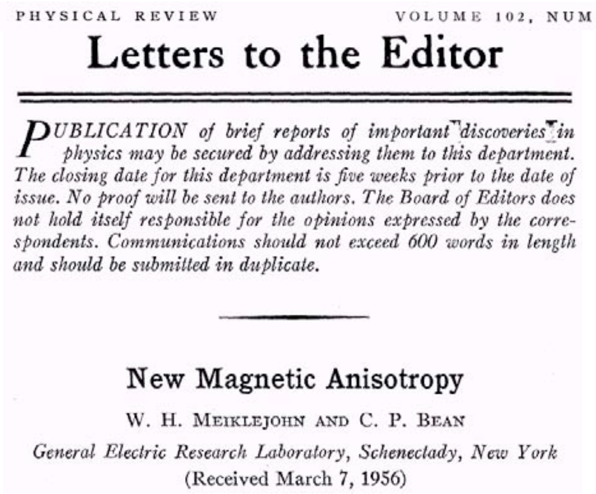

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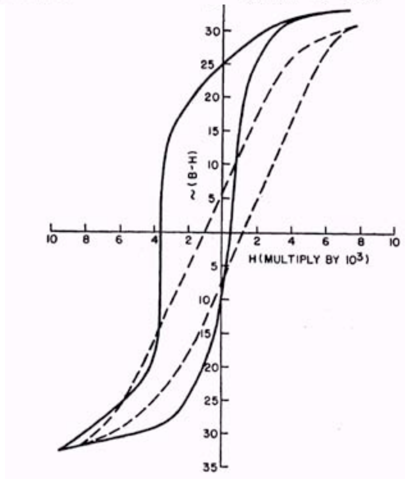
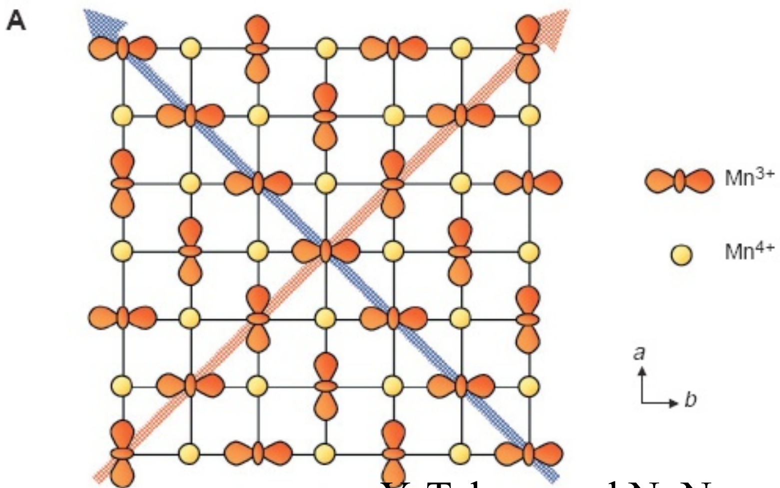


Colossal magneto resistance



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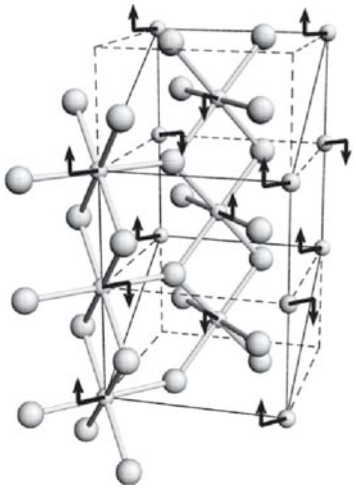

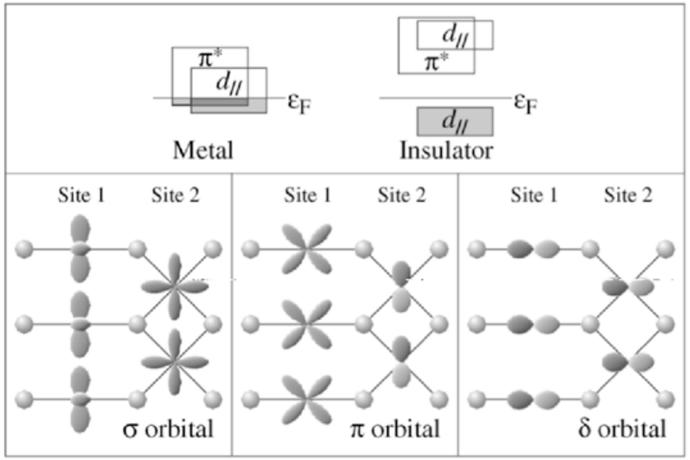

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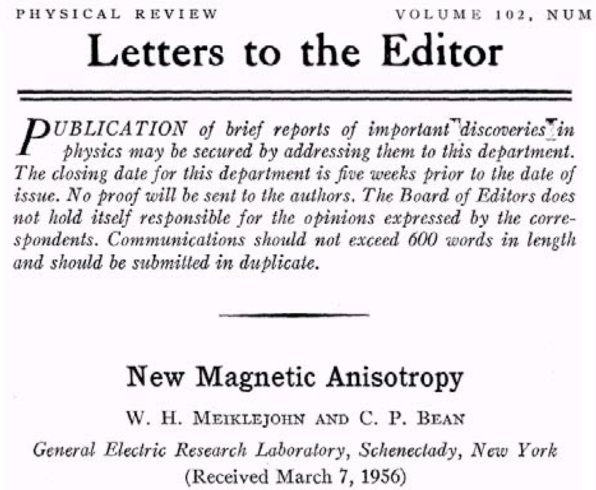

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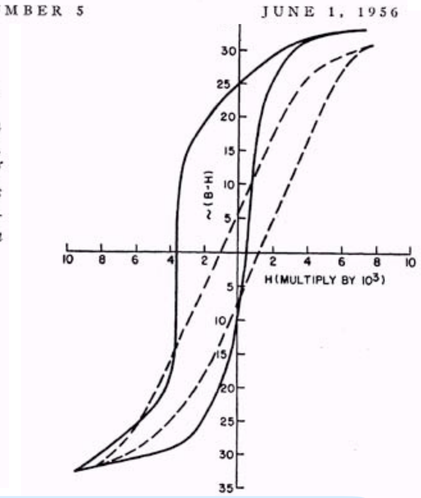

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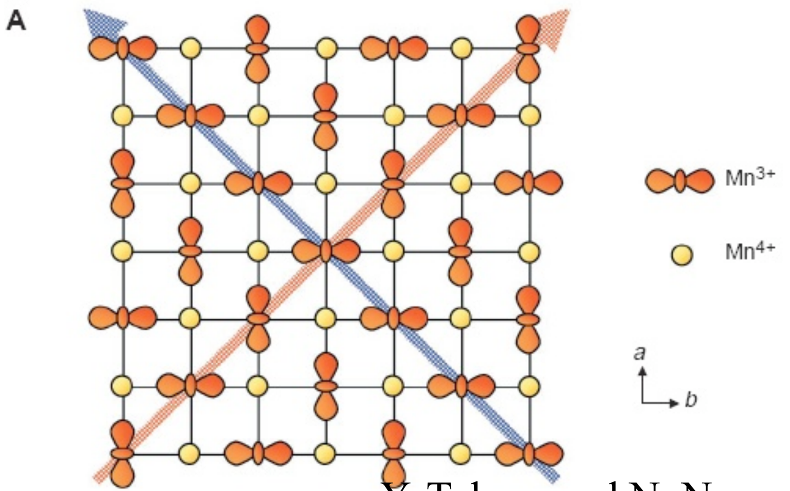

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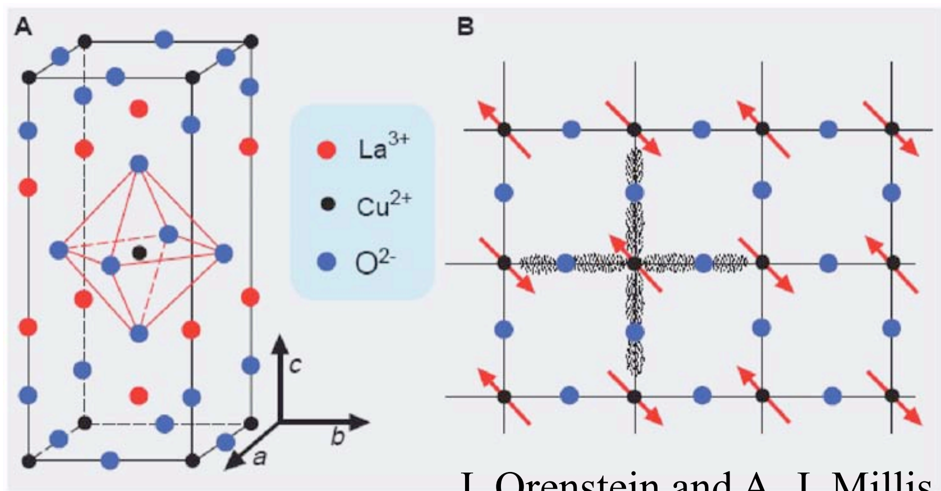
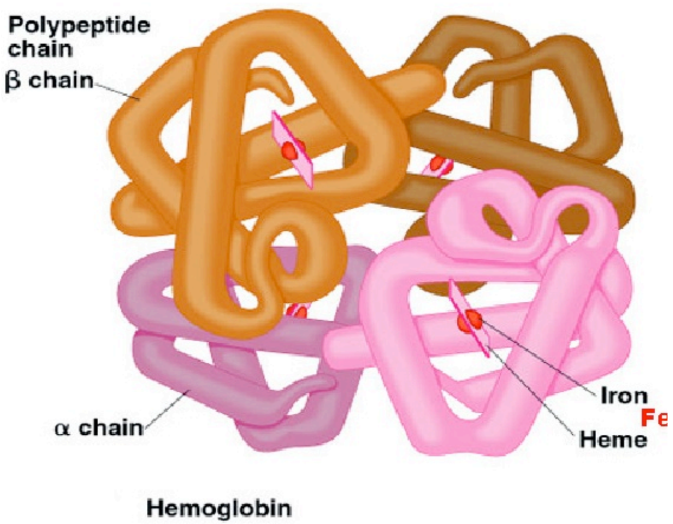
High-Tc Superconductivity

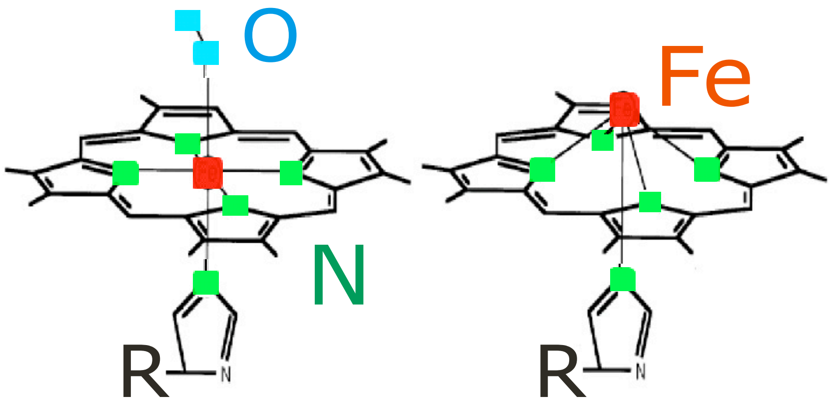


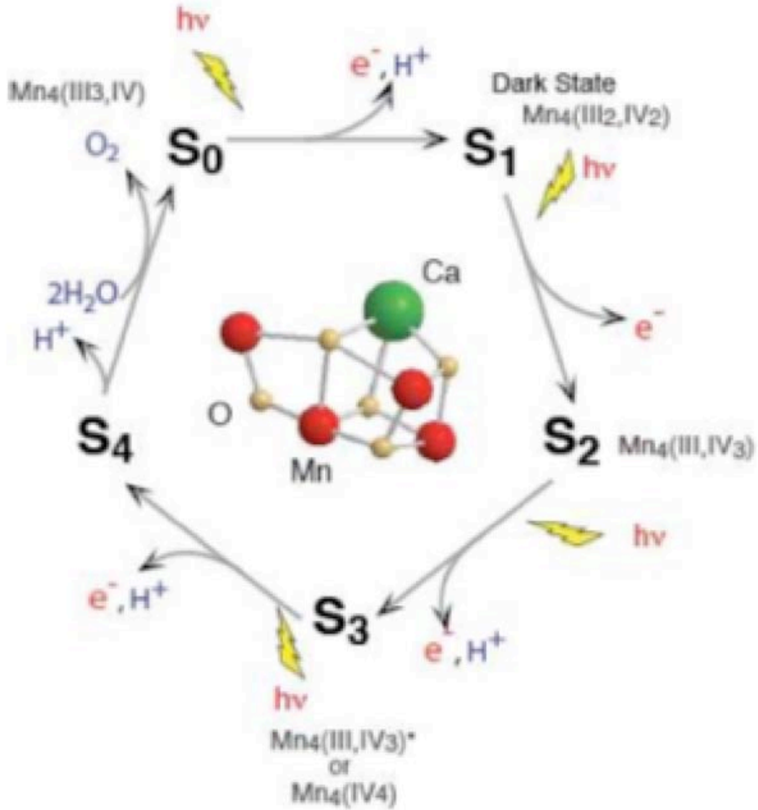
J. Orenstein and A. J. Millis,
Science 288, 468 (2000).

Transition metal compounds show a large variety of properties

Active centers in enzymes





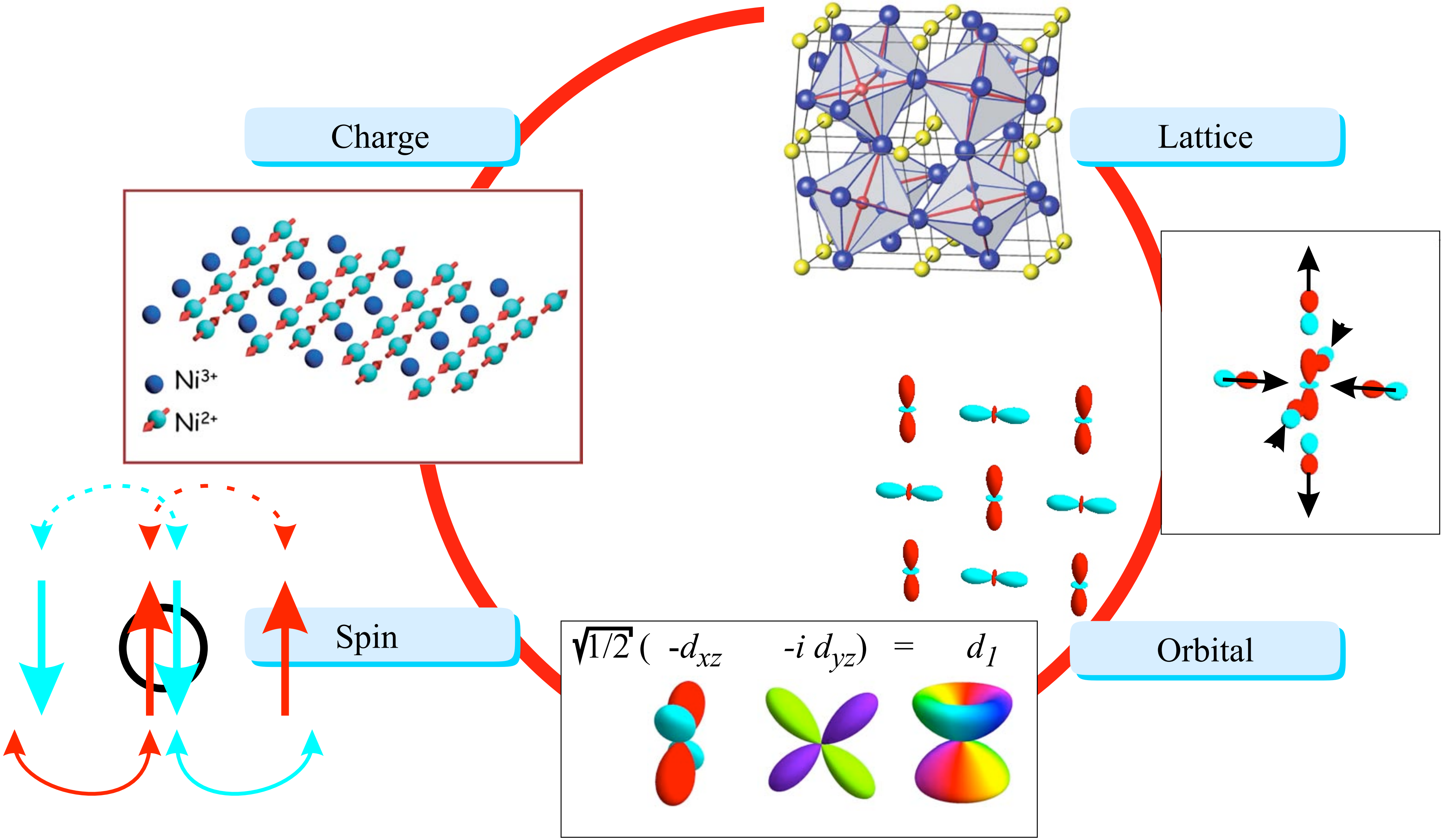


Kok Cycle for water splitting reaction in PSII.

Fe in Heme

Mn in Photo-system II

Interactions between the charge, lattice, orbitals and spins



Need tools to measure

- Spin arrangements (element resolved) of TM multilayers

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- Valence and local symmetry of TM compounds

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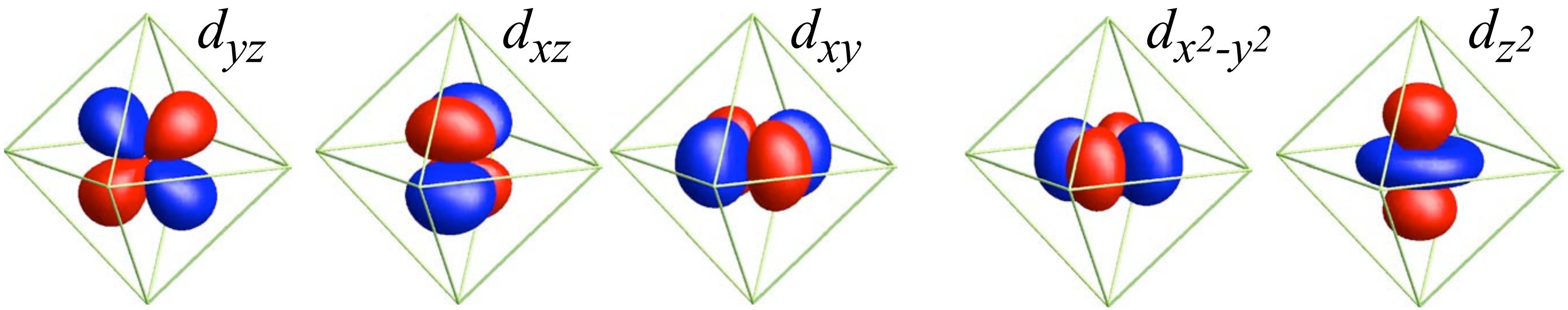
- Valence and local symmetry of TM compounds
- Orbital occupation (The d-shell is 5-fold degenerate)



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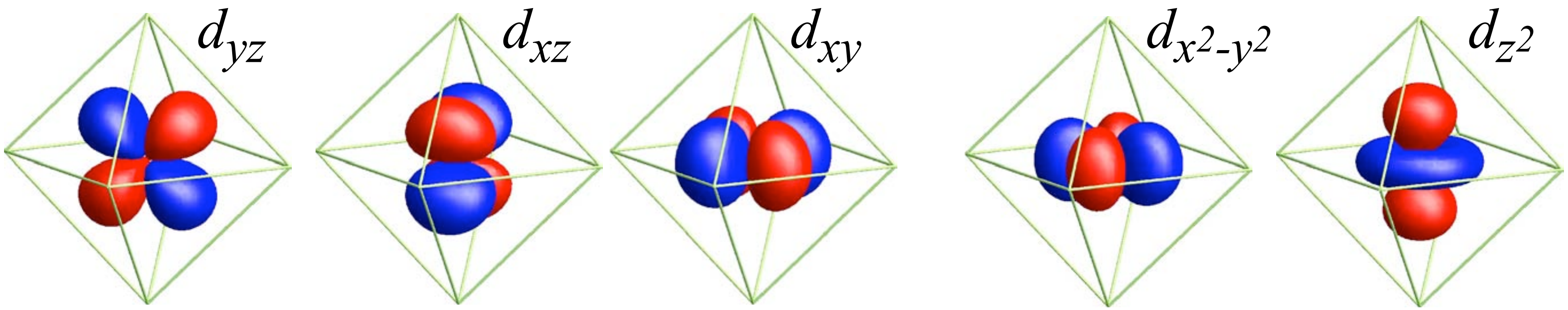
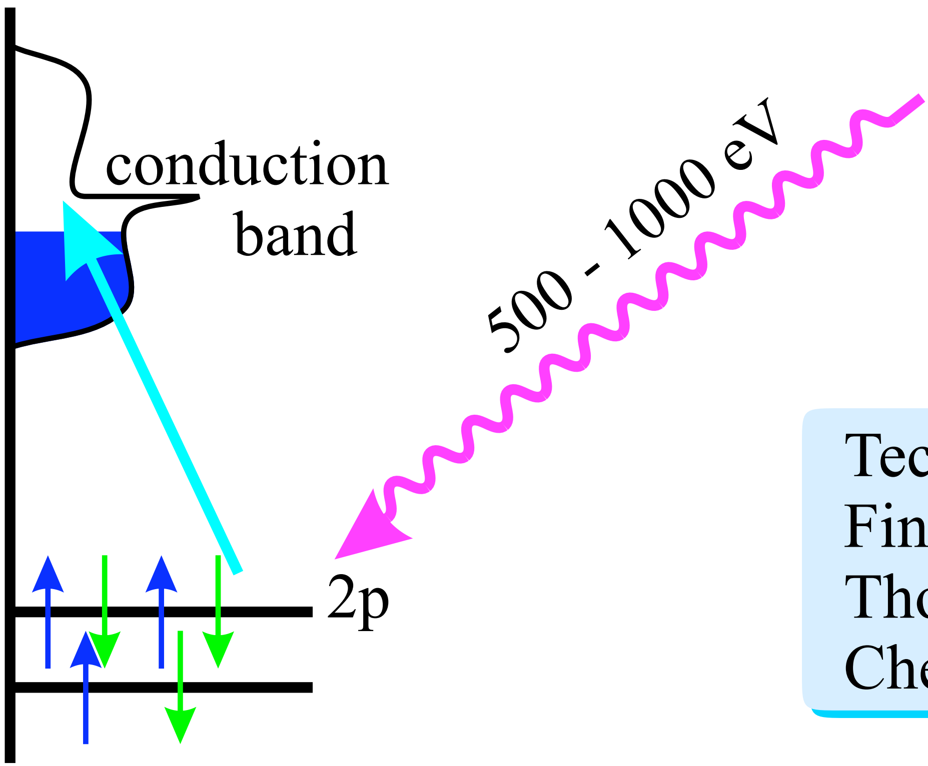


- And excitations (spin-waves - magnons - orbital excitations)

Need tools to measure: Orbital, Spin, Charge

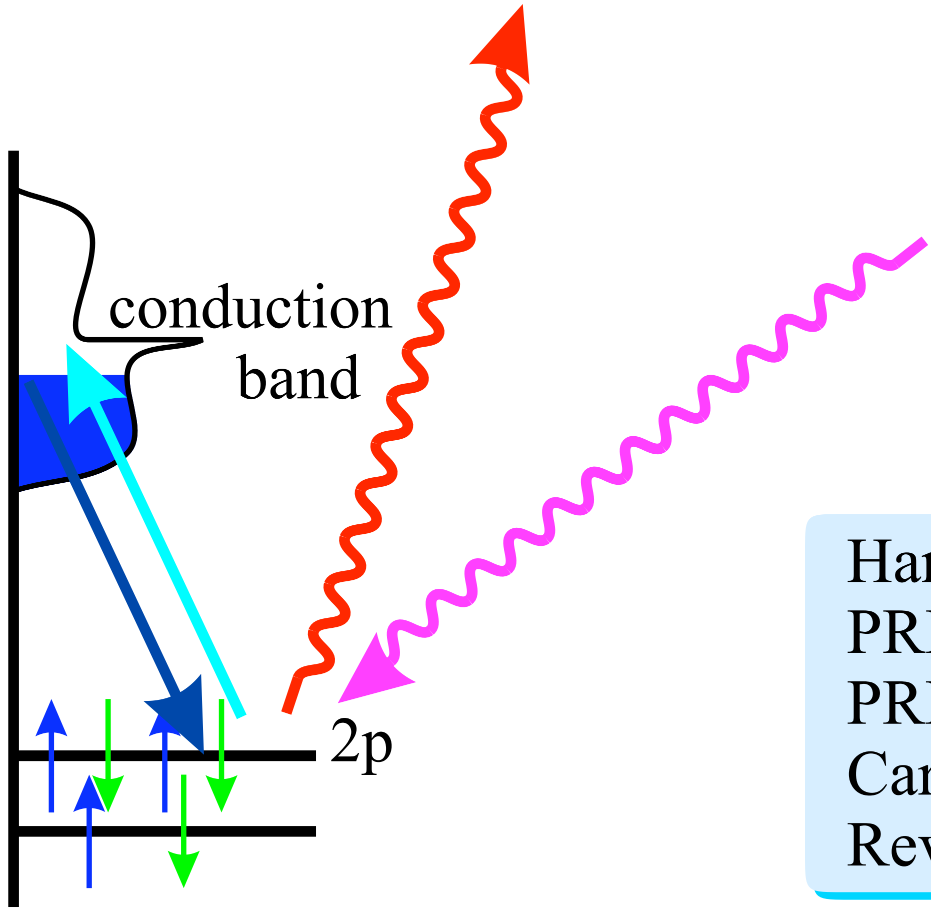
- X-ray Absorption Spectroscopy (XAS) at the TM *2p* to *3d* edge



Technique developed in late 1980's:
Fink, Sawatzky, Fuggle
Thole, van der Laan
Chen, Sette

Need tools to measure: Orbital, Spin, Charge

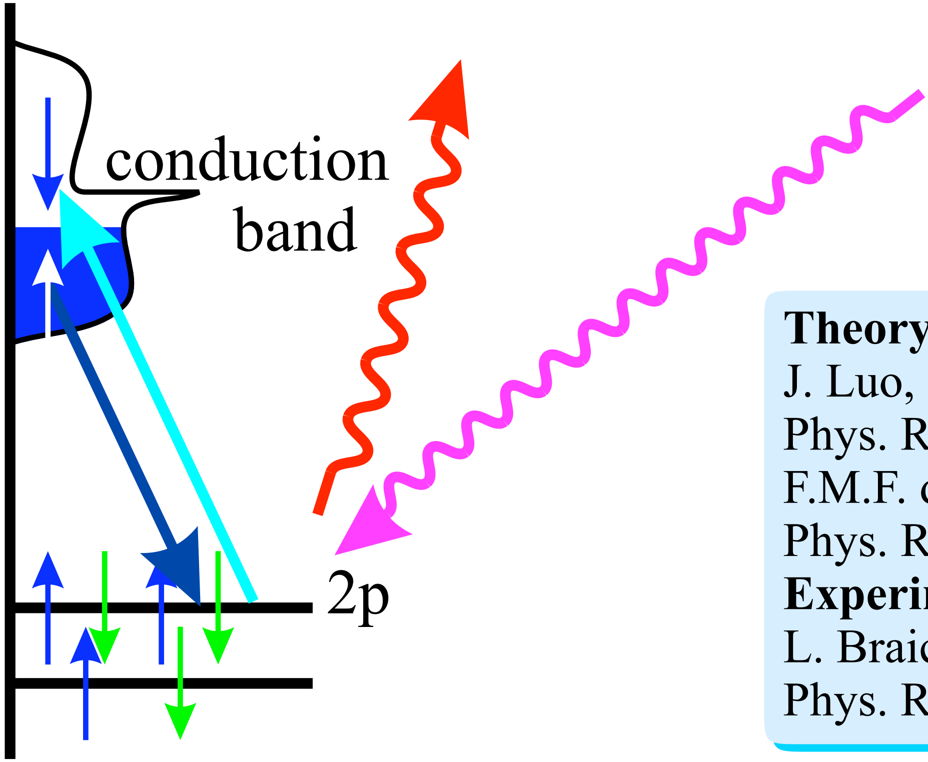
- X-ray Absorption Spectroscopy (XAS) at the TM *2p* to *3d* edge
- Resonant X-ray Diffraction (RXD)



Hannon, Trammel, Bloom, Gibbs
PRL **61**, 1245 (1988)
PRB **43**, 5663 (1991)
Carra, Thole
Rev. Mod. Phys. 66, 1509 (1994).

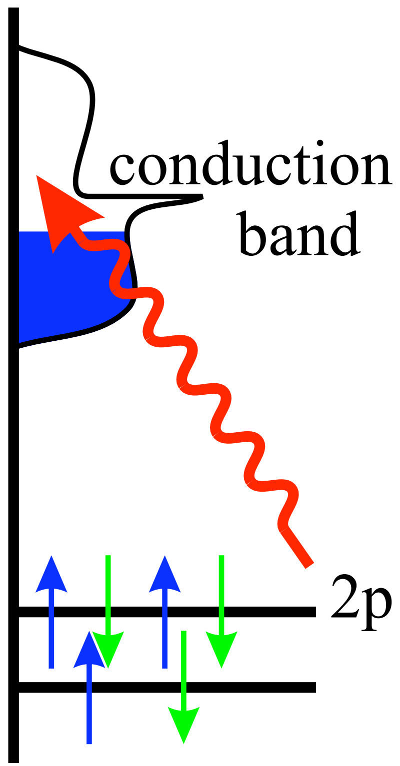
Need tools to measure: Orbital, Spin, Charge

- X-ray Absorption Spectroscopy (XAS) at the TM *2p* to *3d* edge
- Resonant X-ray Diffraction (RXD)
- Resonant Inelastic X-ray Scattering (RIXS)

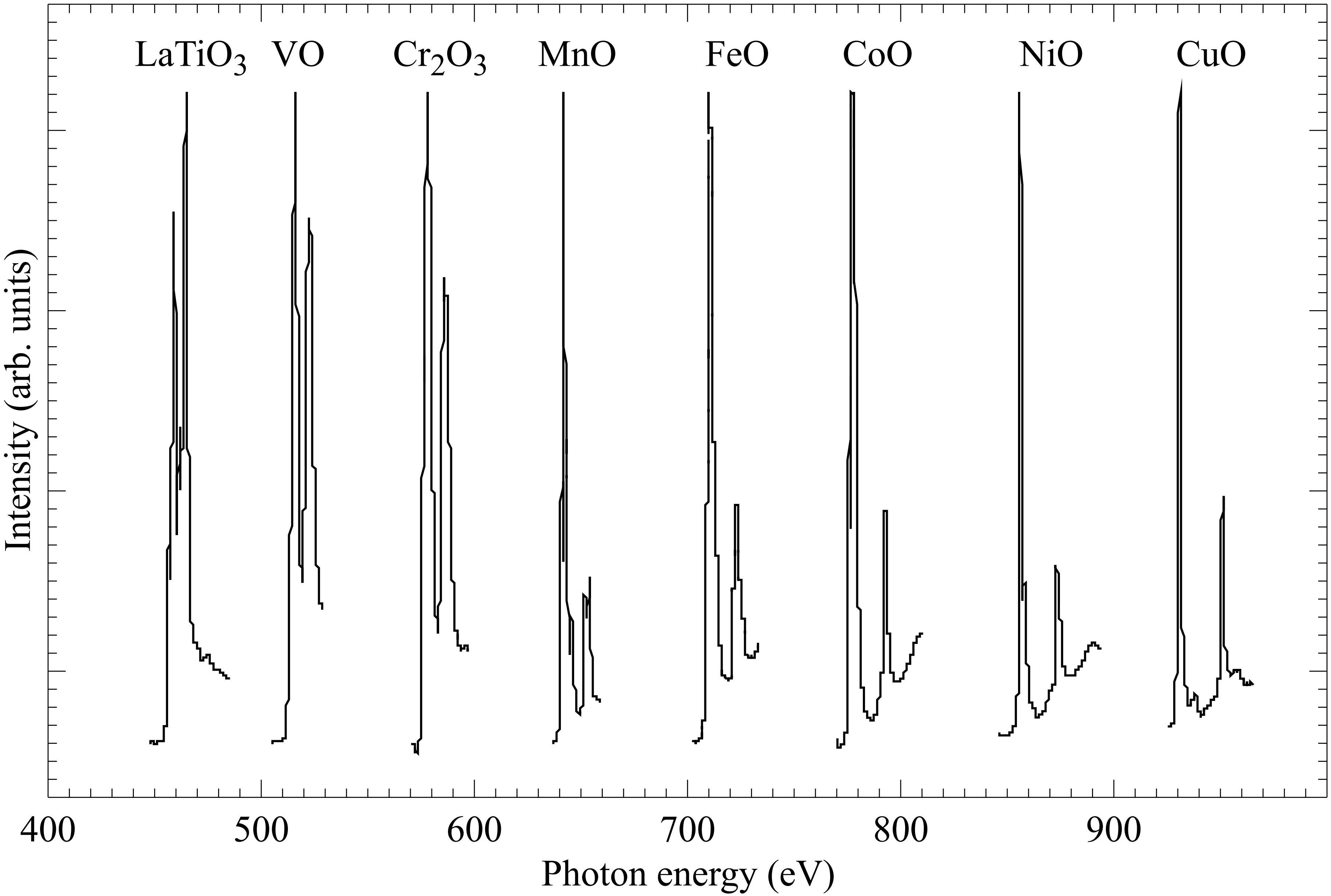


Theory prediction of magnetic excitations
J. Luo, G.T. Trammell, and J.P. Hannon,
Phys. Rev. Lett. **71**, 287 (1993).
F.M.F. de Groot, P. Kuiper, and G.A. Sawatzky,
Phys. Rev. B **57**, 14584 (1998).
Experimental realization
L. Braicovich, G. Ghiringhelli, N. B. Brookes *et al.*
Phys. Rev. Lett. **102**, 167401 (2009).

X-ray Absorption Spectroscopy

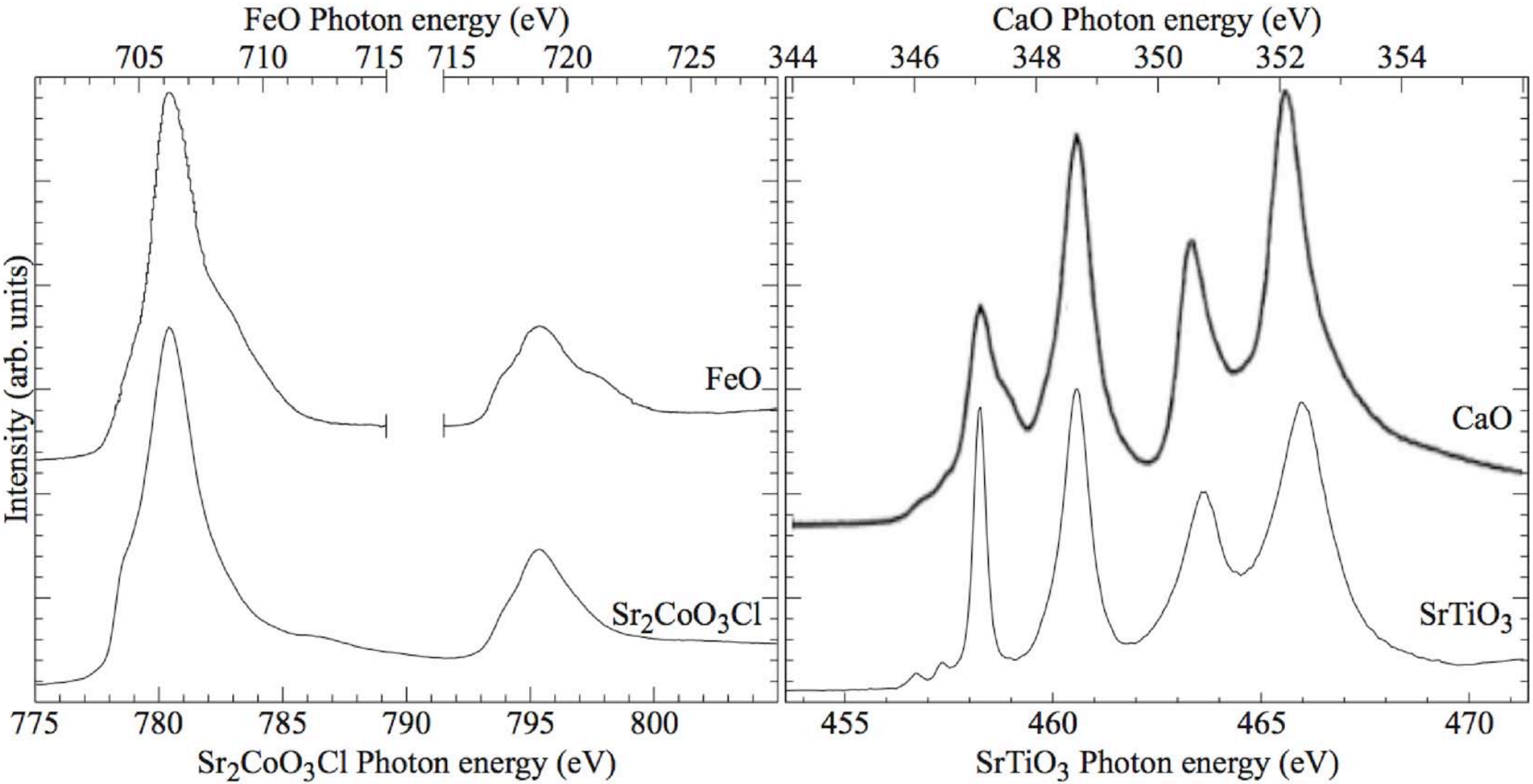


X-ray Absorption Spectroscopy: Some observations



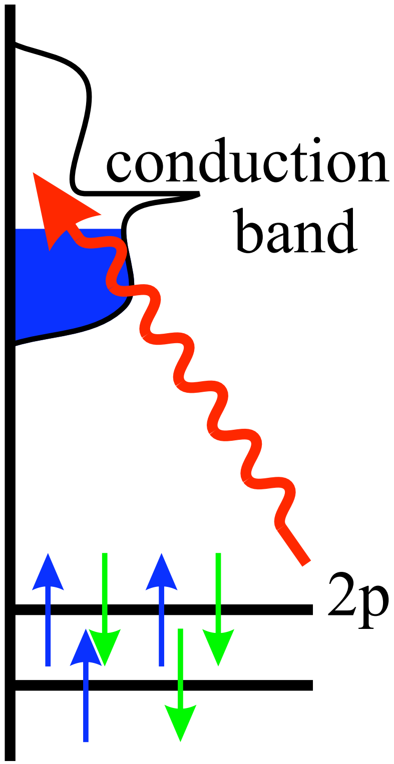
X-ray Absorption Spectroscopy: Some observations

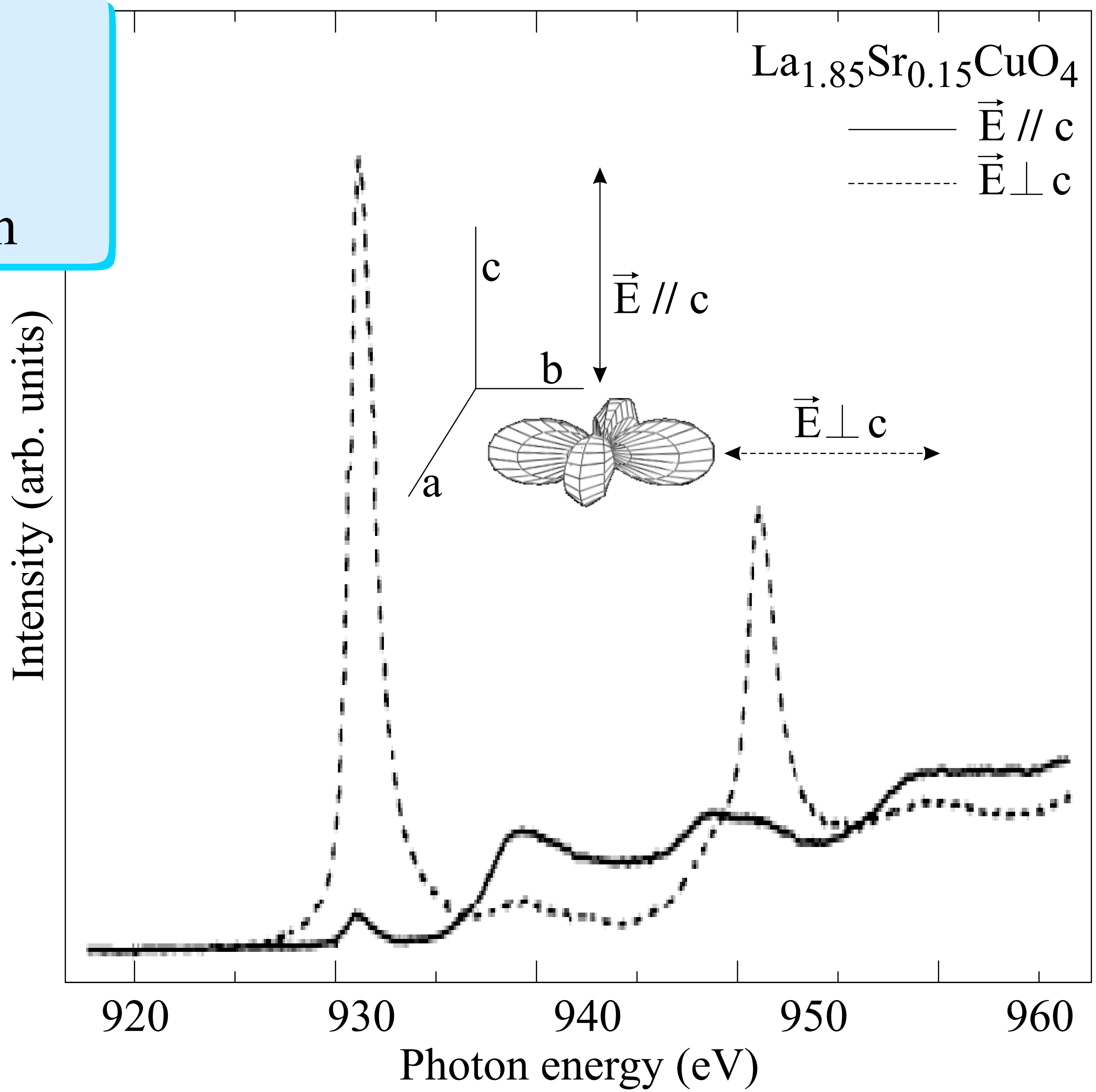
Valence dependence - ground state symmetry determines the line shape



X-ray Absorption Spectroscopy: Some observations

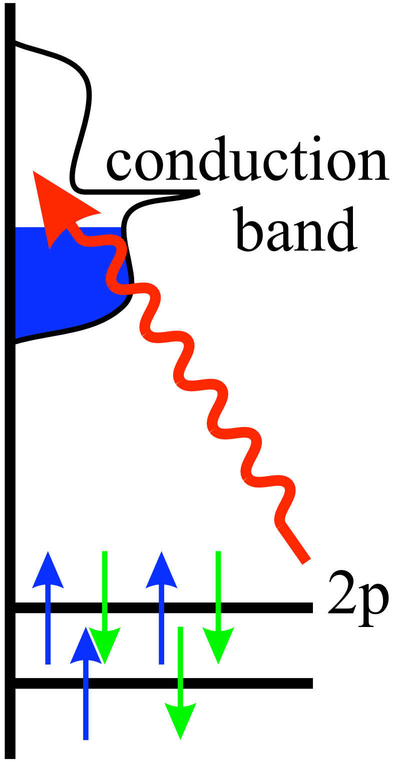
Polarized XAS
Sensitive to
Orbital occupation
natural linear dichroism

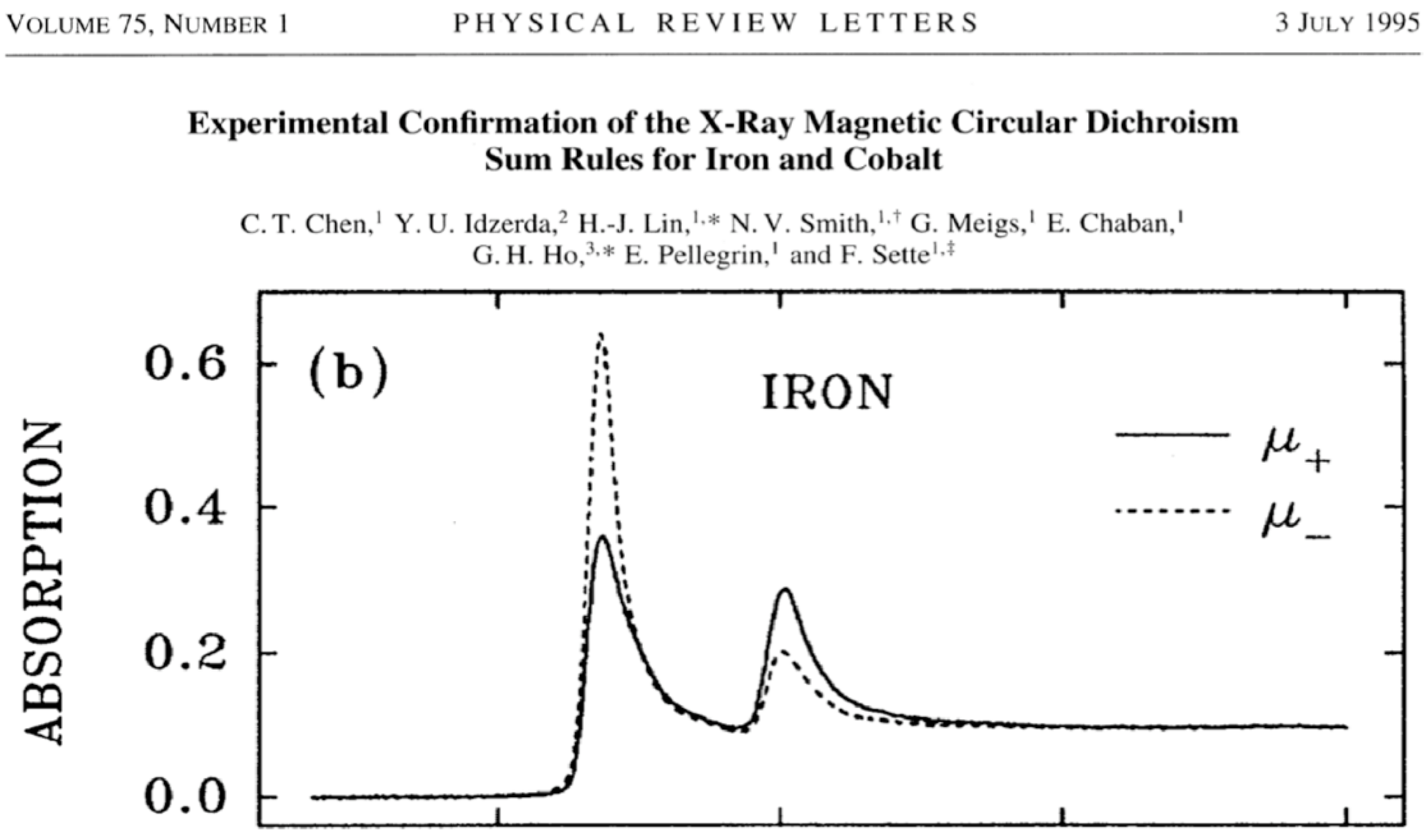




X-ray Absorption Spectroscopy: Some observations

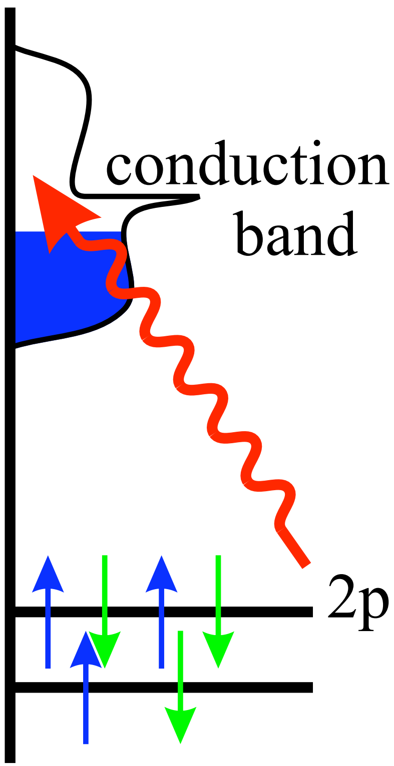
Polarized XAS
Sensitive to
Magnetic moments
magnetic circular dichroism

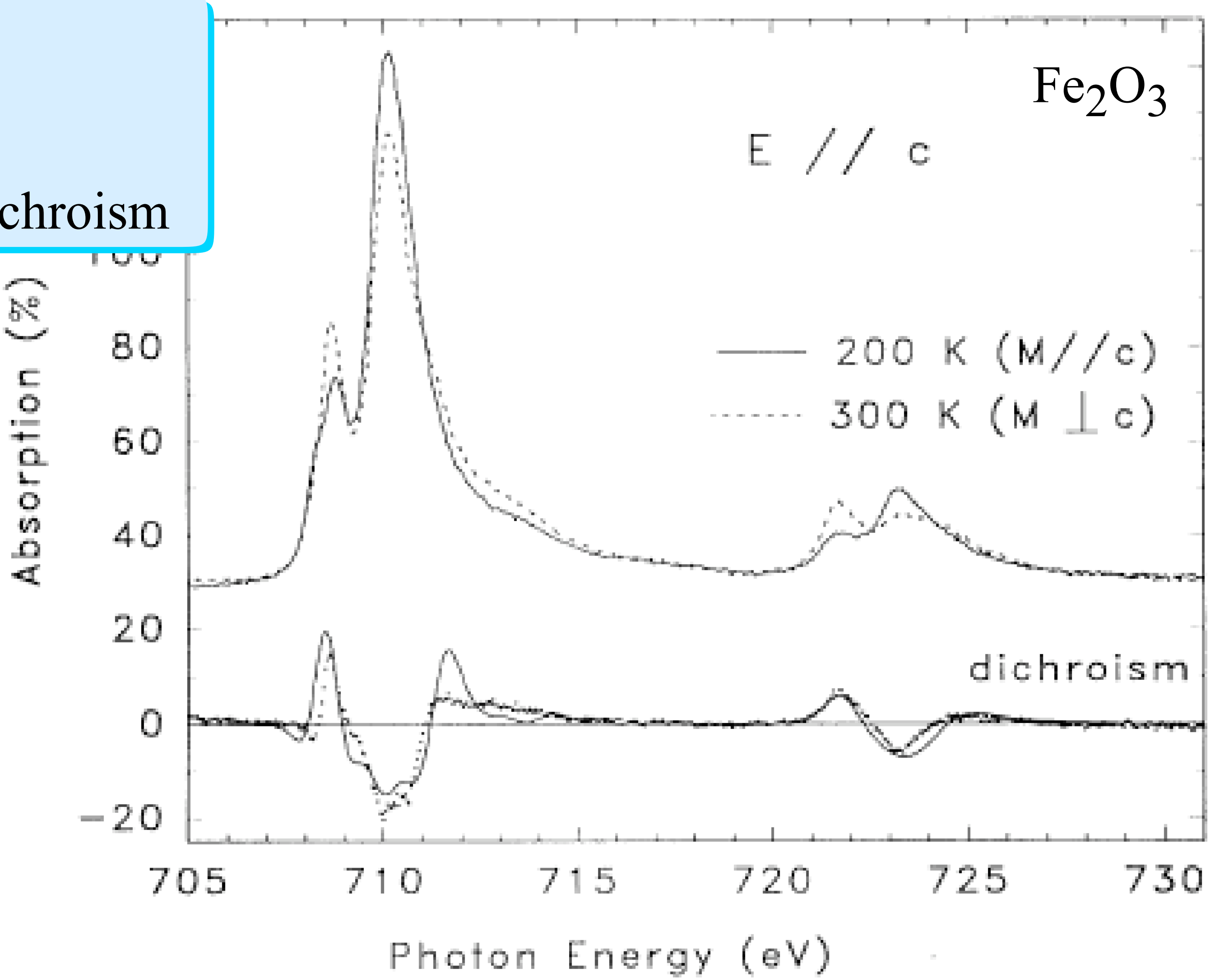




X-ray Absorption Spectroscopy: Some observations

Polarized XAS
Sensitive to
Spin orientation
magnetic linear dichroism





X-ray Absorption Spectroscopy: A band picture

RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 40, NUMBER 1 1 JULY 1989

X-ray absorption of $YBa_2Cu_3O_7$: A band picture

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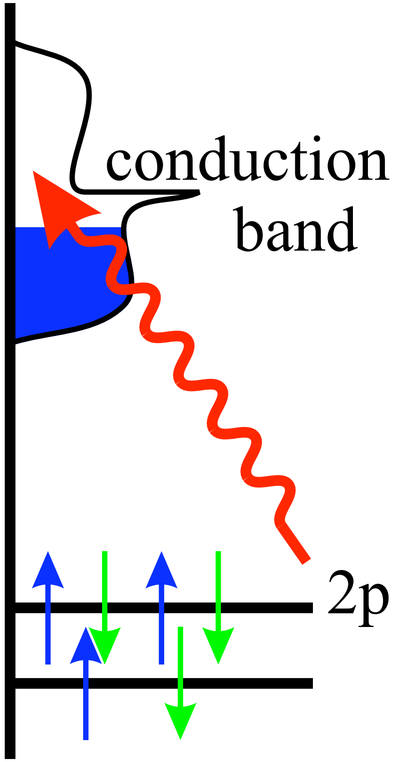
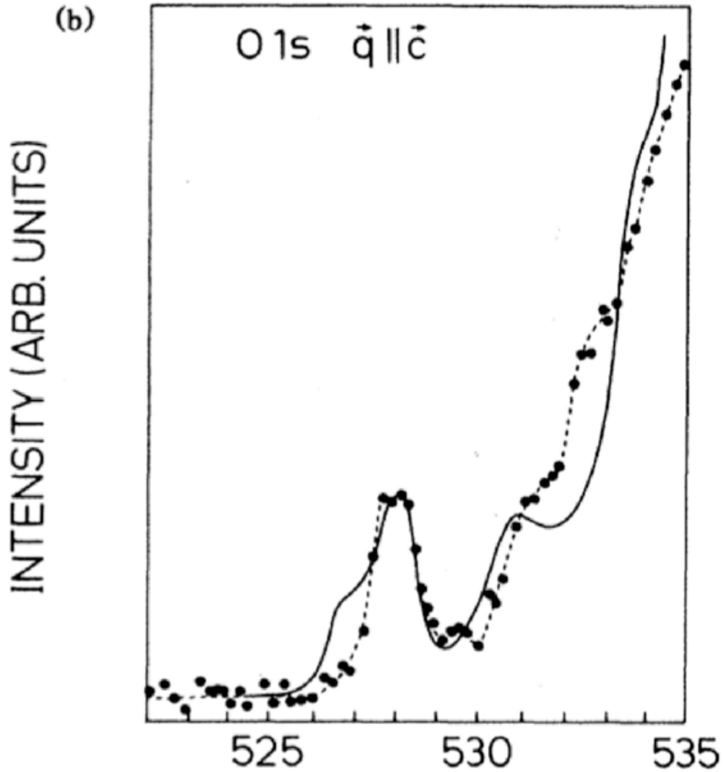
Max-Planck-Institut für Festkörperforschung, D-7000 Stuttgart 80, Heisenbergstrasse 1, Federal Republic of Germany





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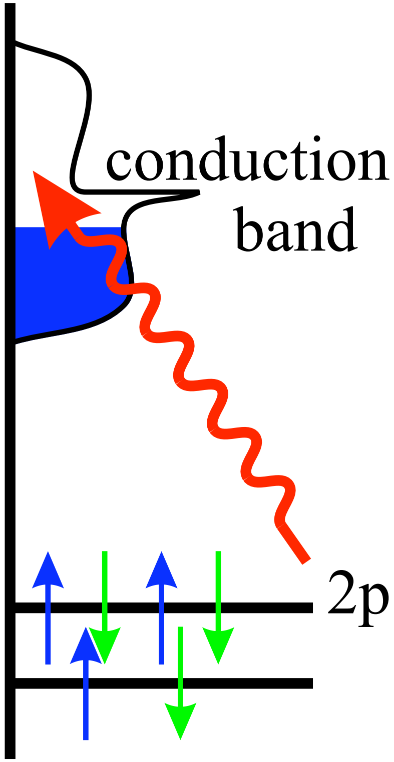
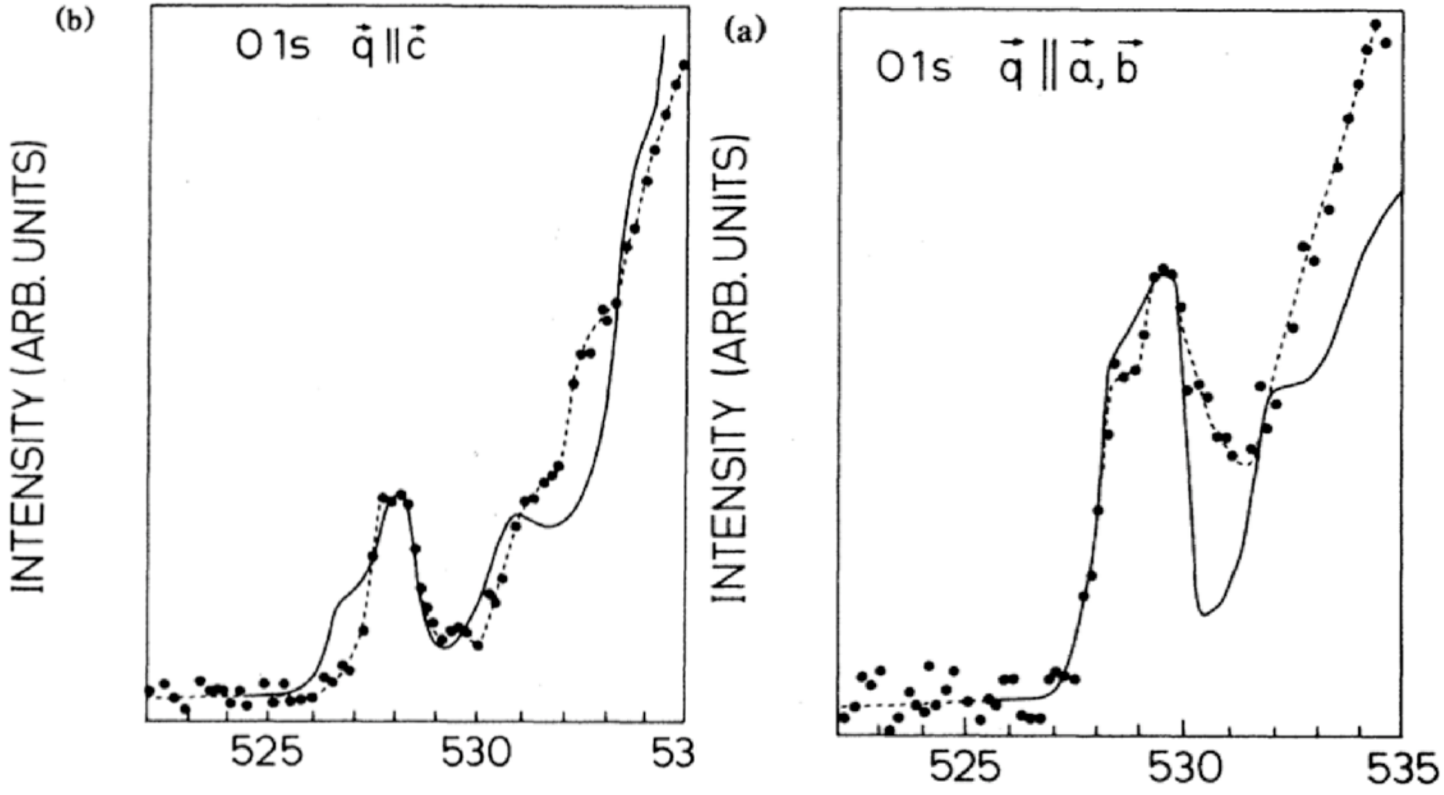
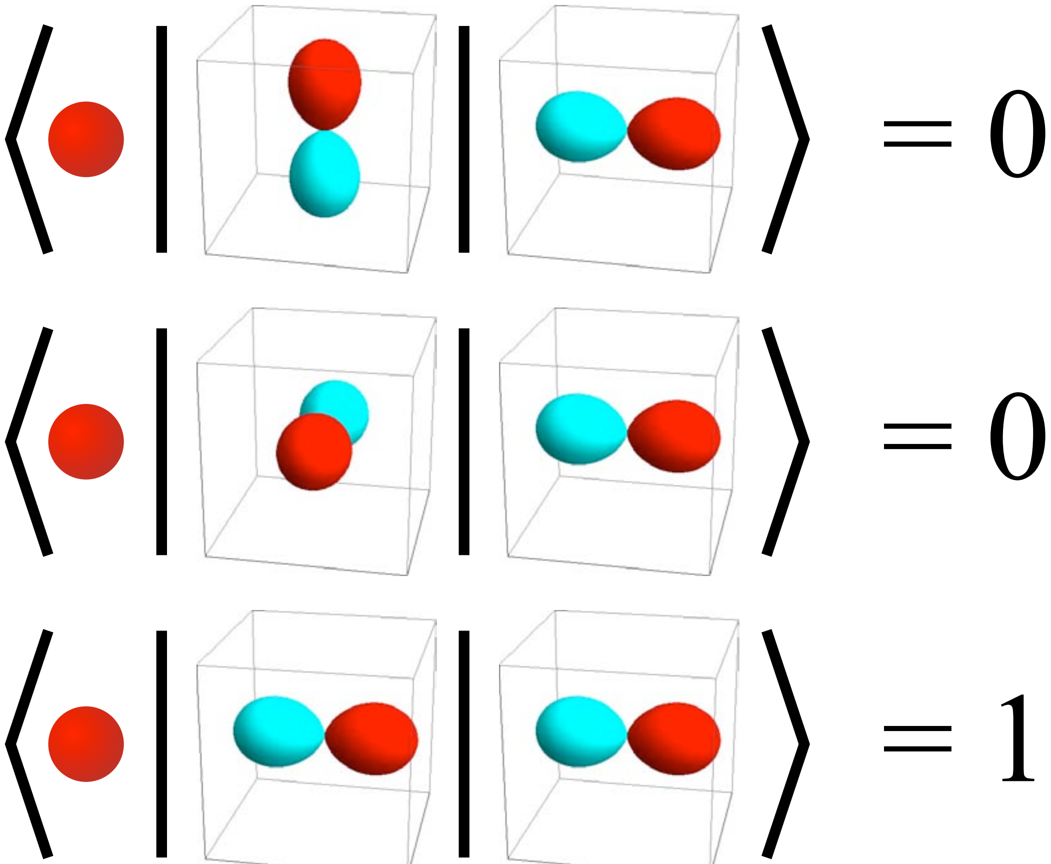




X-ray Absorption Spectroscopy: One electron selection rules

$$\mu_q(h\nu) = \sum_{\Phi_f} |\langle \Phi_f | r C_q^{(1)} | \Phi_i \rangle|^2 \delta(E_i - E_f + h\nu)$$



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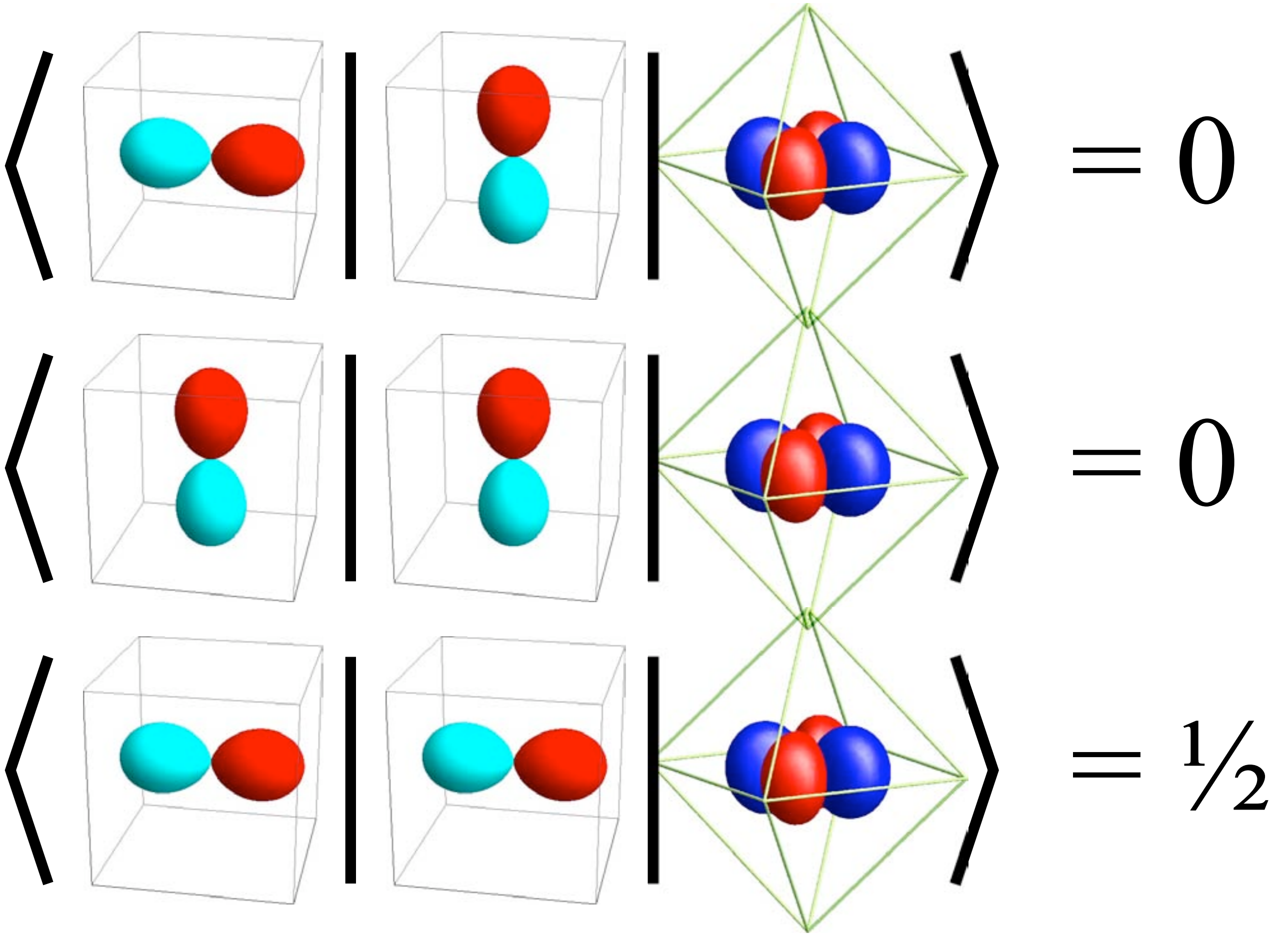

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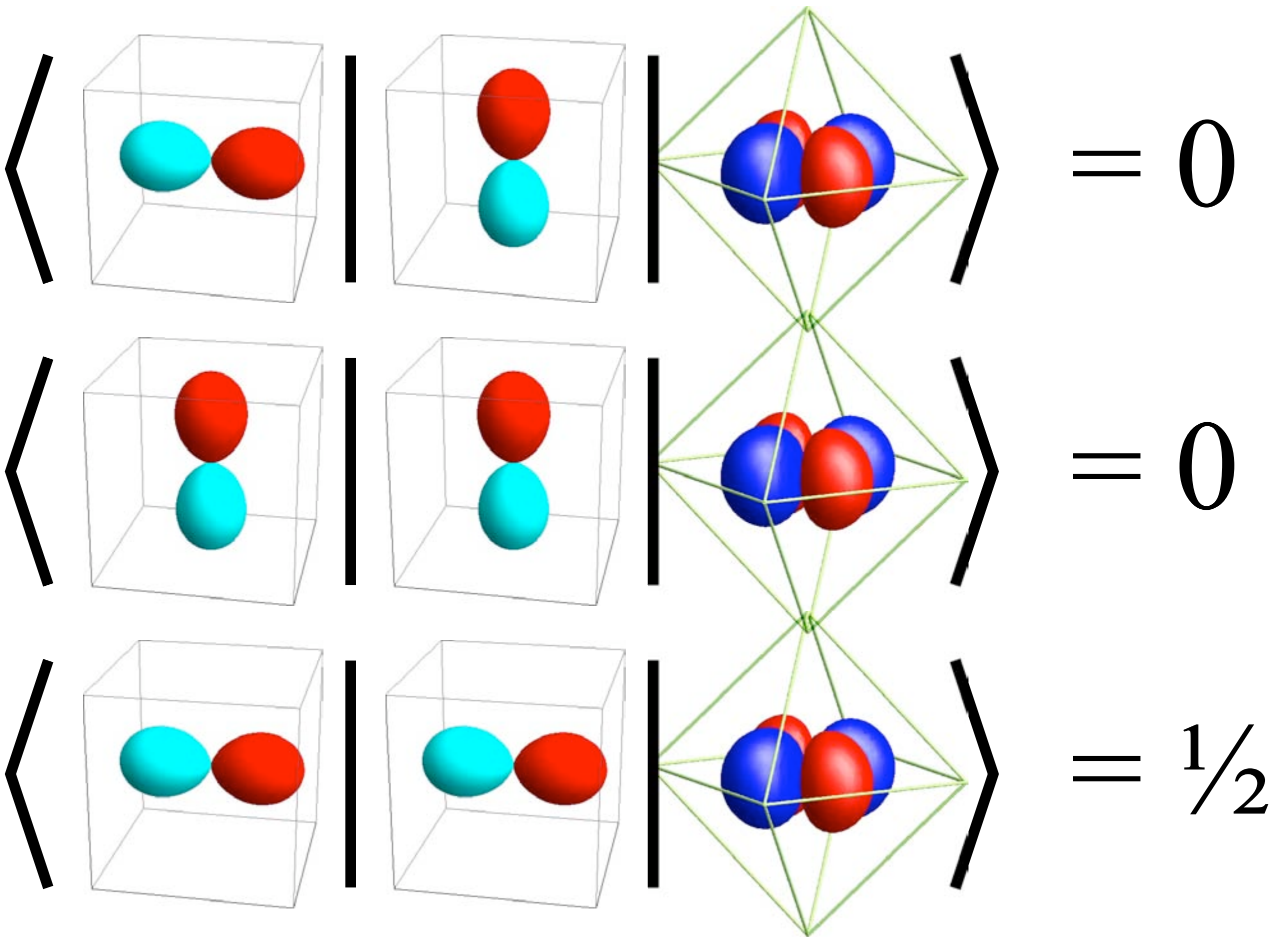

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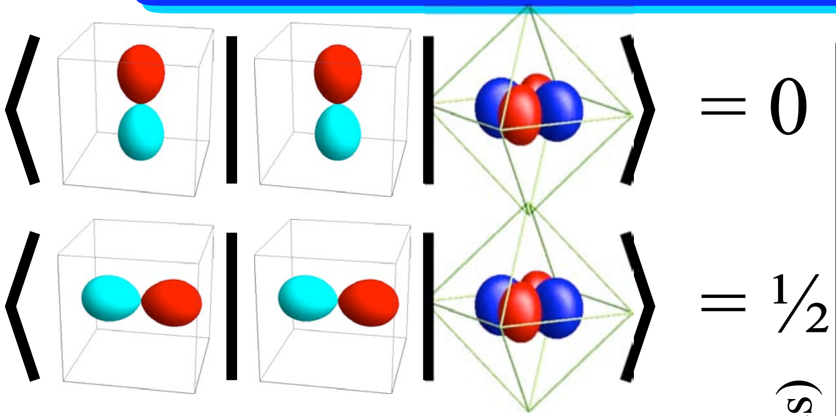
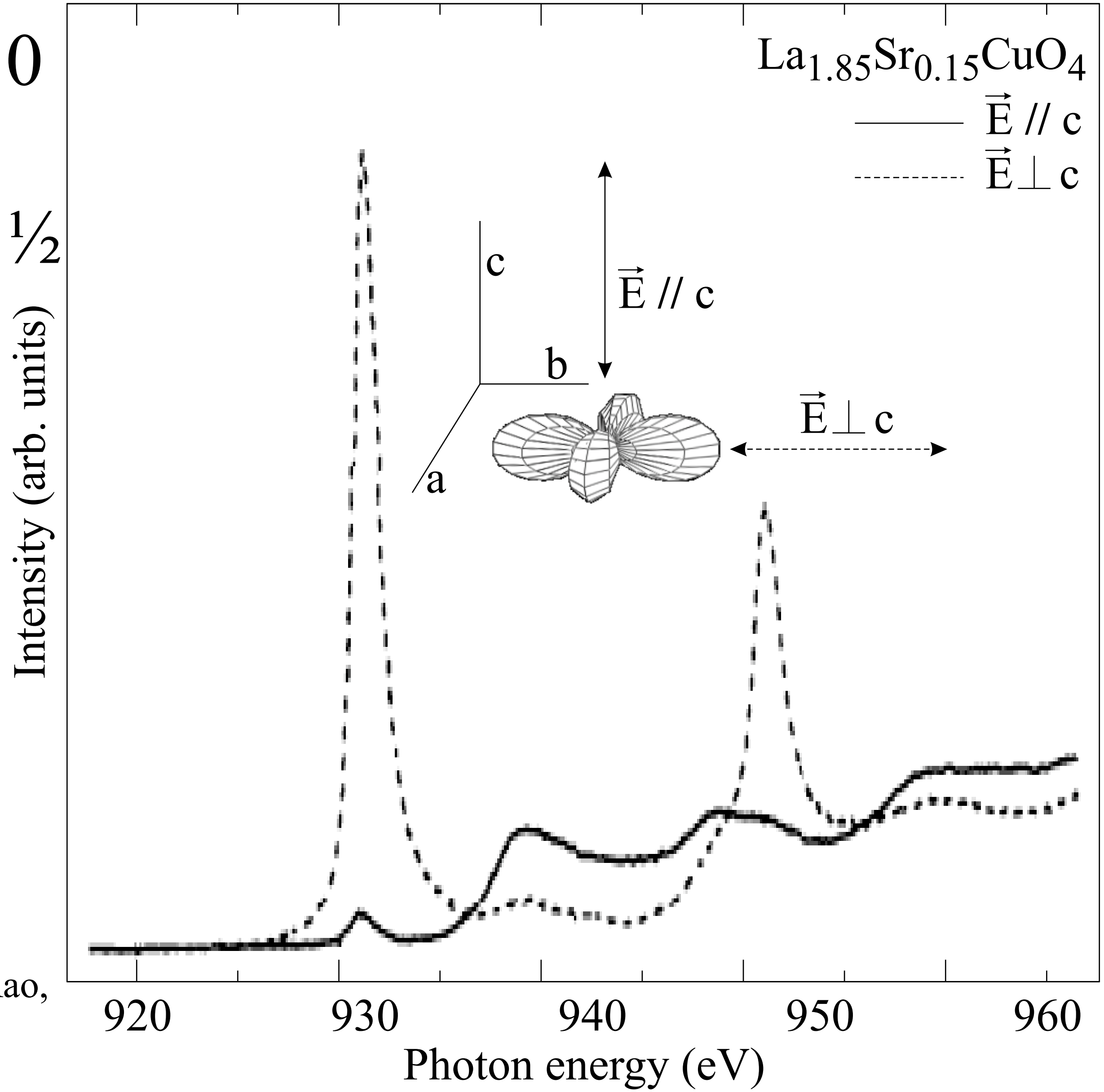
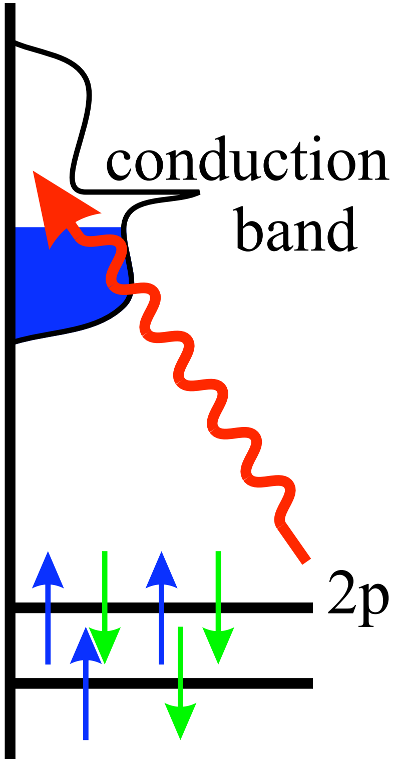
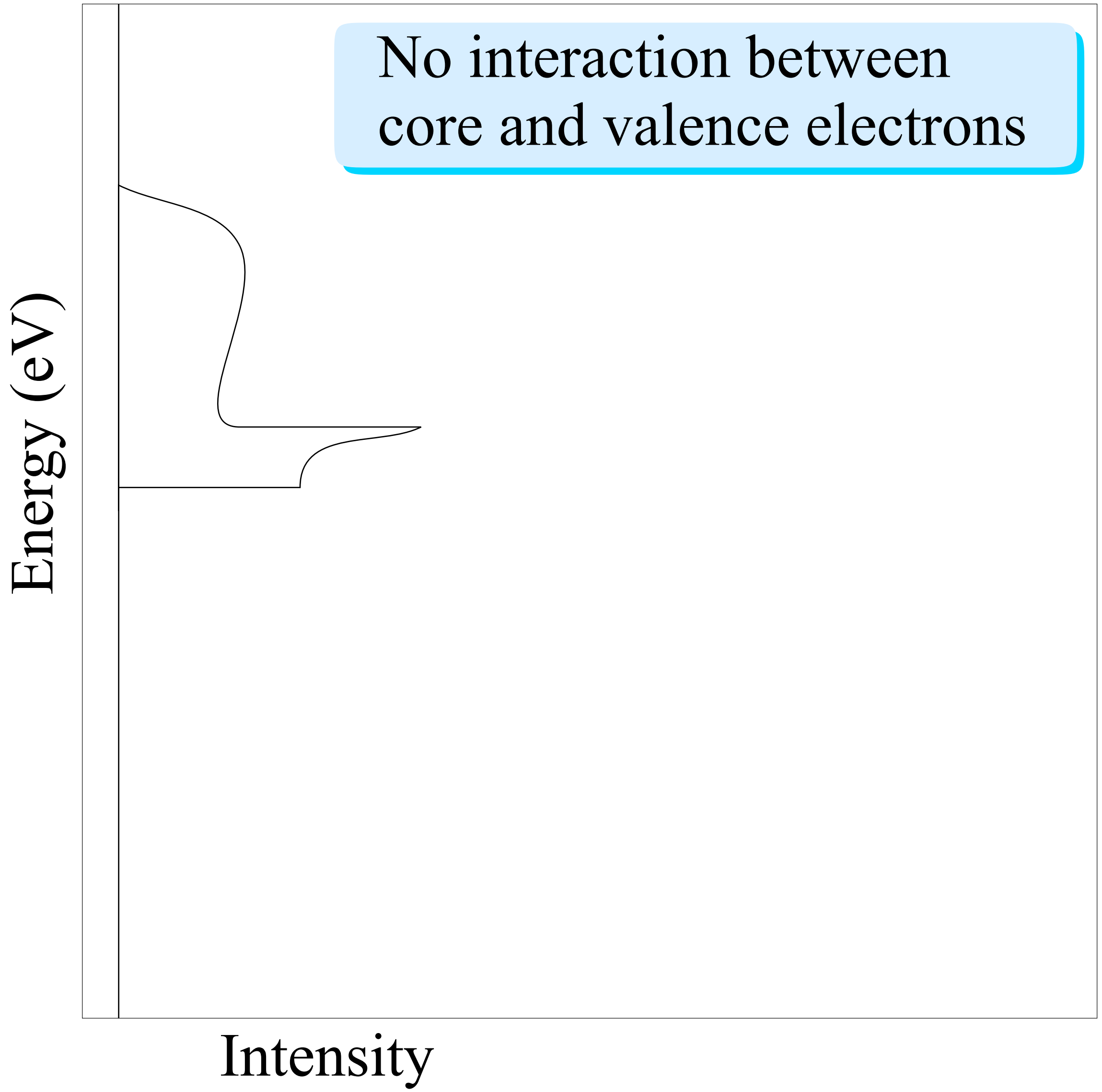




C. T. Chen, L. H. Tjeng, J. Kwo, H. L. Kao, P. Rudolf, F. Sette, and R. M. Fleming, Phys. Rev. Lett. 68, 2543 (1992).

X-ray Absorption Spectroscopy: Excitons





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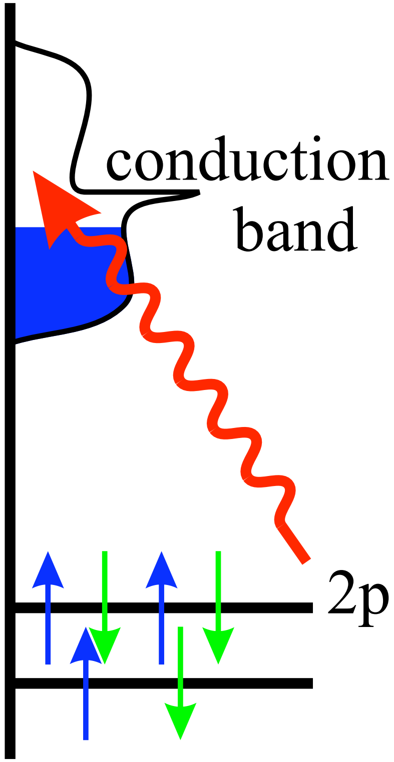

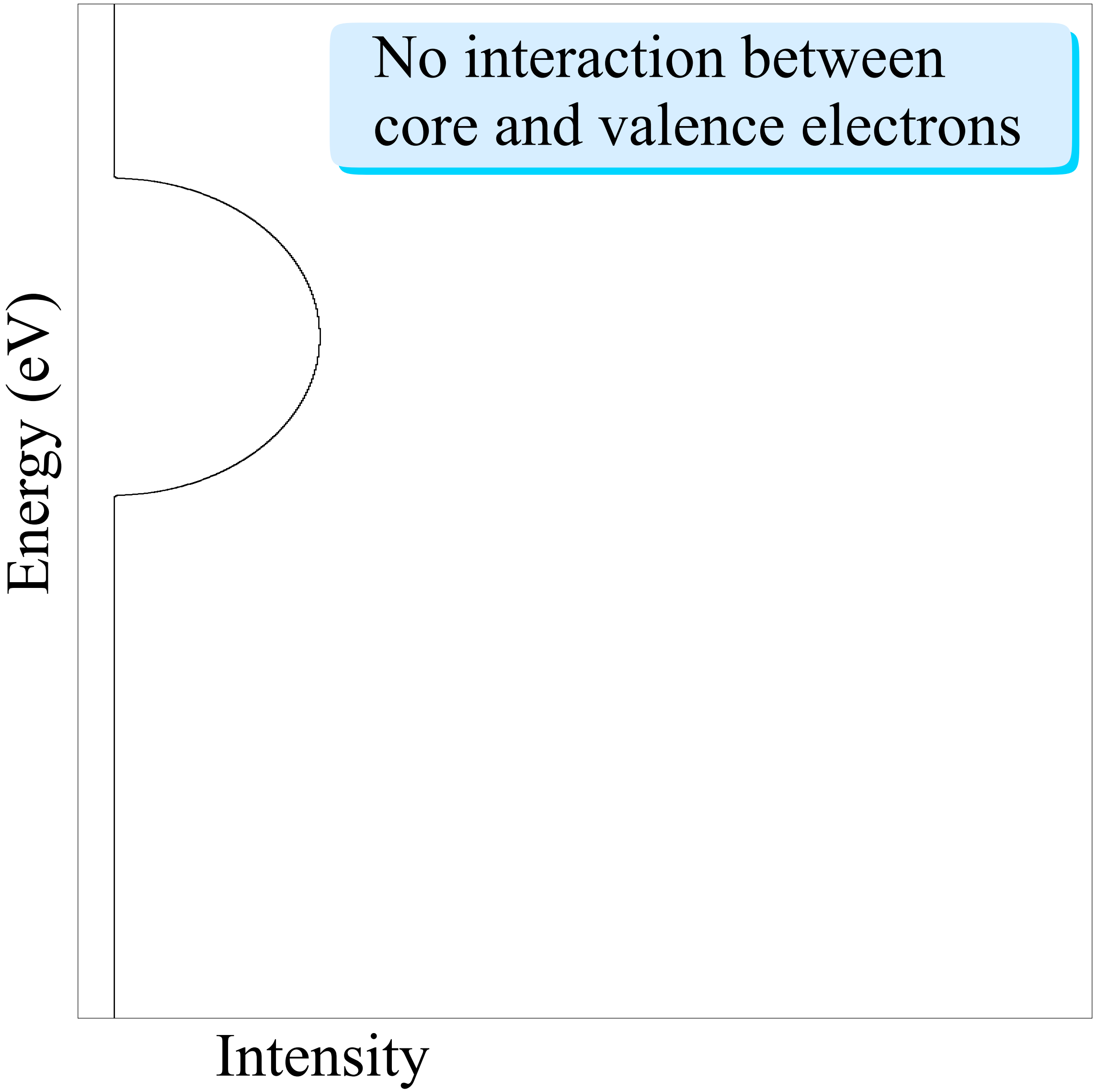

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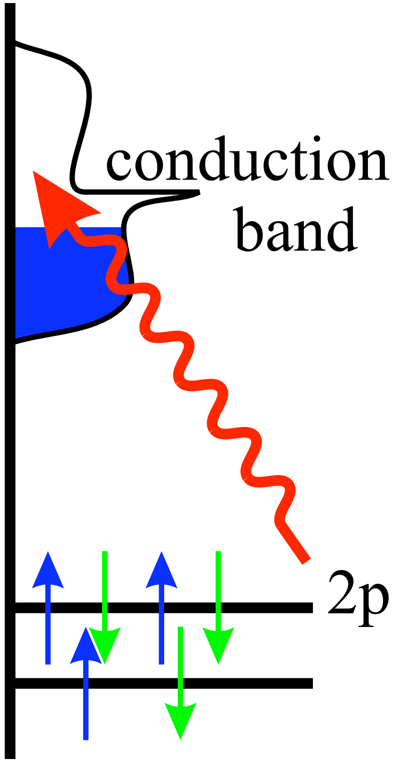

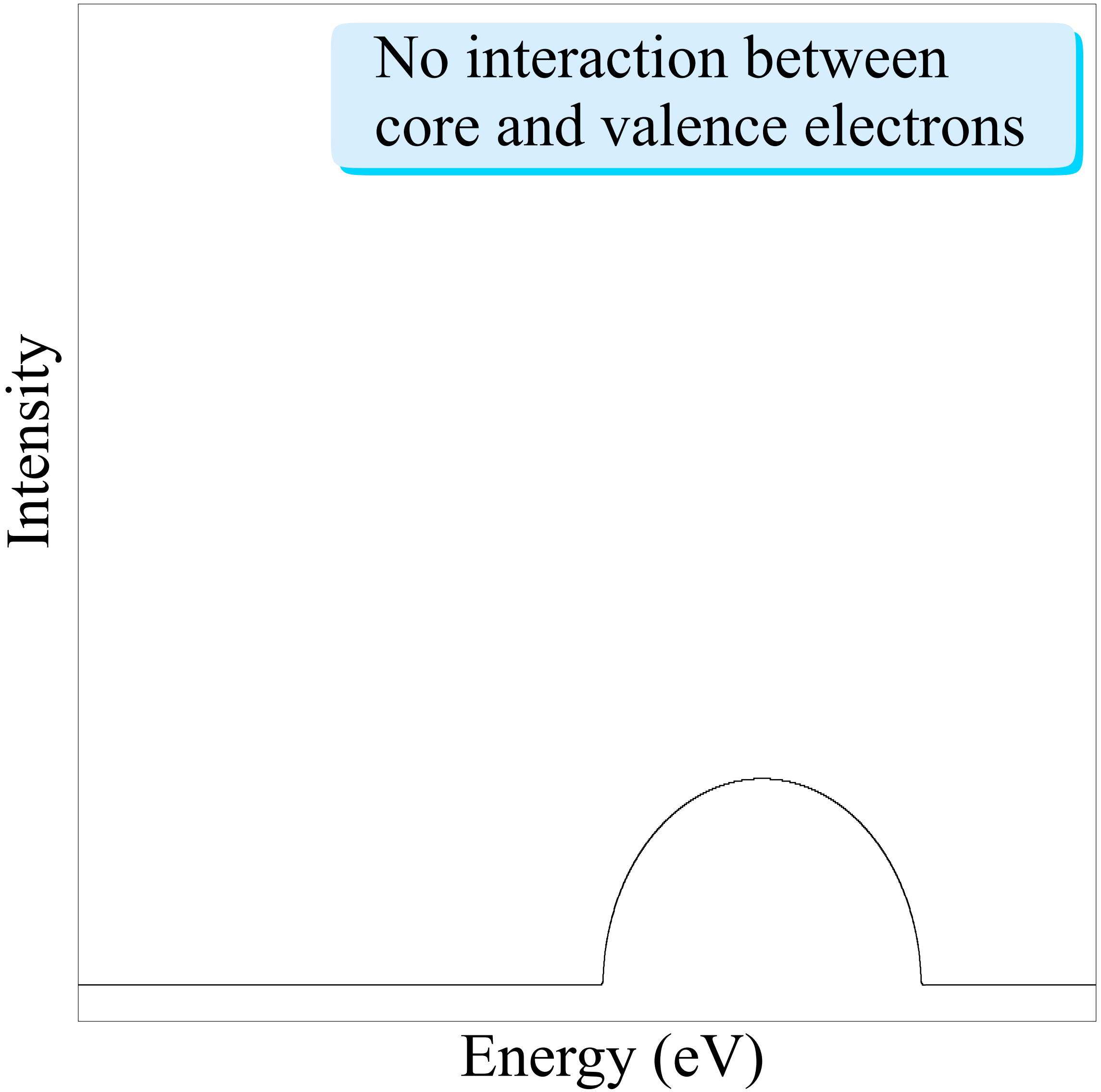

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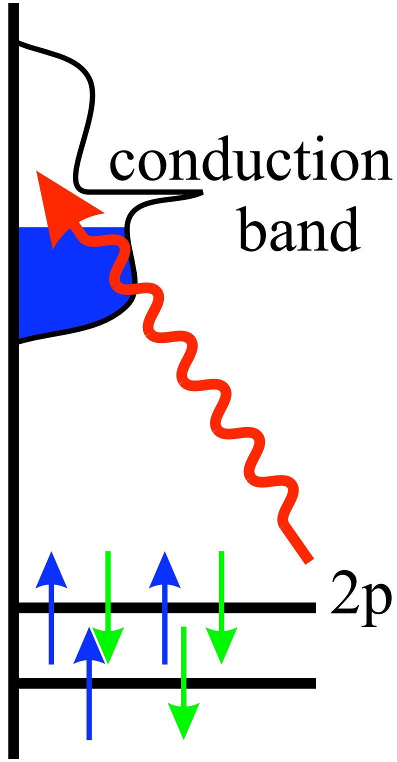

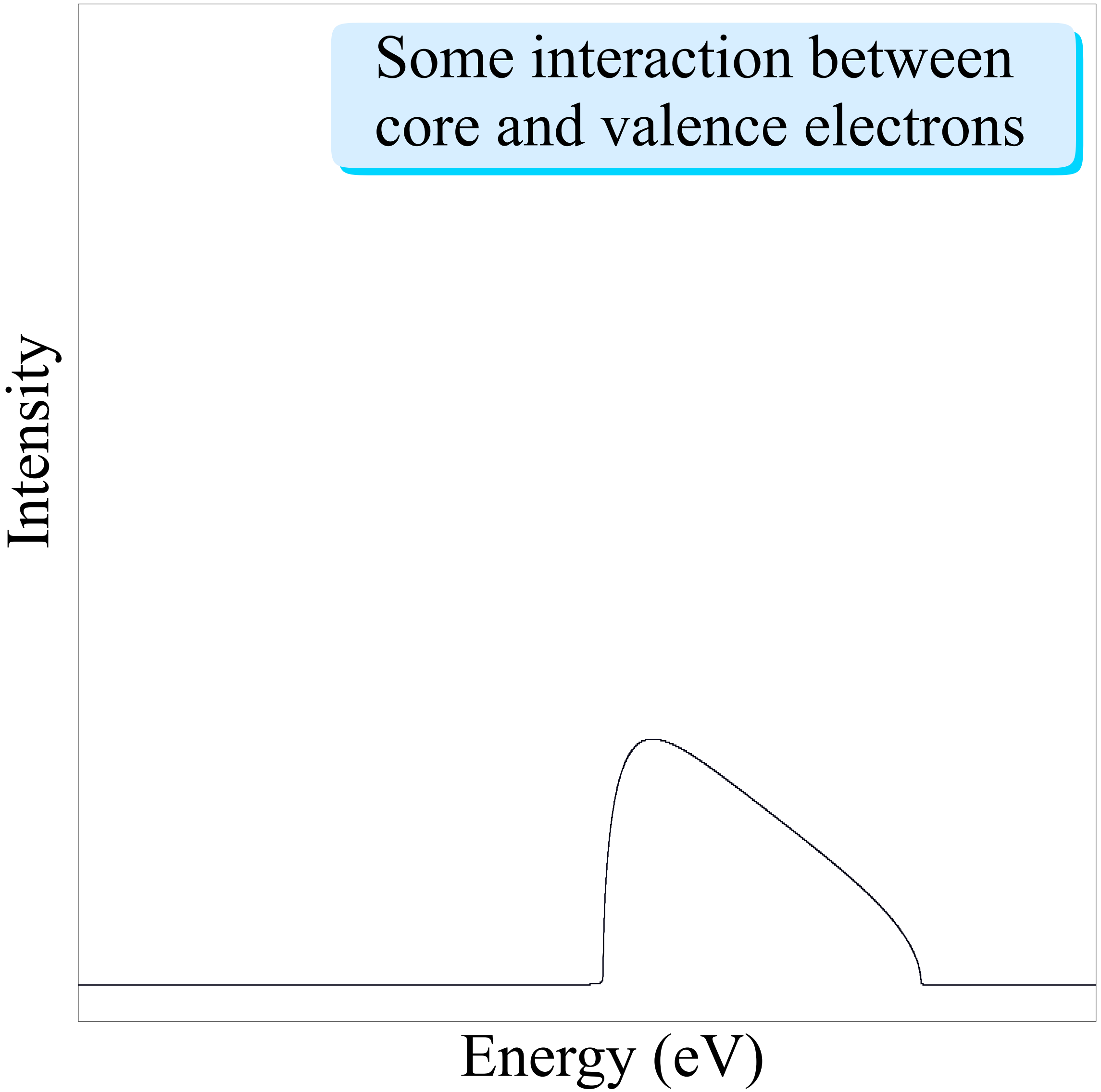

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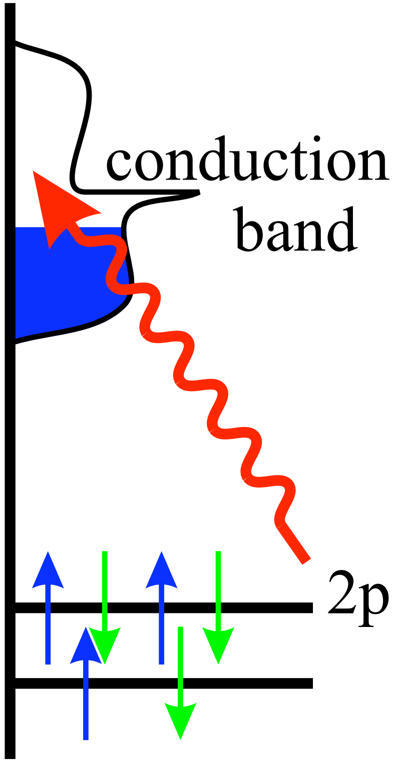

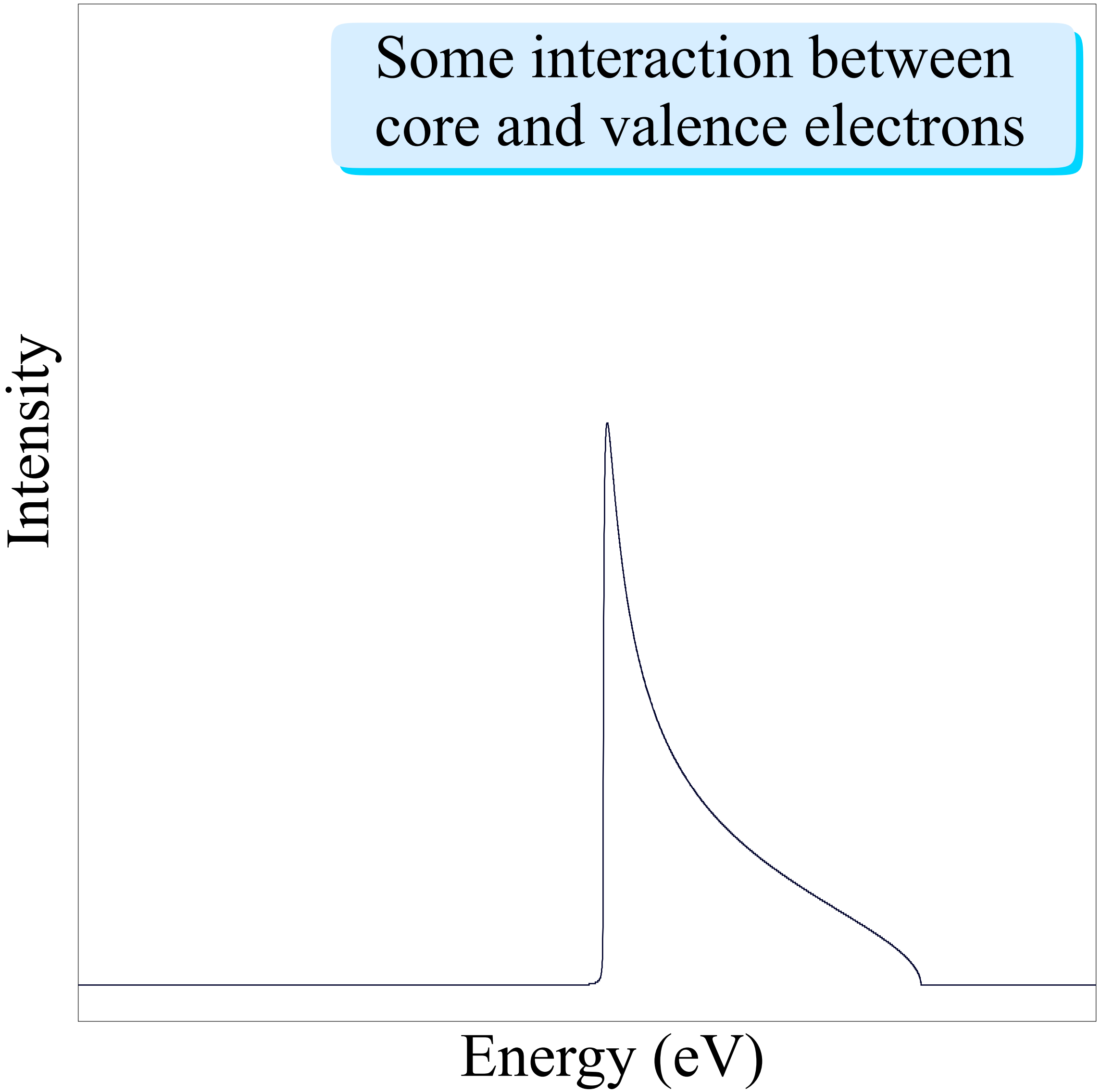

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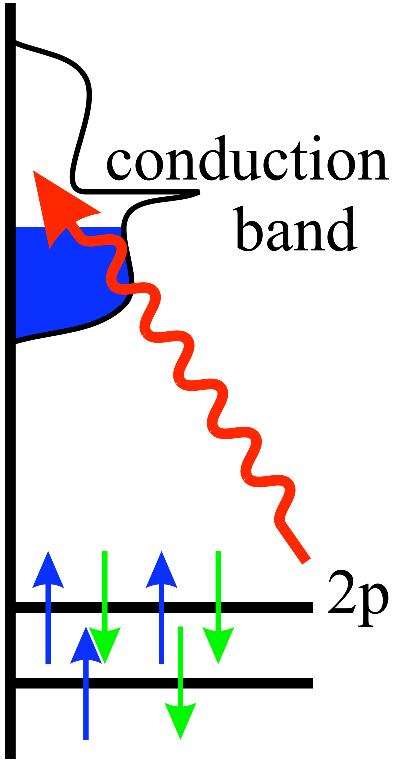

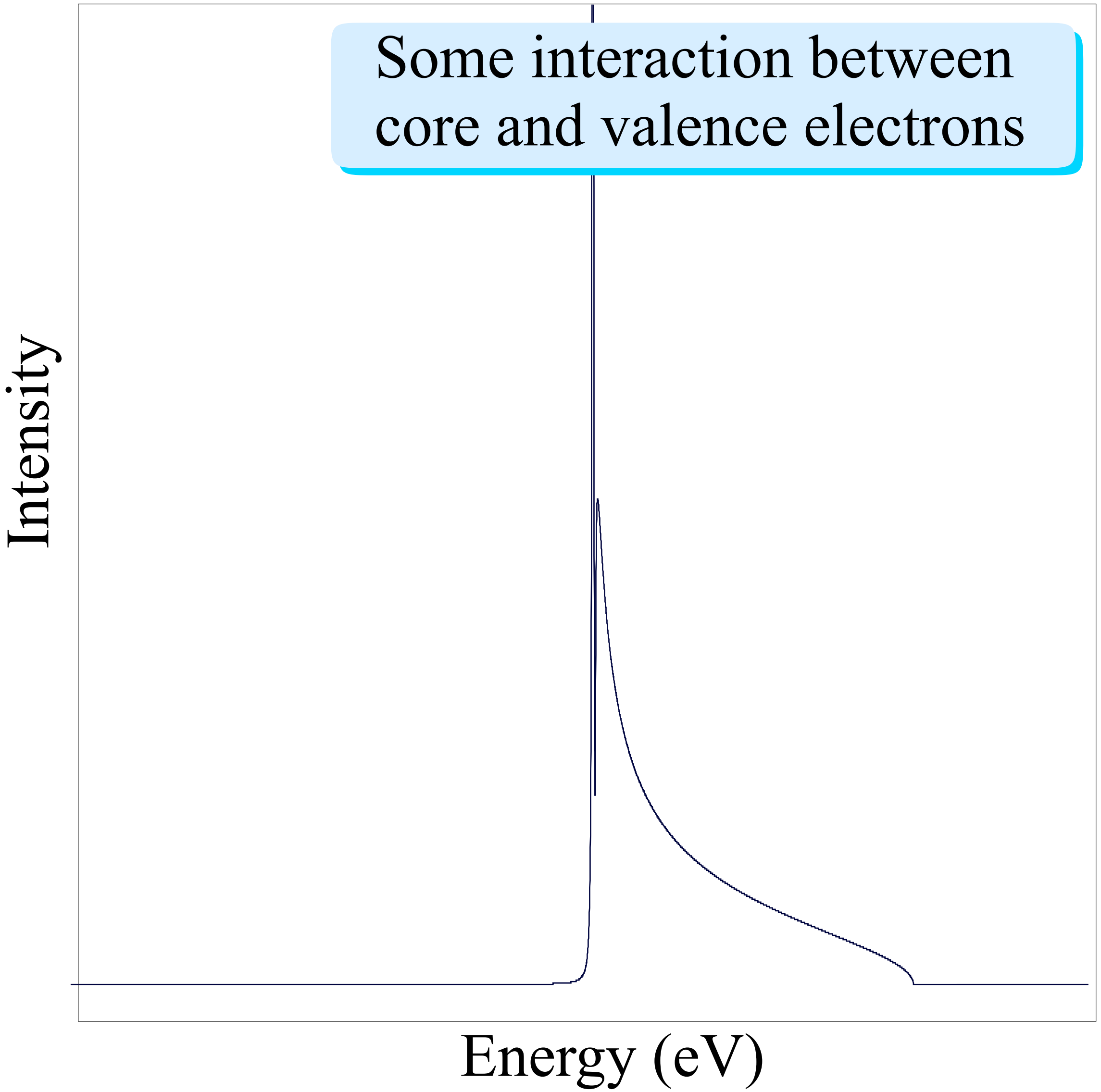

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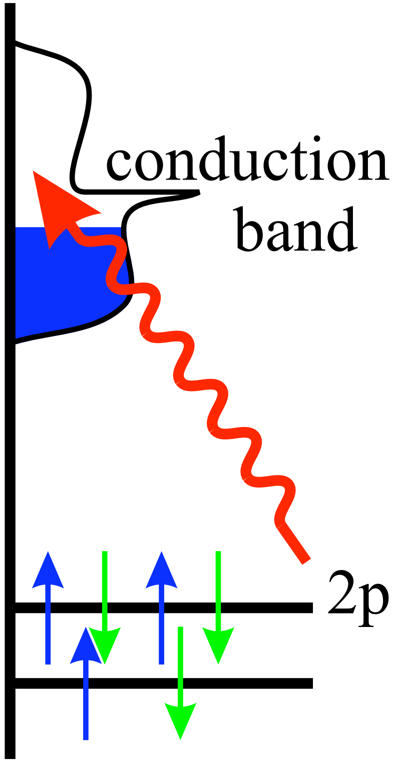

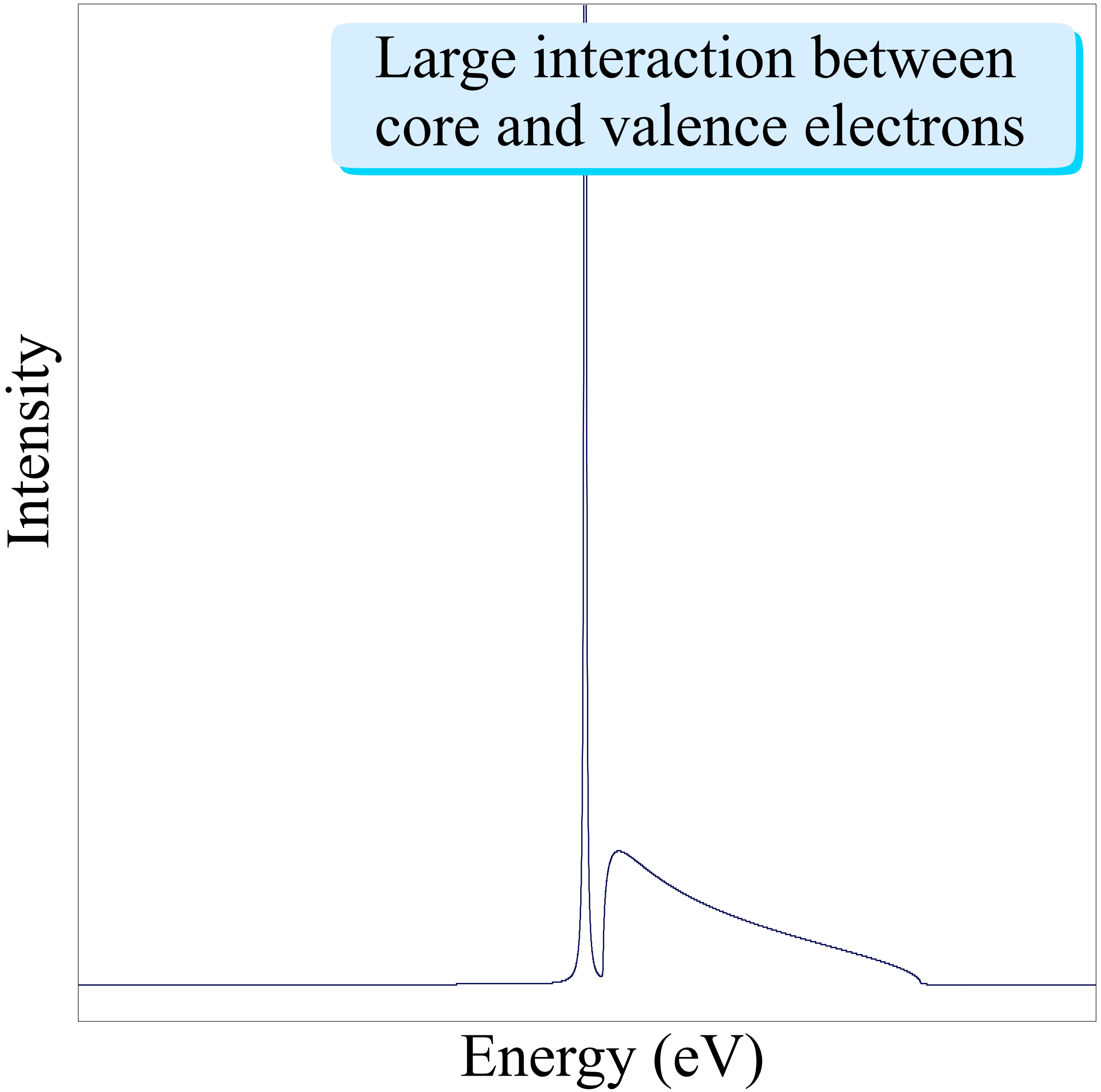

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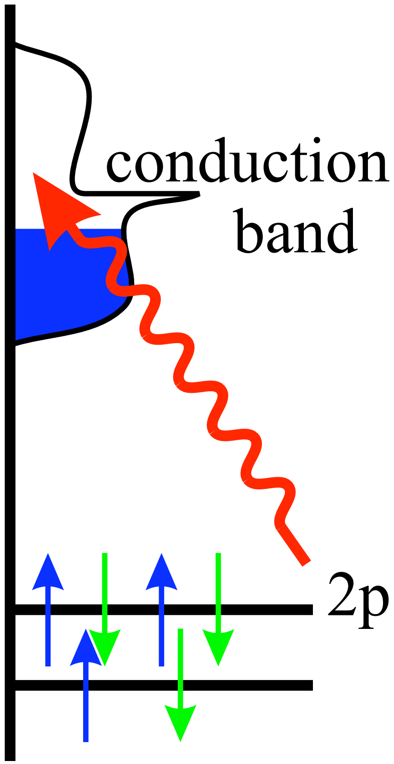

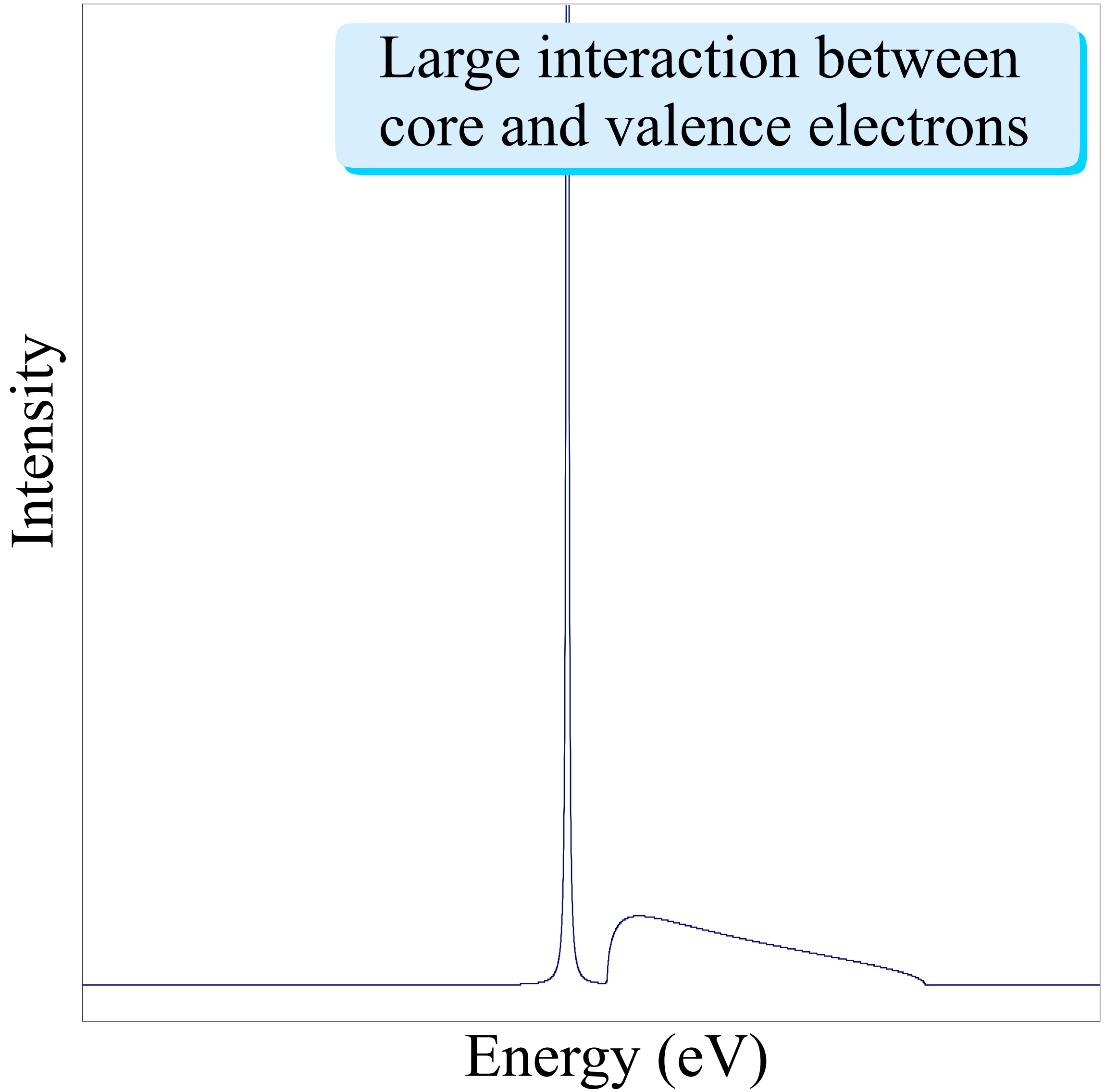

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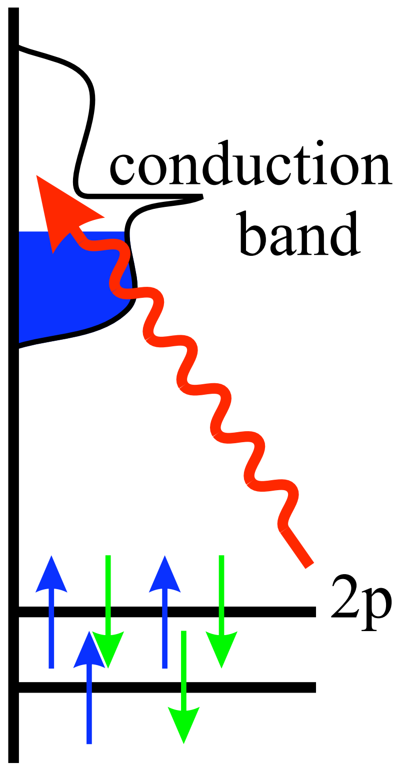

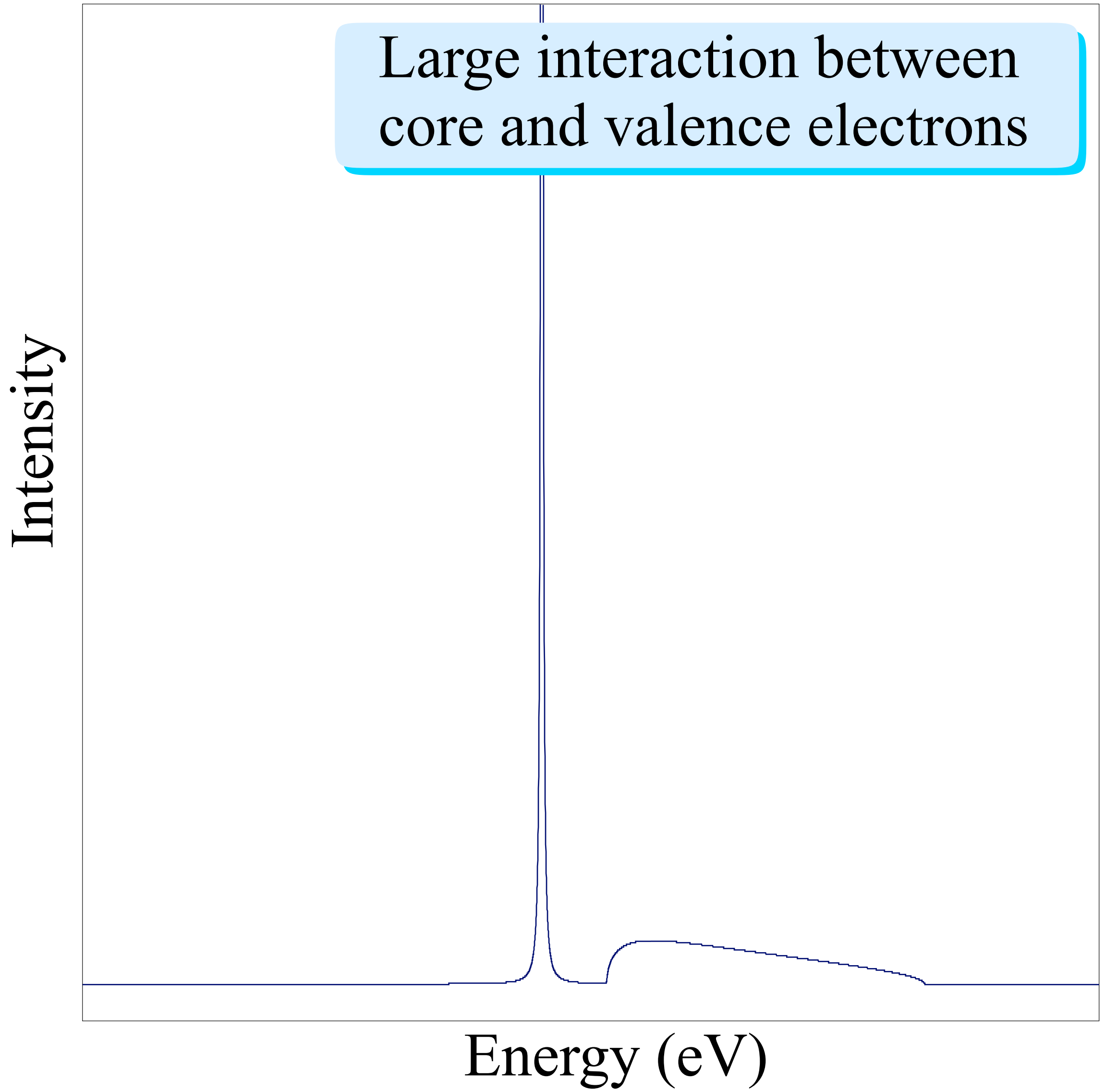

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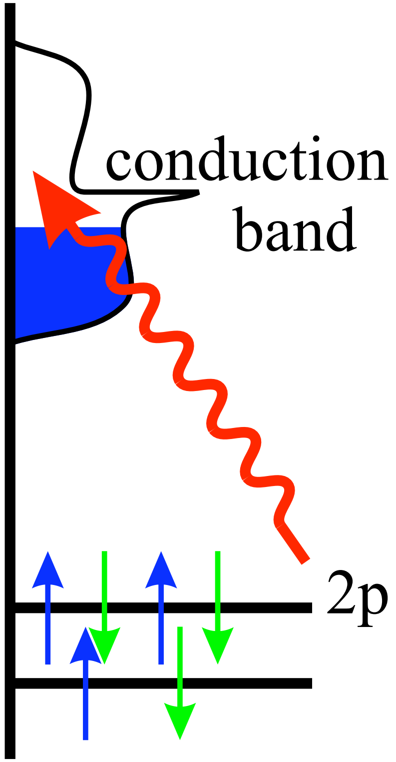

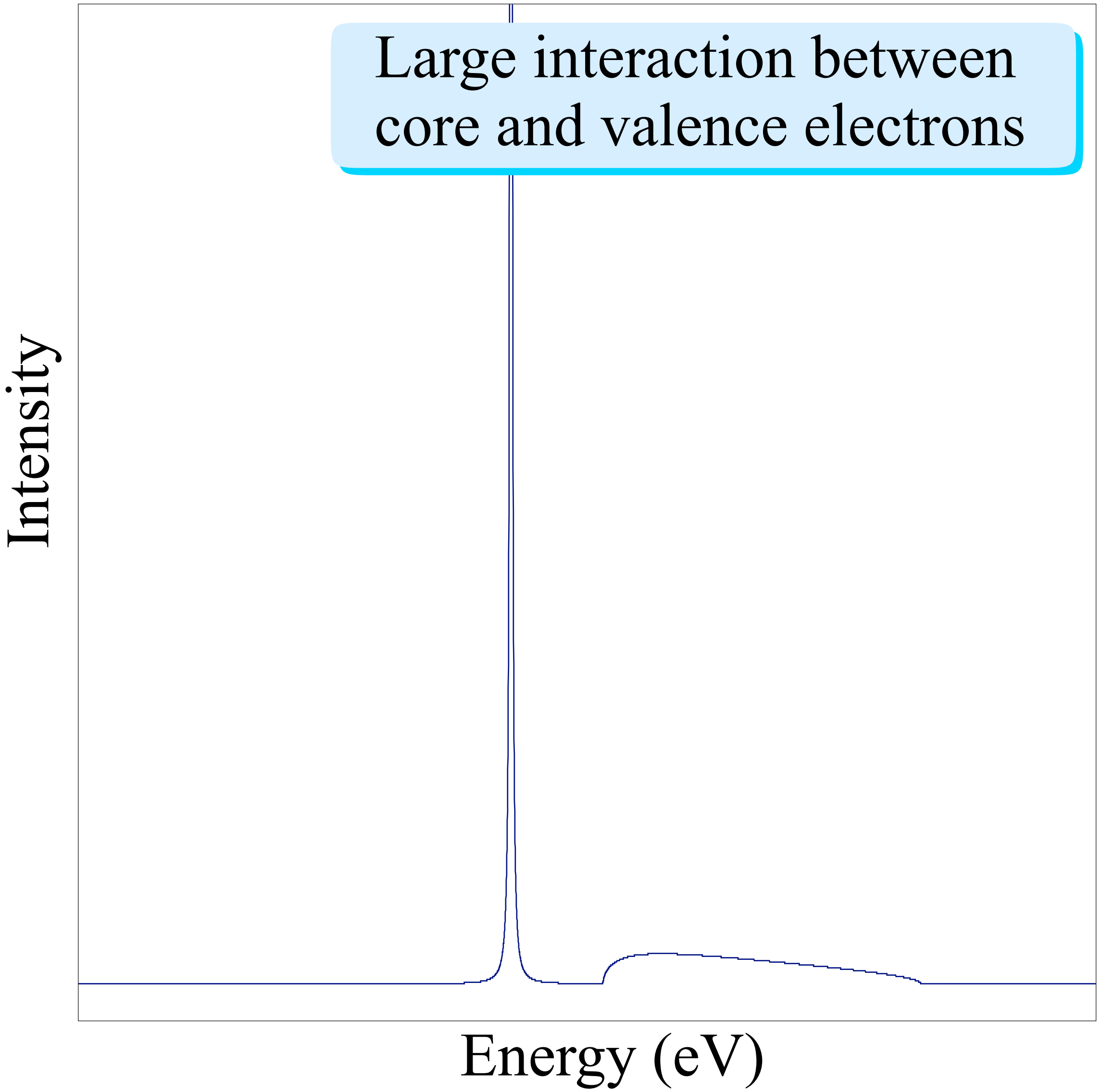

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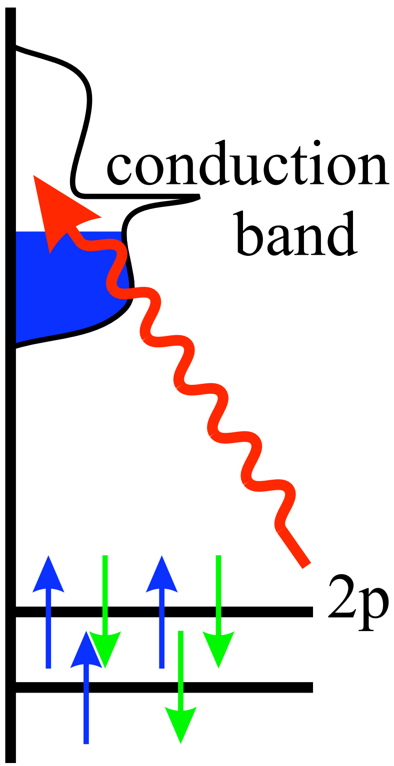

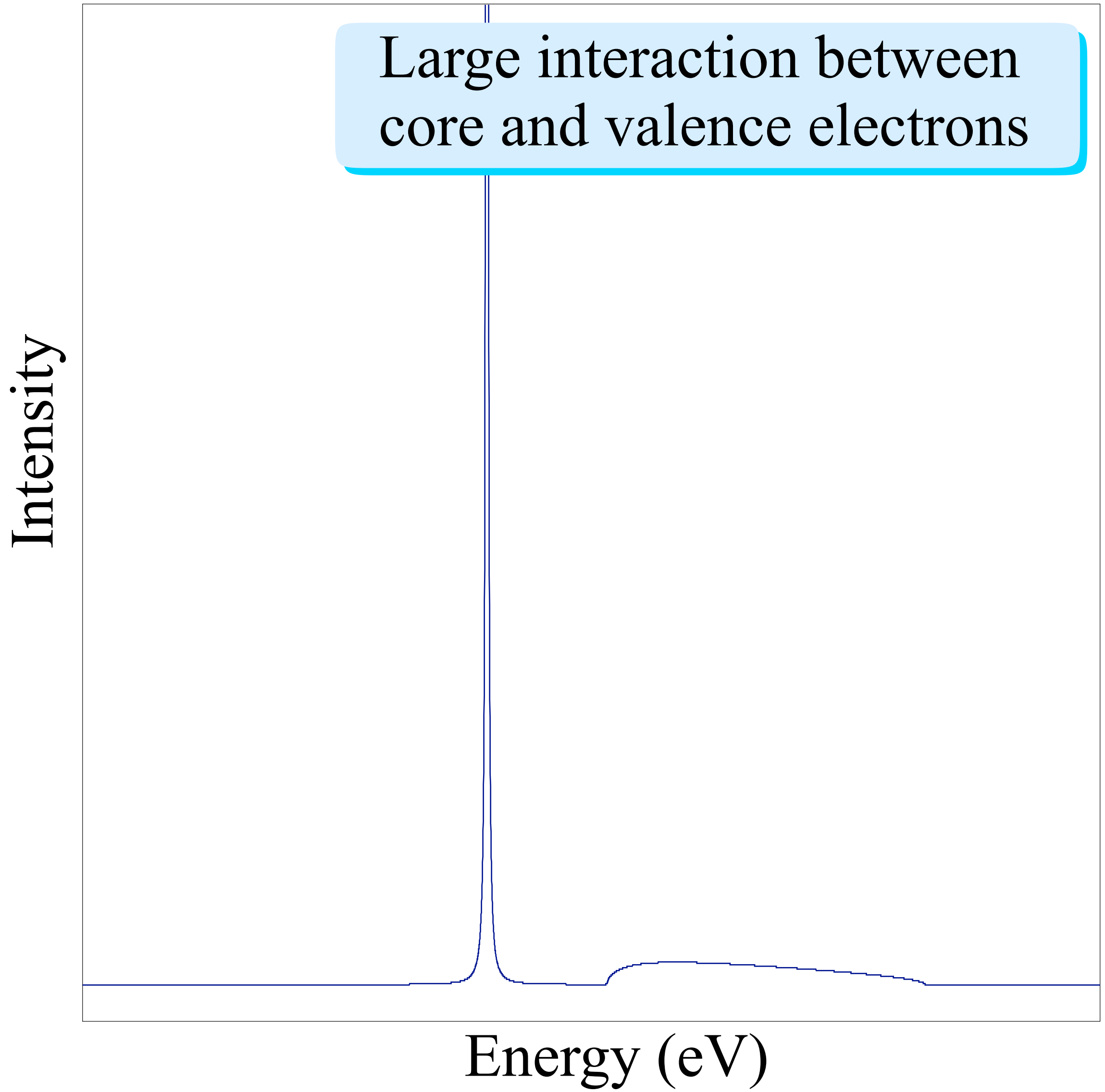

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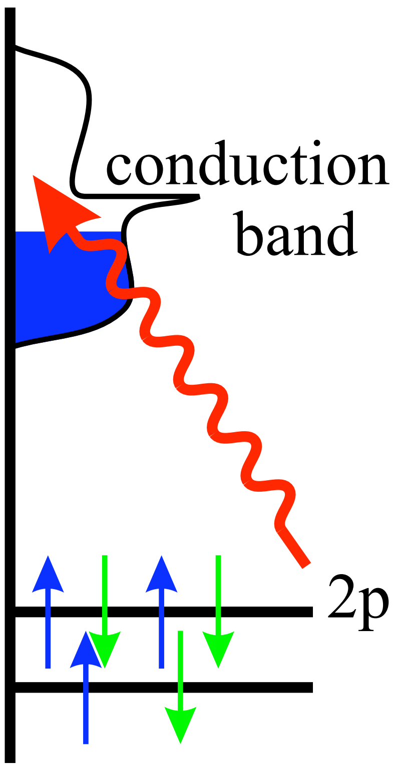

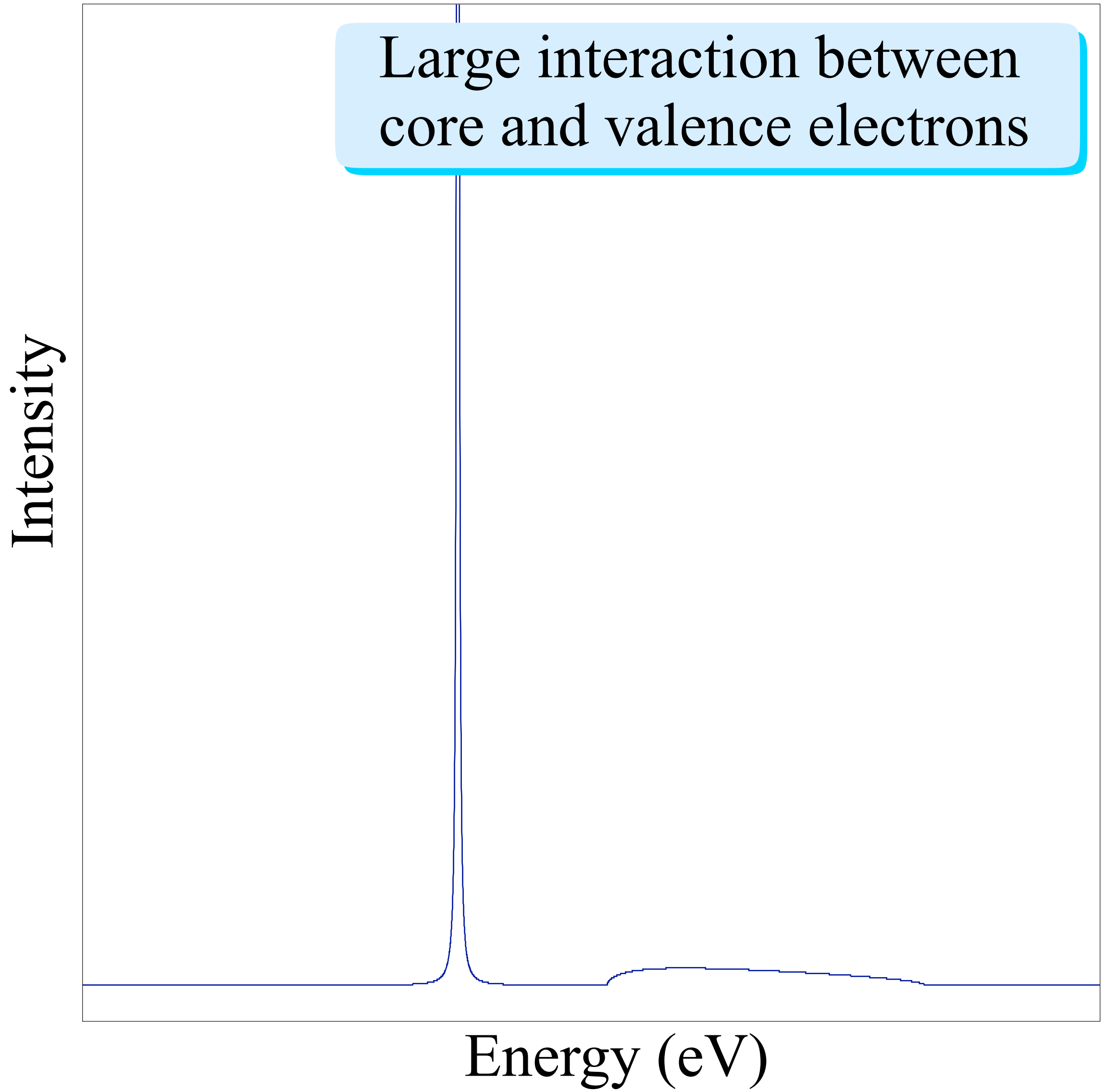

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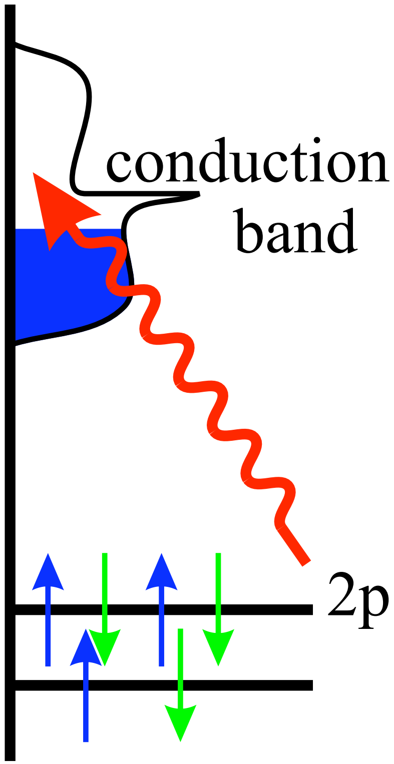

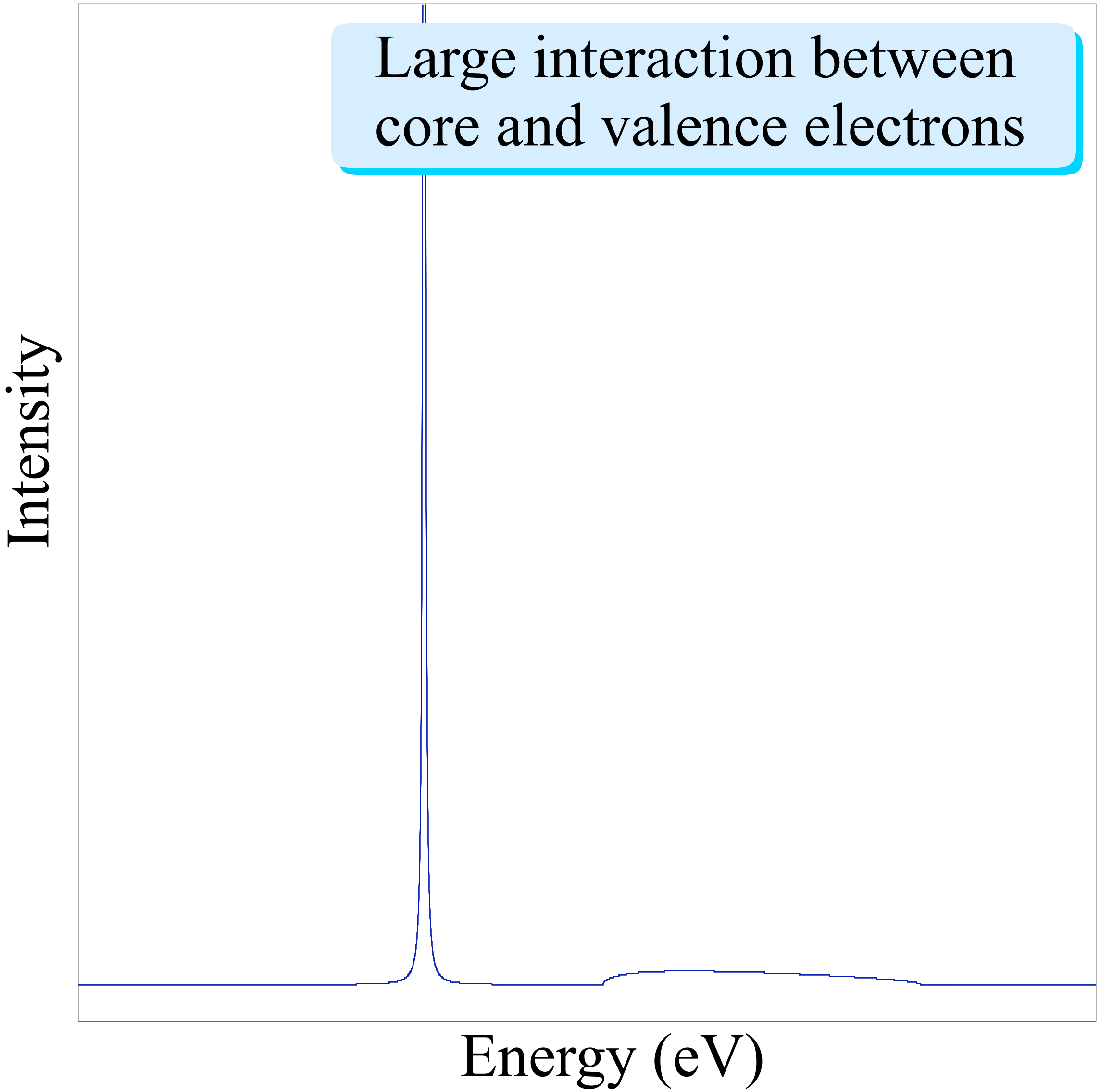

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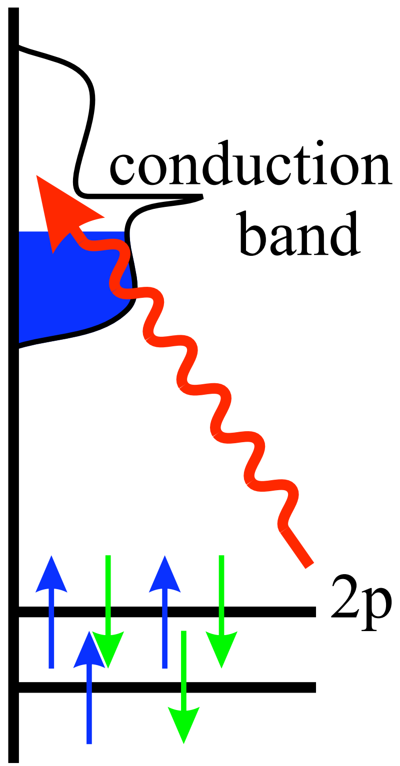

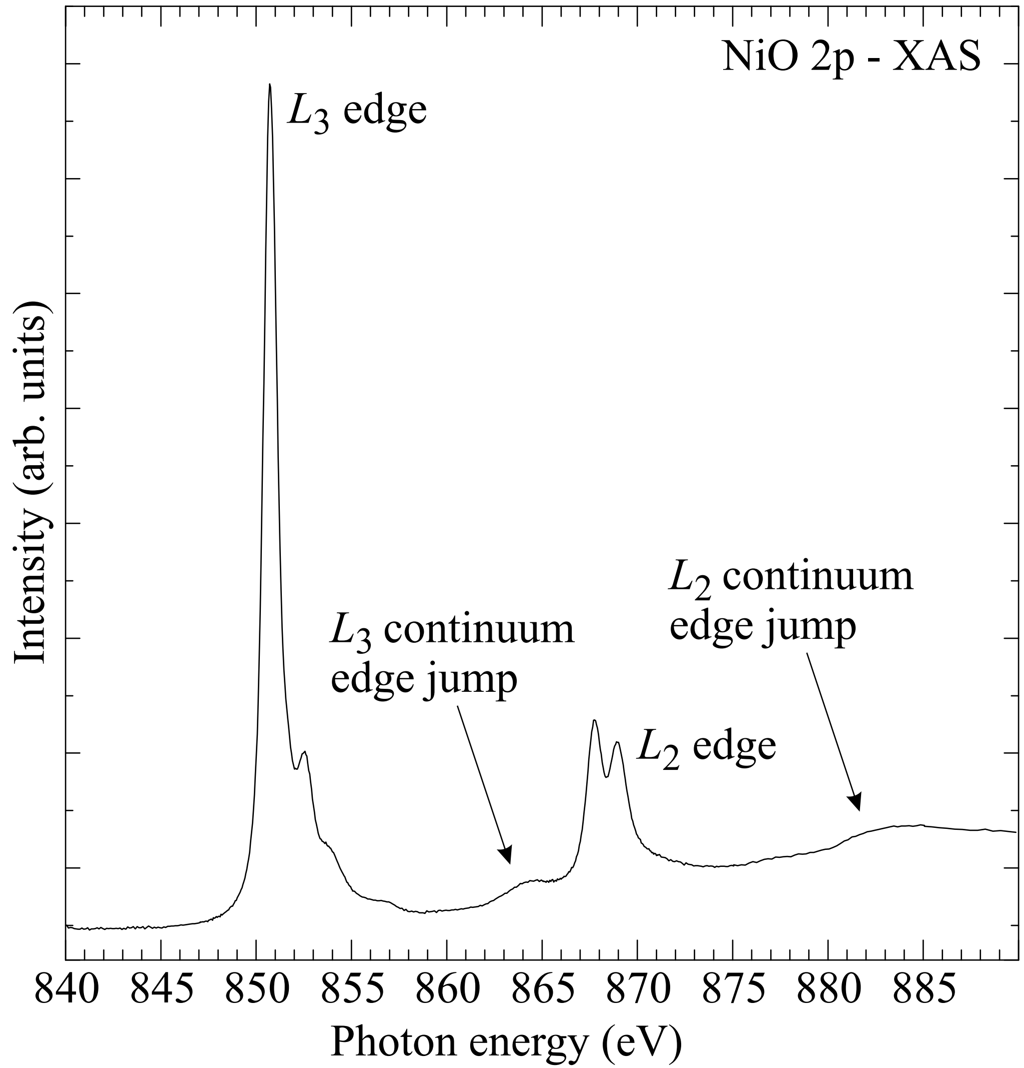

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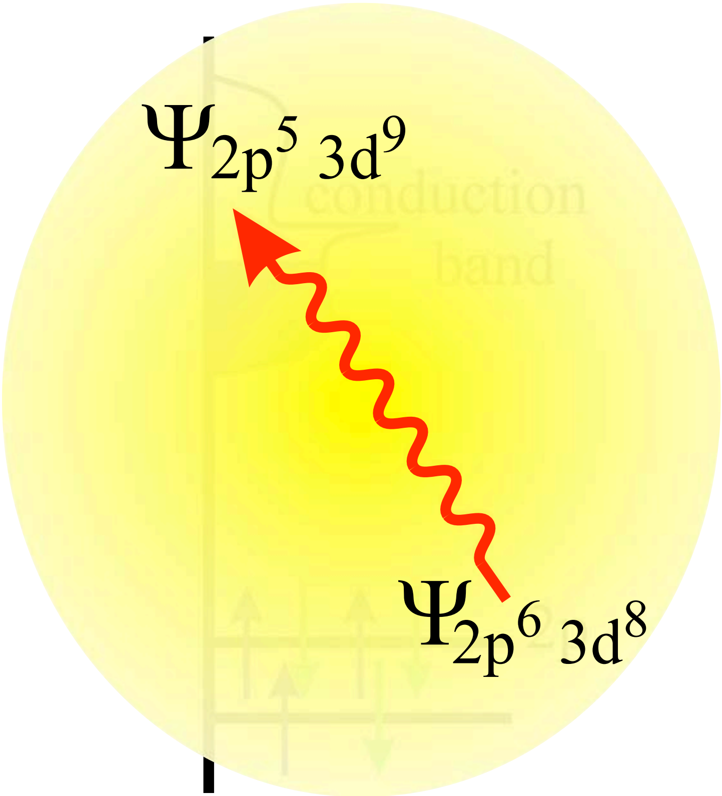
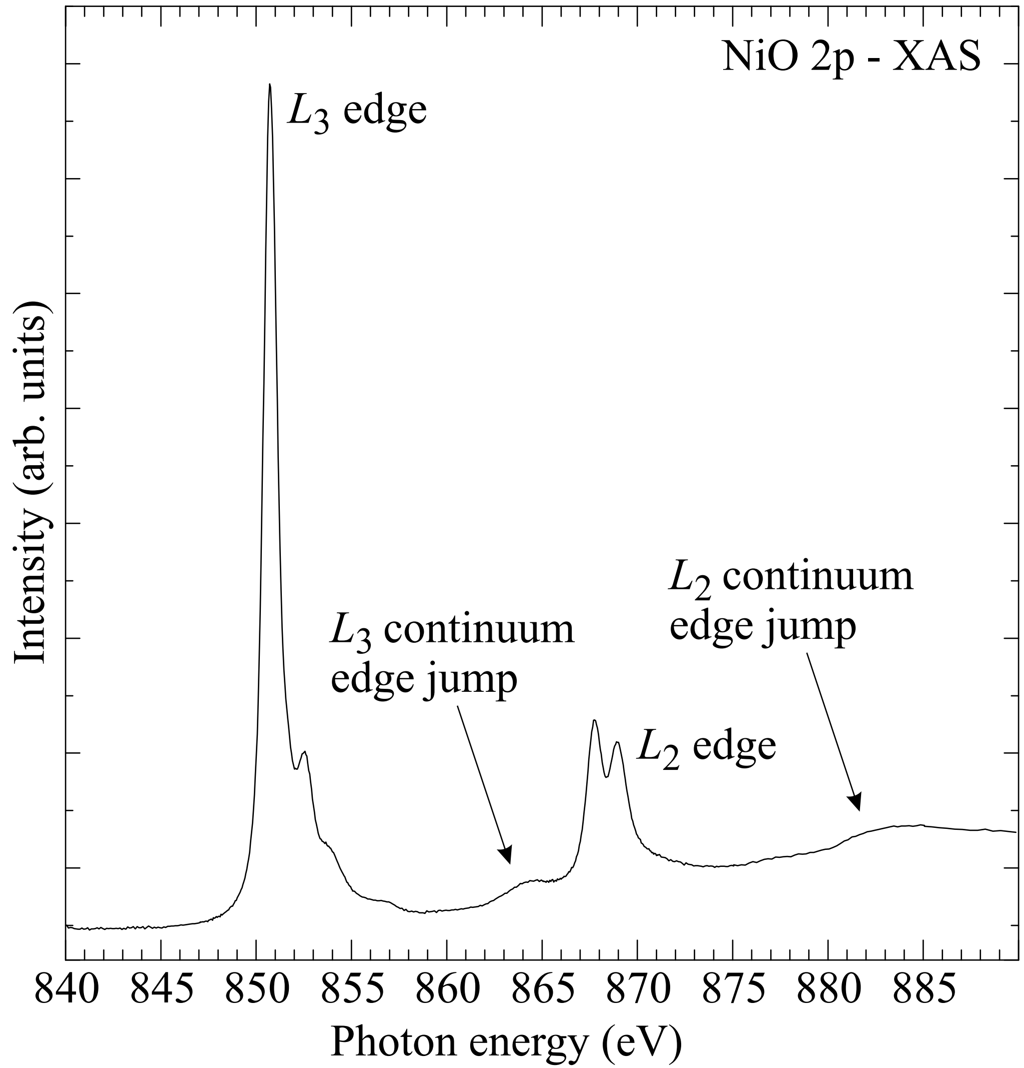
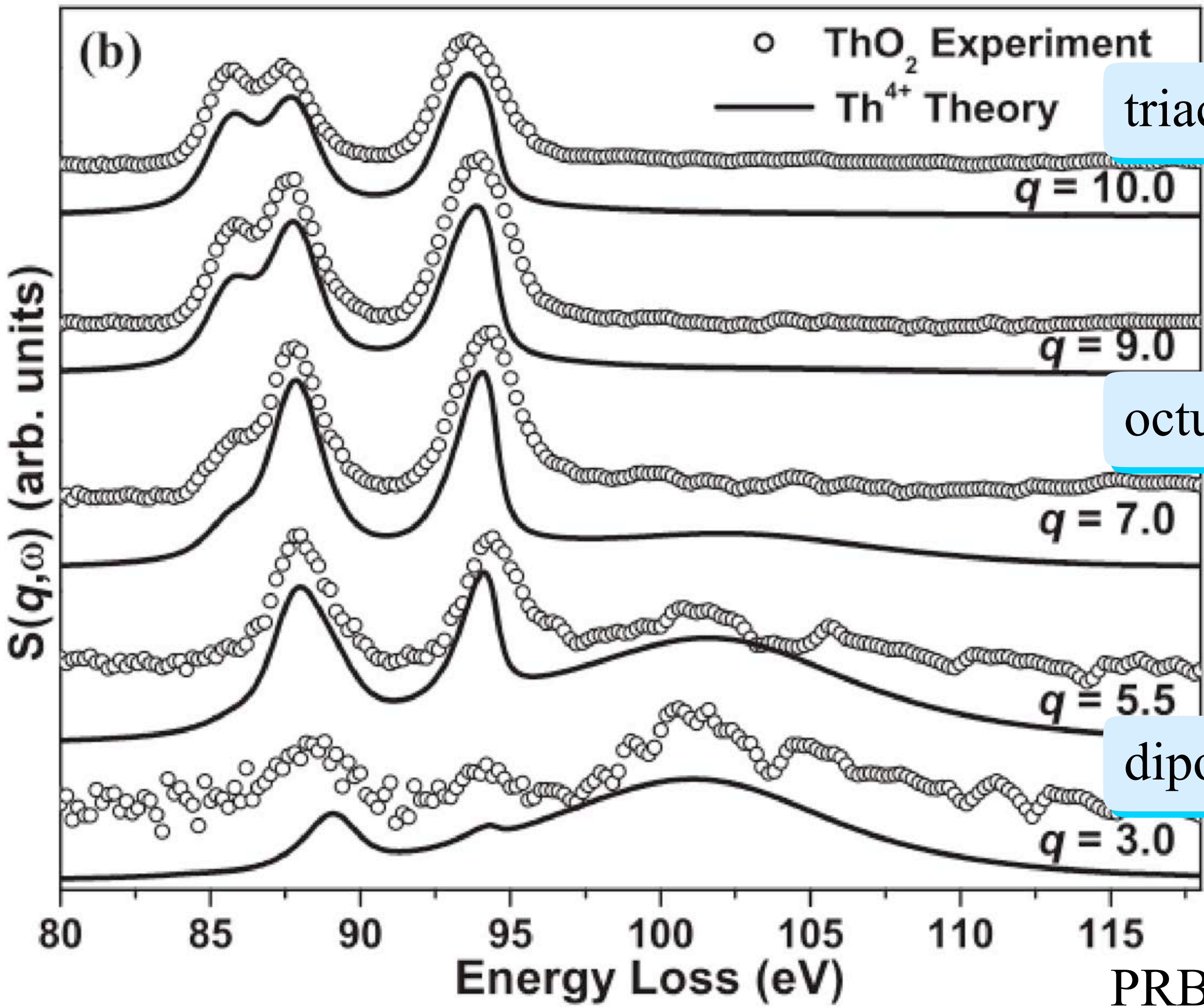




X-ray Absorption Spectroscopy: Excitons and continuum excitations



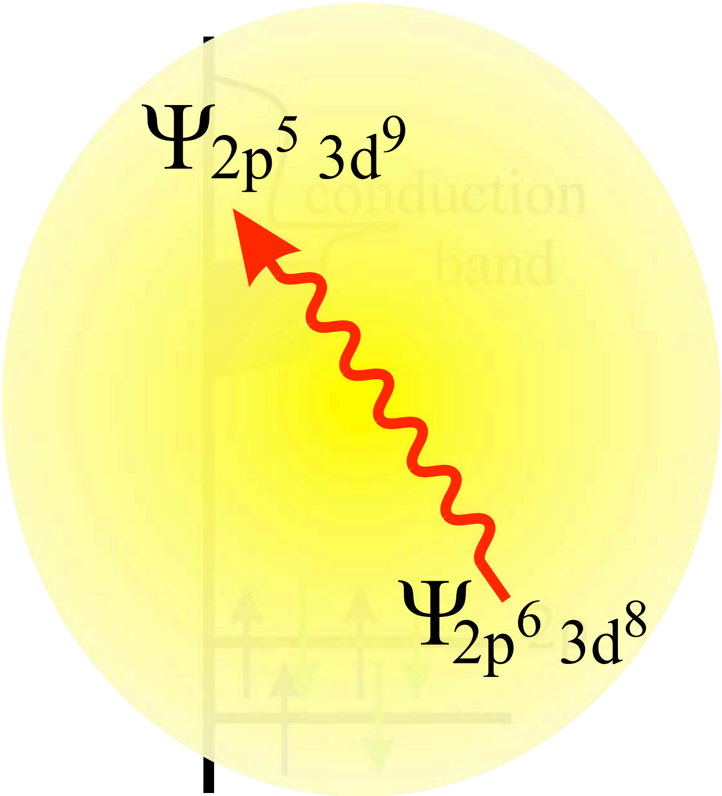
triacontadipole transitions

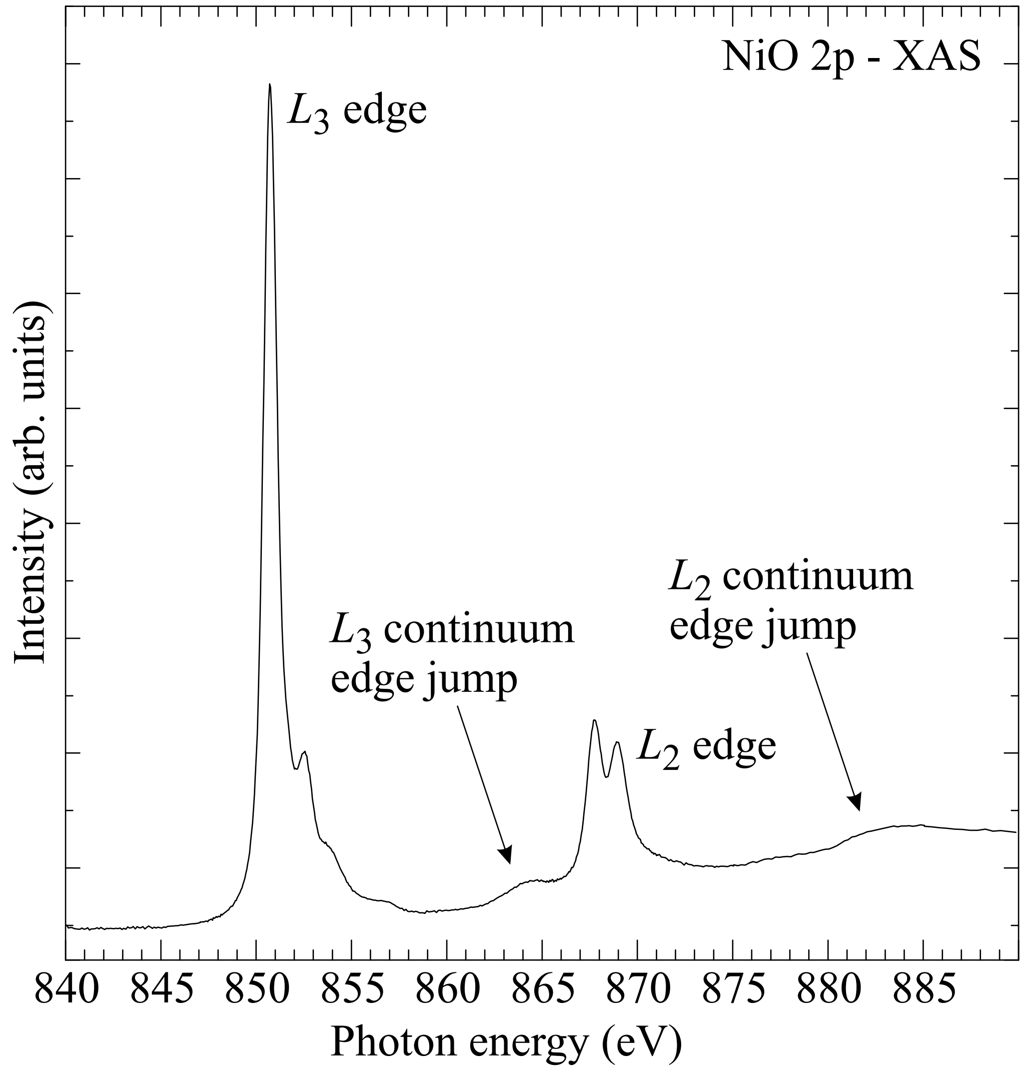
octupole transitions

dipole transitions

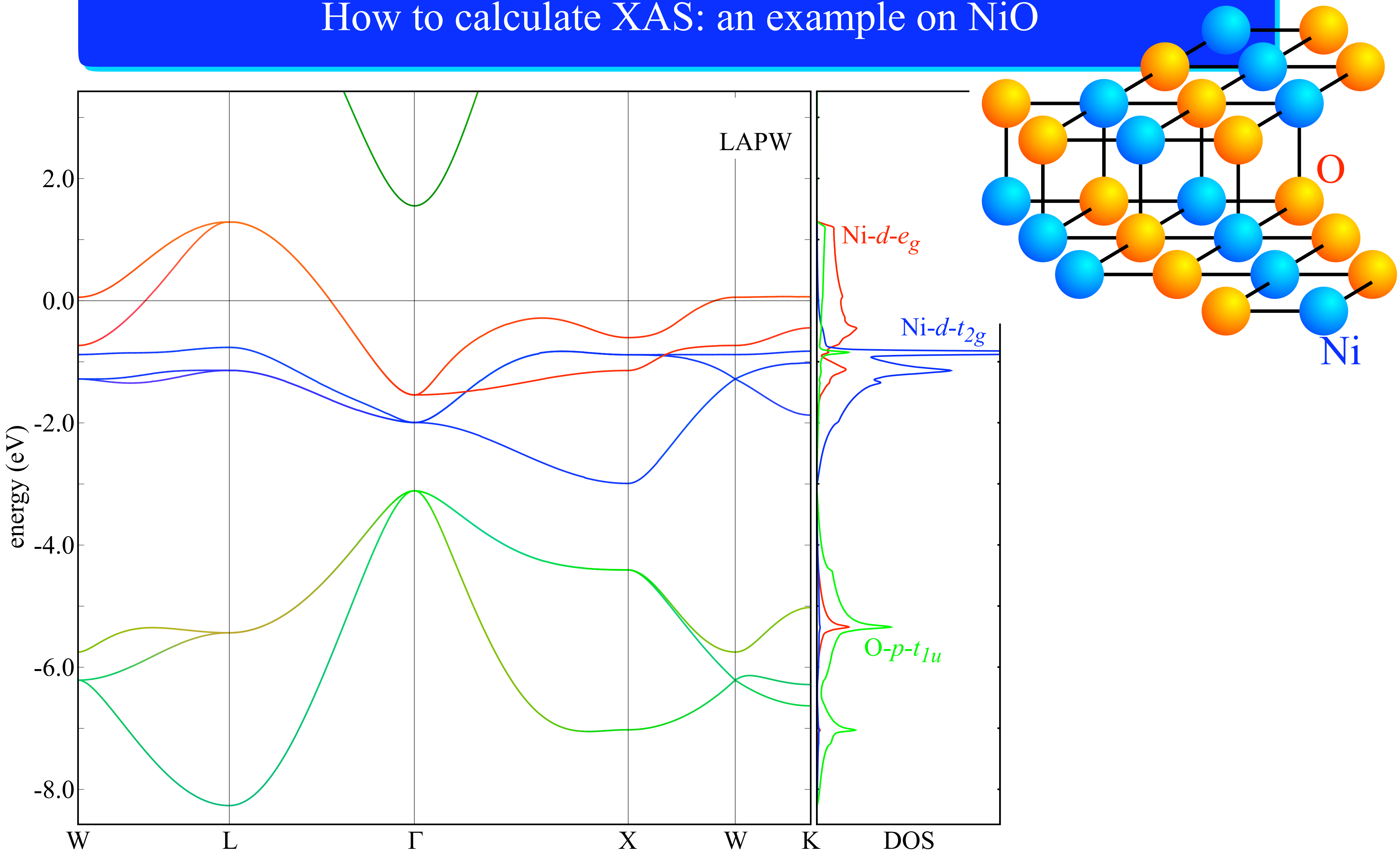
PRB **84,** 075134 (2011)

X-ray Absorption Spectroscopy: Excitons

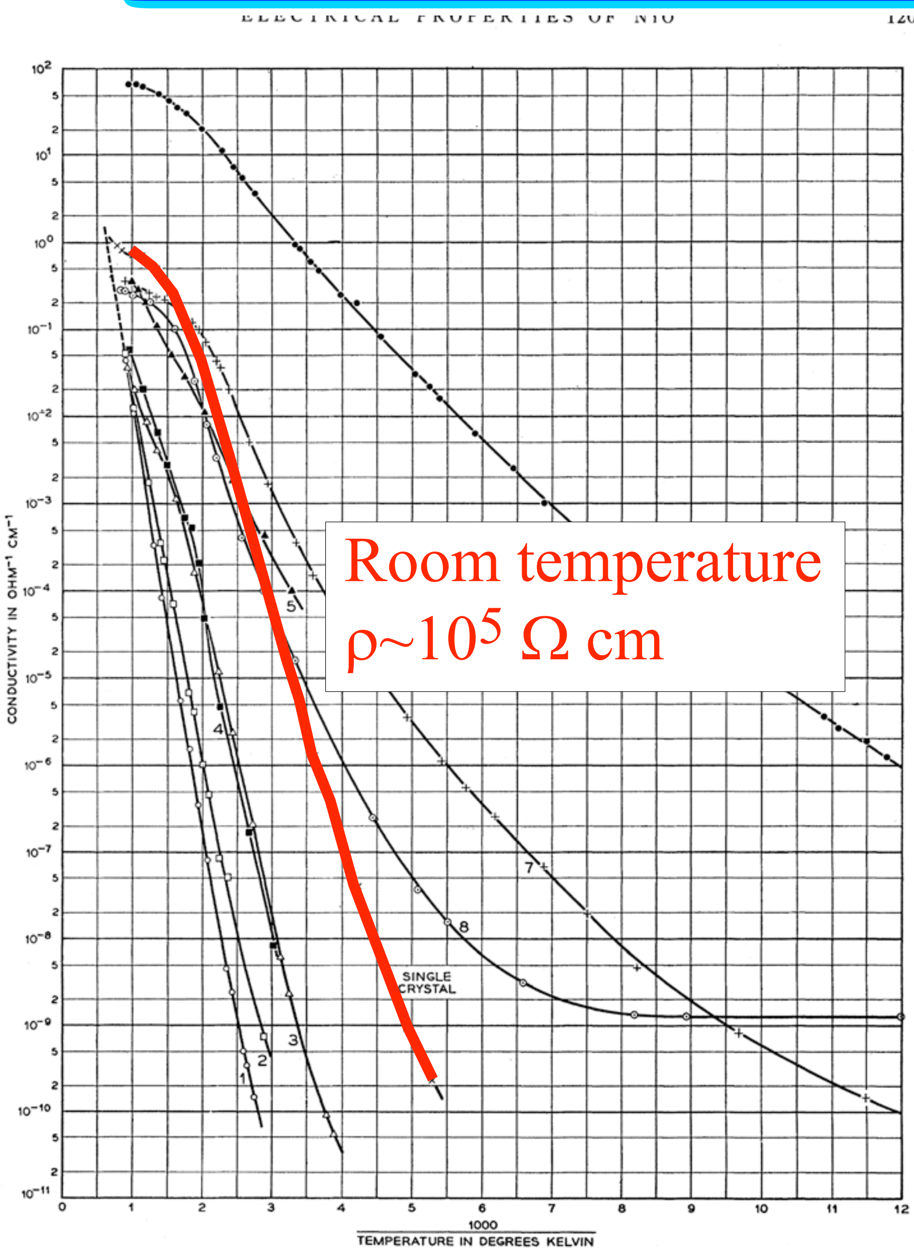




How to calculate XAS: an example on NiO

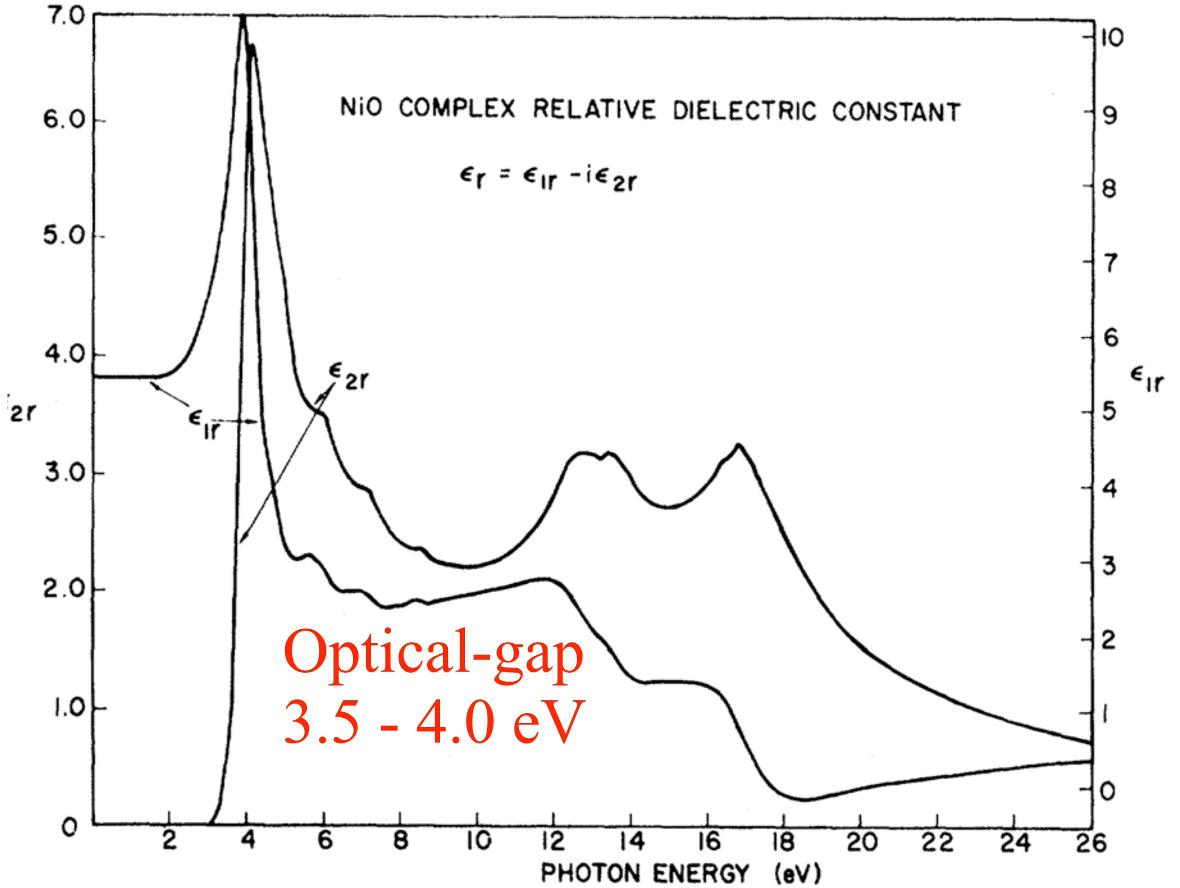


Within LDA NiO is a metal; experimentally it is a good insulator

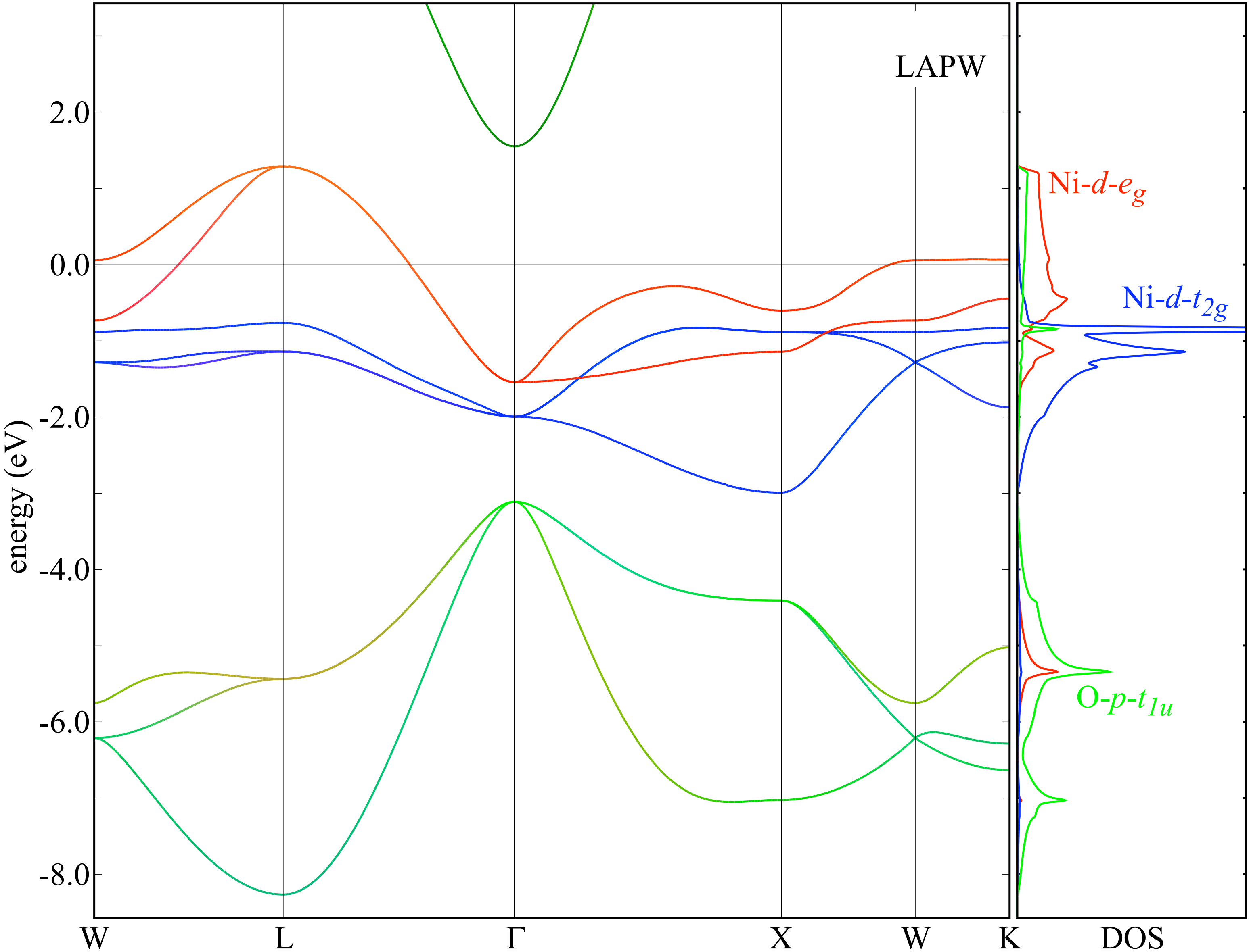


F. J. Morin Phys. Rev. **93**, 1199 (1954)

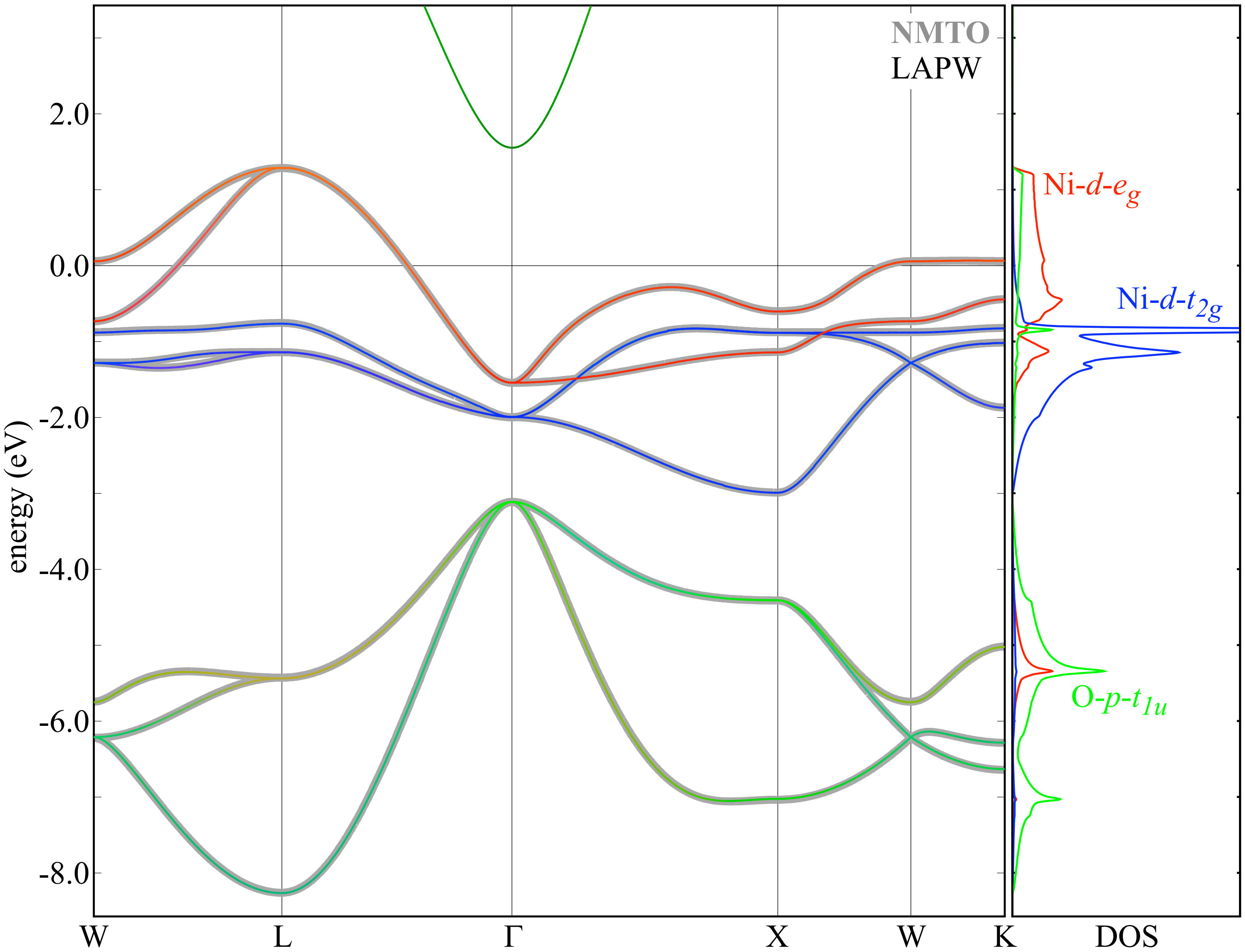
R. Newman and R. M. Chrenko
Phys. Rev. **114** 1507 (1959)



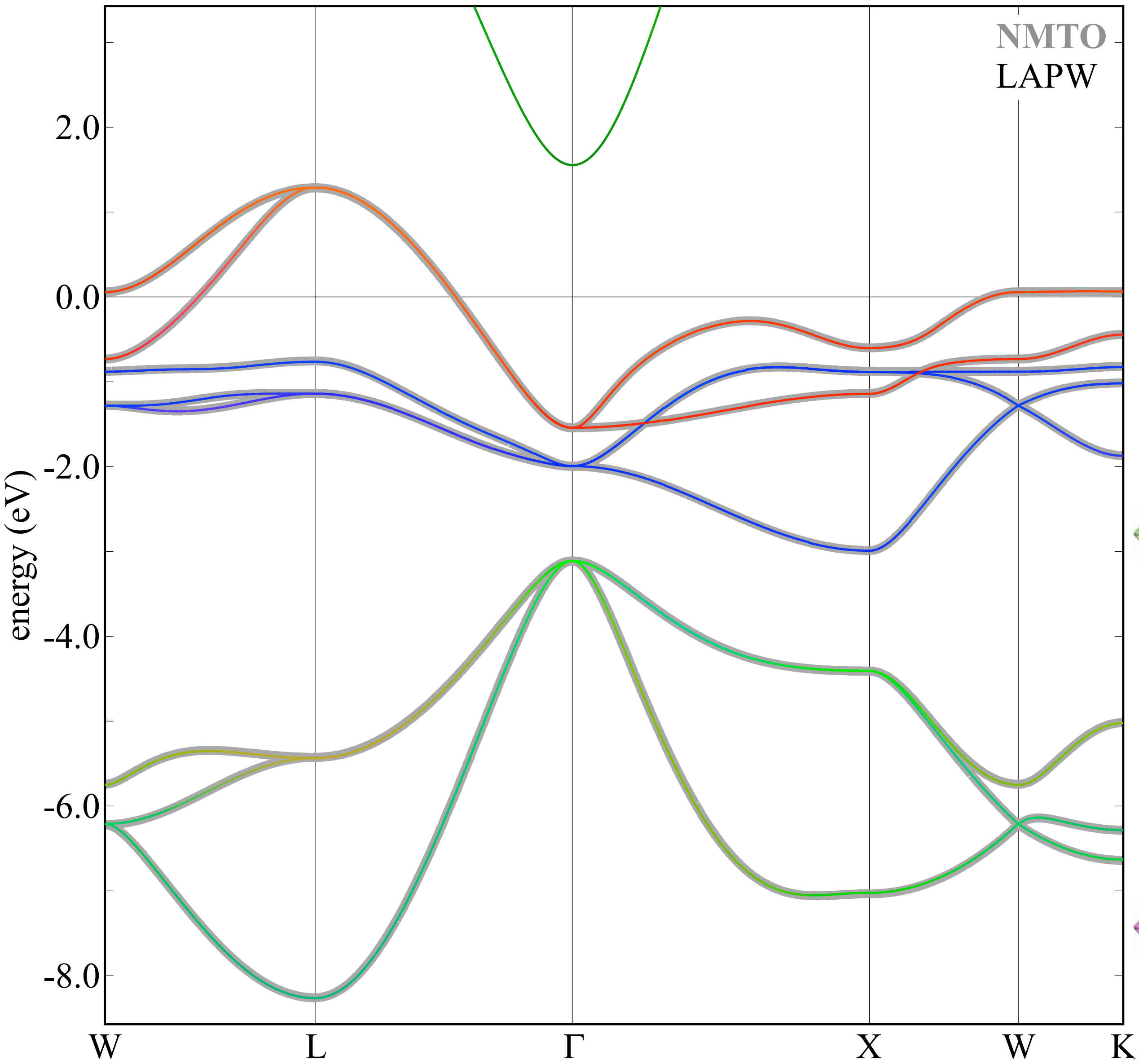
Although NiO is metal in LDA there are many things correct

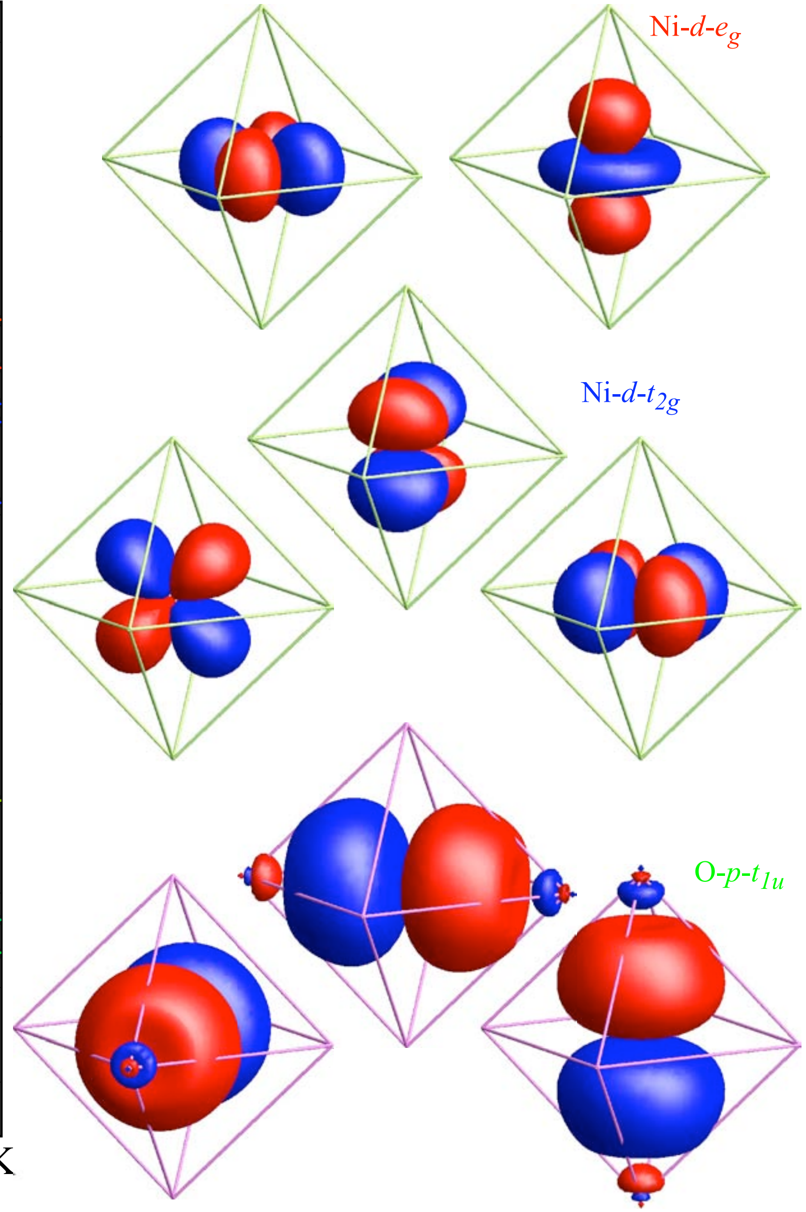


Use the LAPW potential for an NMTO calculation



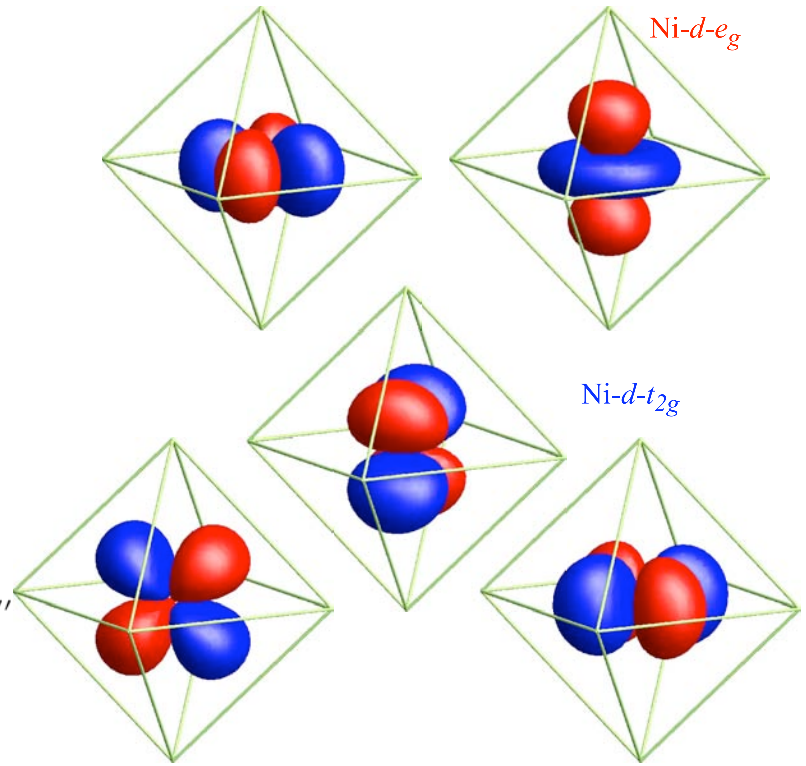
Obtain Wannier orbitals from the Muffin Tin Orbitals

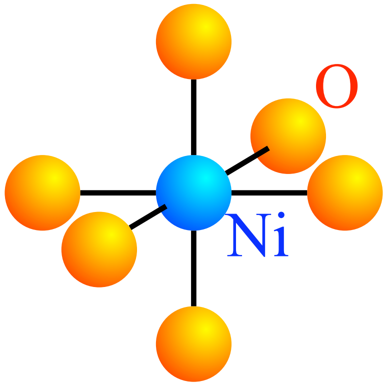




Full multiplet Ligand Field model based on LDA

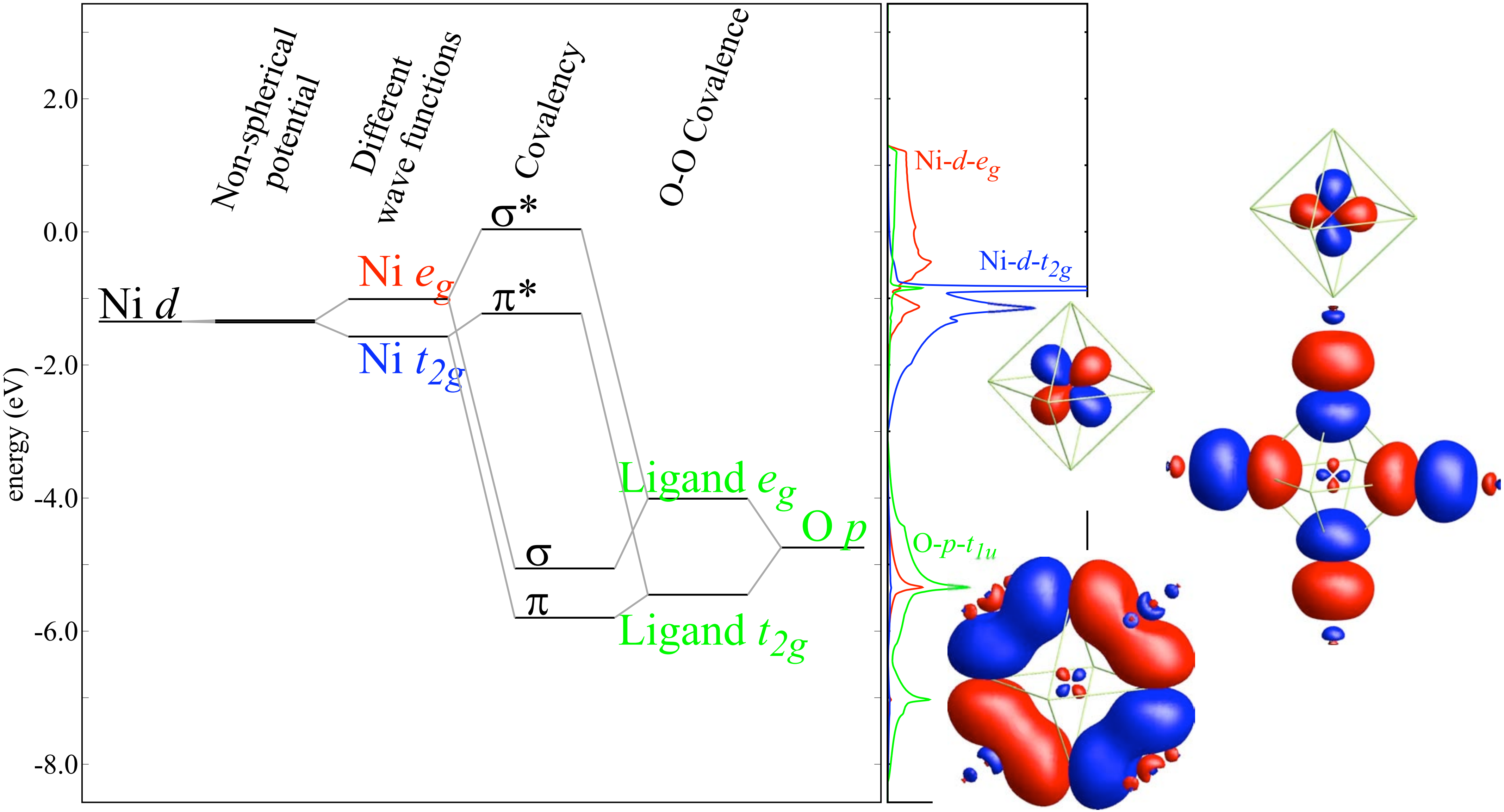
$$
\begin{aligned}
H_i = &\sum_{\sigma,\tau,\tau'} \varepsilon_{\tau,\tau'} \; d^\dagger_{\sigma,\tau} d_{\sigma,\tau'} \\
&+ \sum_{\sigma,\tau,\tau'} t_{\tau,\tau'} \; (d^\dagger_{\sigma,\tau} L_{\sigma,\tau'} + L^\dagger_{\sigma,\tau} d_{\sigma,\tau'}) \\
&+ \sum_{\sigma,\tau,\tau'} t'_{\tau,\tau'} \; L^\dagger_{\sigma,\tau} L_{\sigma,\tau'} \\
&+ \sum_{\sigma,\tau} H_{EX} \; \sigma \; d^\dagger_{\sigma,\tau} d_{\sigma,\tau} \\
&+ \sum_{\sigma,\sigma',\tau,\tau'} \zeta_{\sigma,\sigma',\tau,\tau'} \; d^\dagger_{\sigma,\tau} d_{\sigma',\tau'} \\
&+ \sum_{\sigma,,,,,\tau'''} U_{\sigma,\sigma',\sigma'',\sigma''',\tau,\tau',\tau'',\tau'''} \; d^\dagger_{\sigma,\tau} d^\dagger_{\sigma',\tau'} d_{\sigma'',\tau''} d_{\sigma''',\tau'''}
\end{aligned}
$$



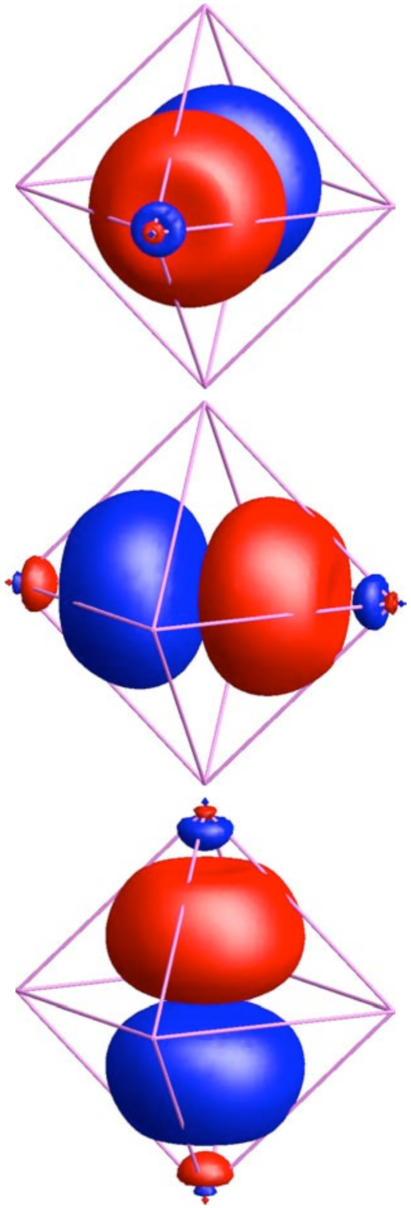


$$
U_{\sigma,,,,,,,,\tau'''} = \frac{1}{2} \delta_{\sigma,\sigma''} \delta_{\sigma'\sigma'''} \int\int f^*_\tau(r_1) f^*_{\tau'}(r_2) \; \frac{e^2}{|r_1 - r_2|} \; f_{\tau''}(r_1) f_{\tau'''}(r_2) \delta r_1 \delta r_2
$$

One particle energy level diagram obtained from LDA



Two particle interactions on a level beyond LDA

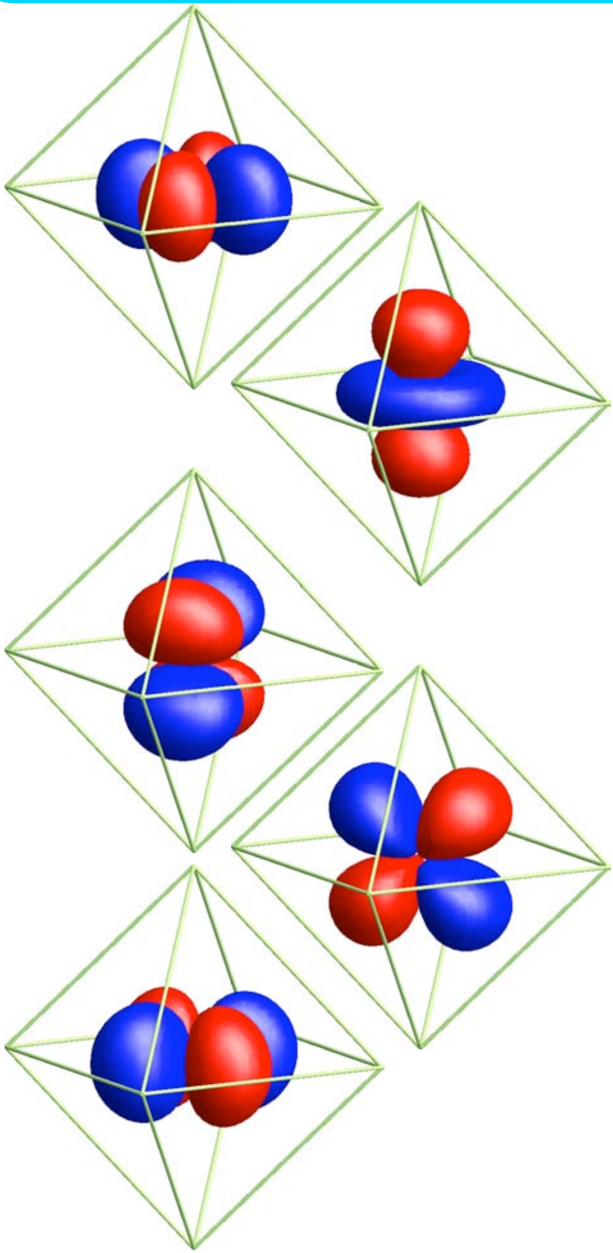


O 2p orbitals

Orbitals are close to completely filled:
Chance that two holes meet on the same orbital is small.

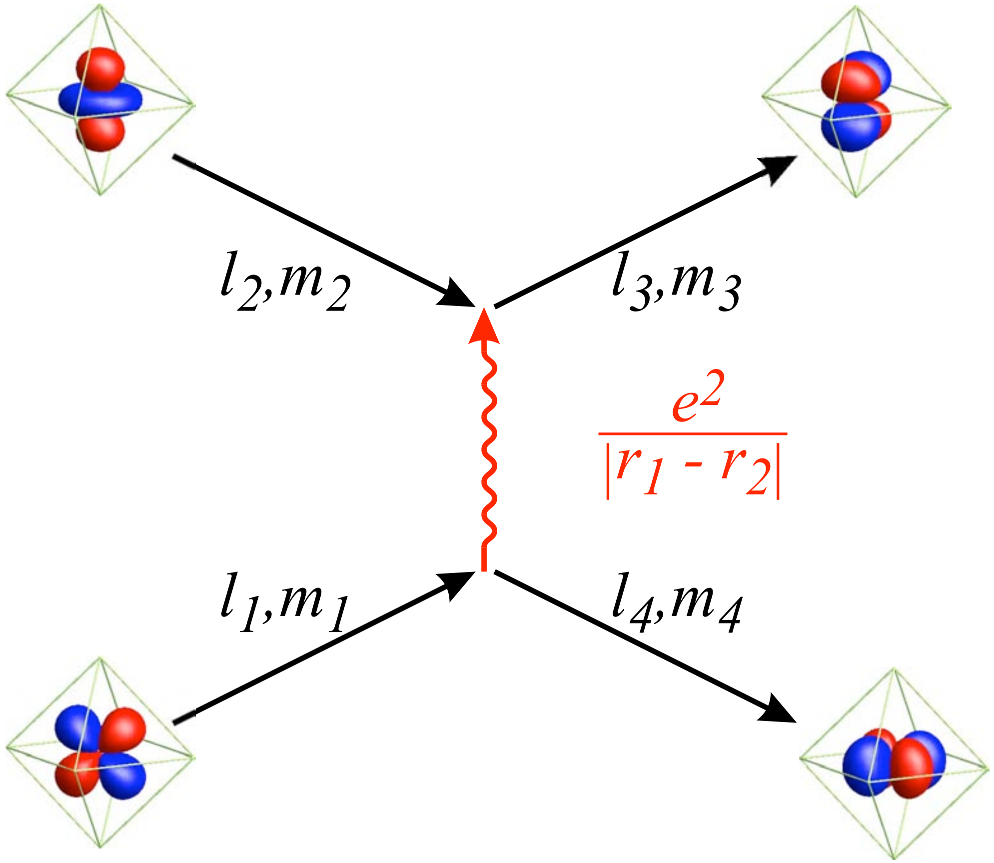
Assume interactions are well treated within the LDA

Two particle interactions on a level beyond LDA

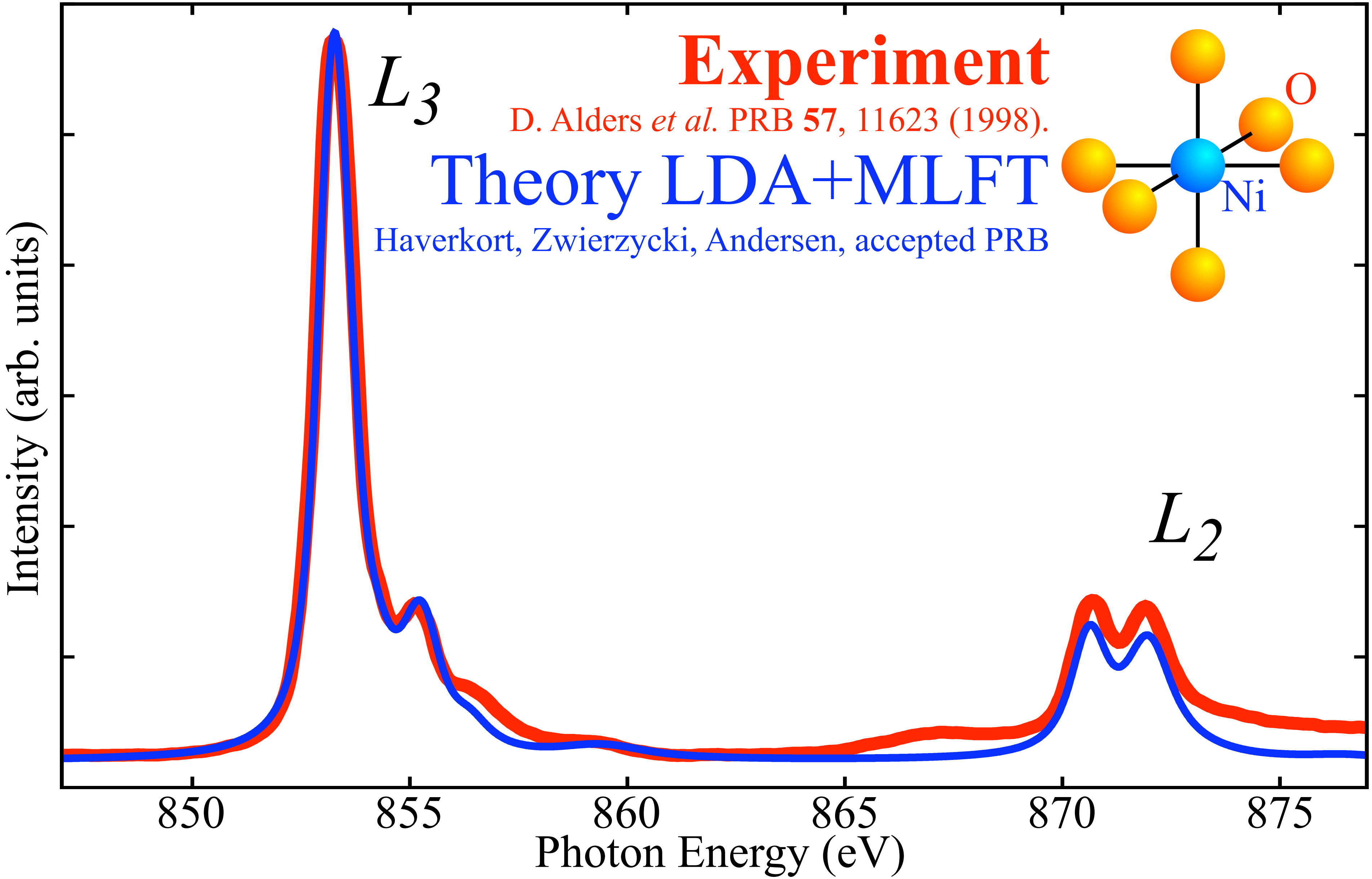


TM 3d orbitals

Include the full Coulomb interaction



2p X-ray Absorption Spectroscopy *ab initio* theory



XAS: Sum rules for circular dichroism orbital and spin moment

VOLUME 68, NUMBER 12 PHYSICAL REVIEW LETTERS 23 MARCH 1992

X-Ray Circular Dichroism as a Probe of Orbital Magnetization

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VOLUME 70, NUMBER 5 PHYSICAL REVIEW LETTERS 1 FEBRUARY 1993

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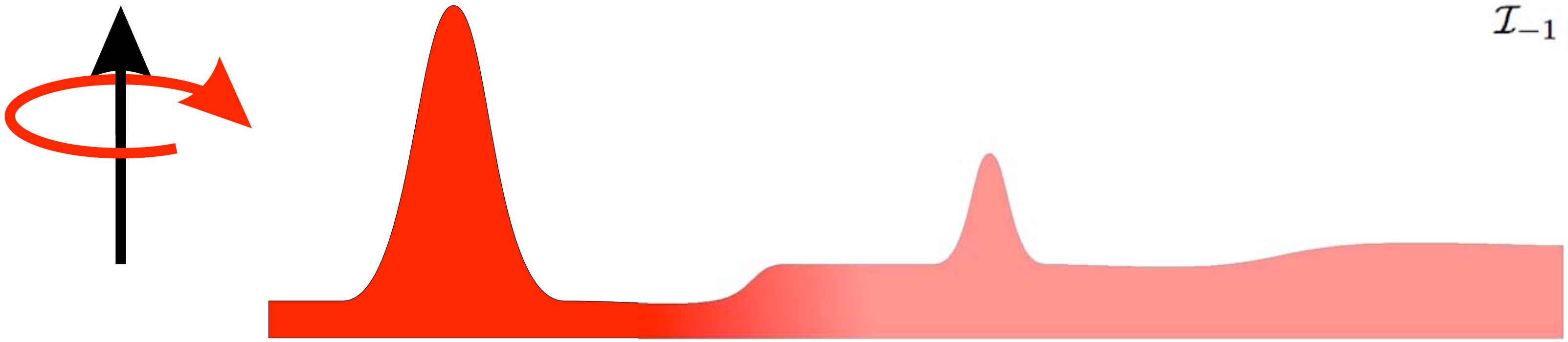

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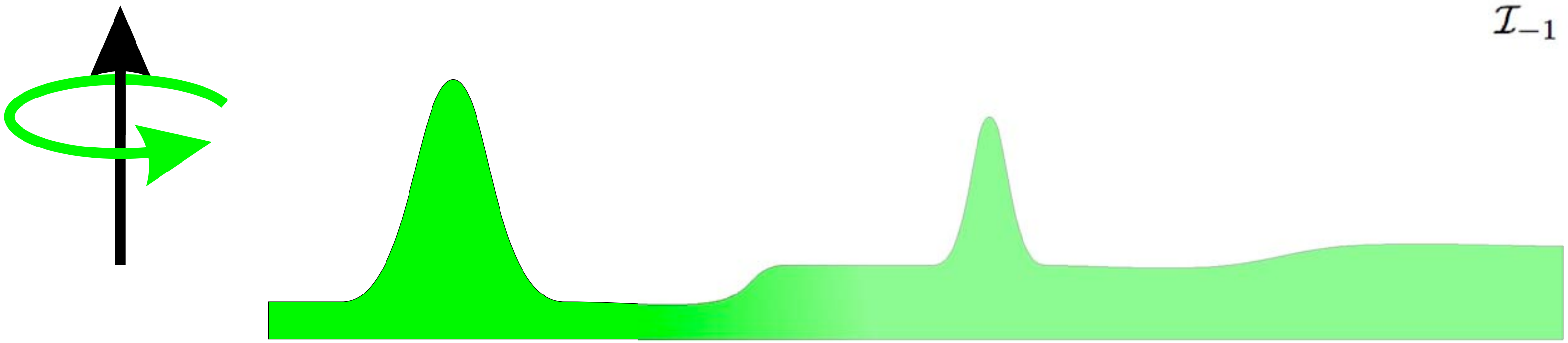

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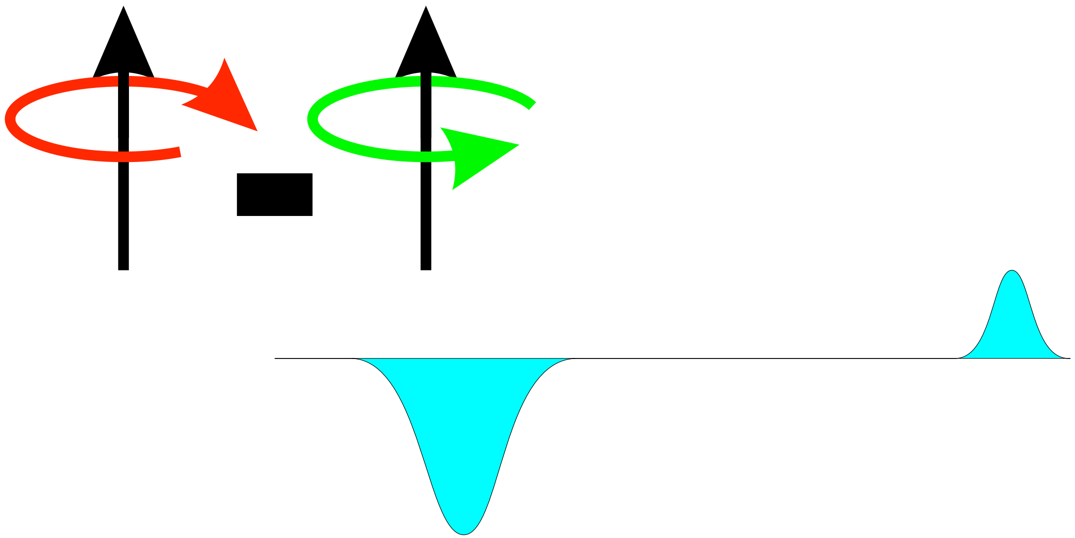

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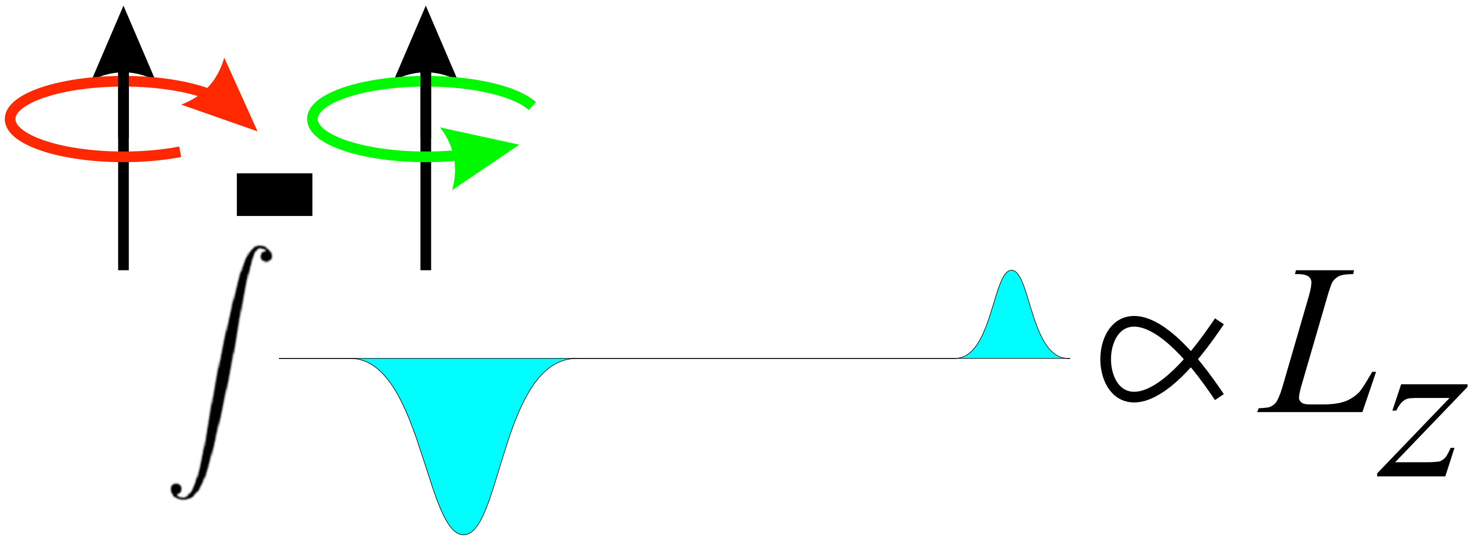

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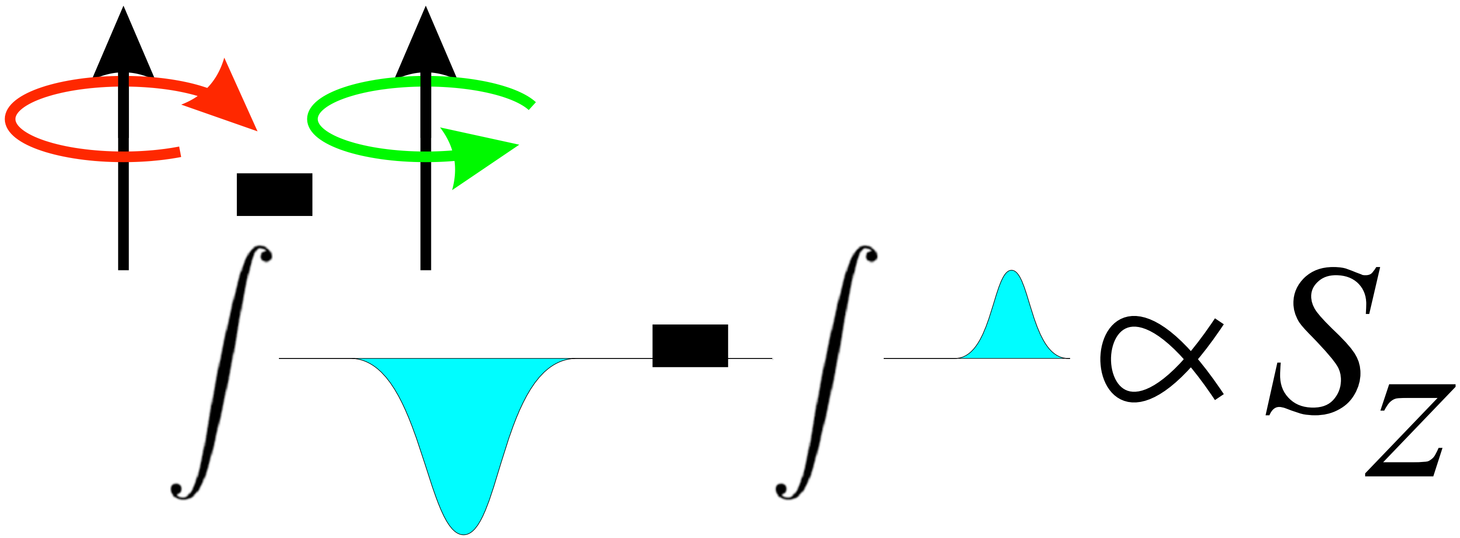

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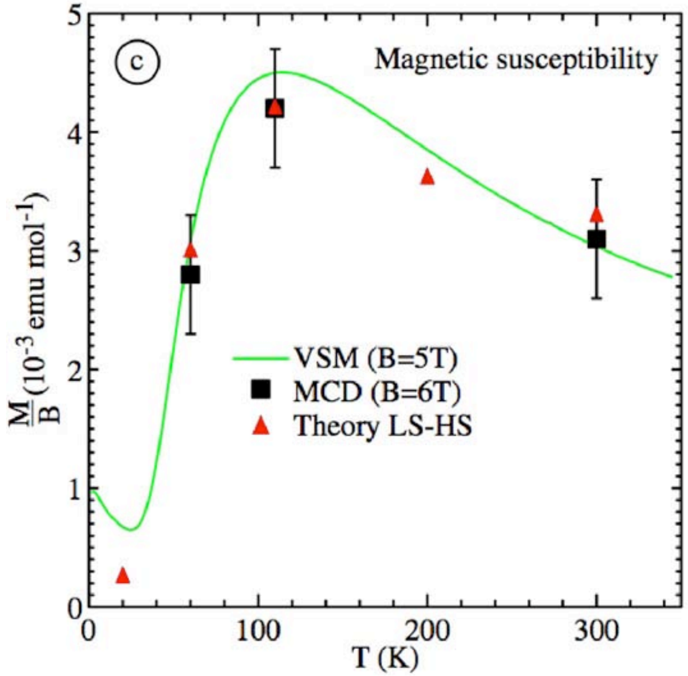
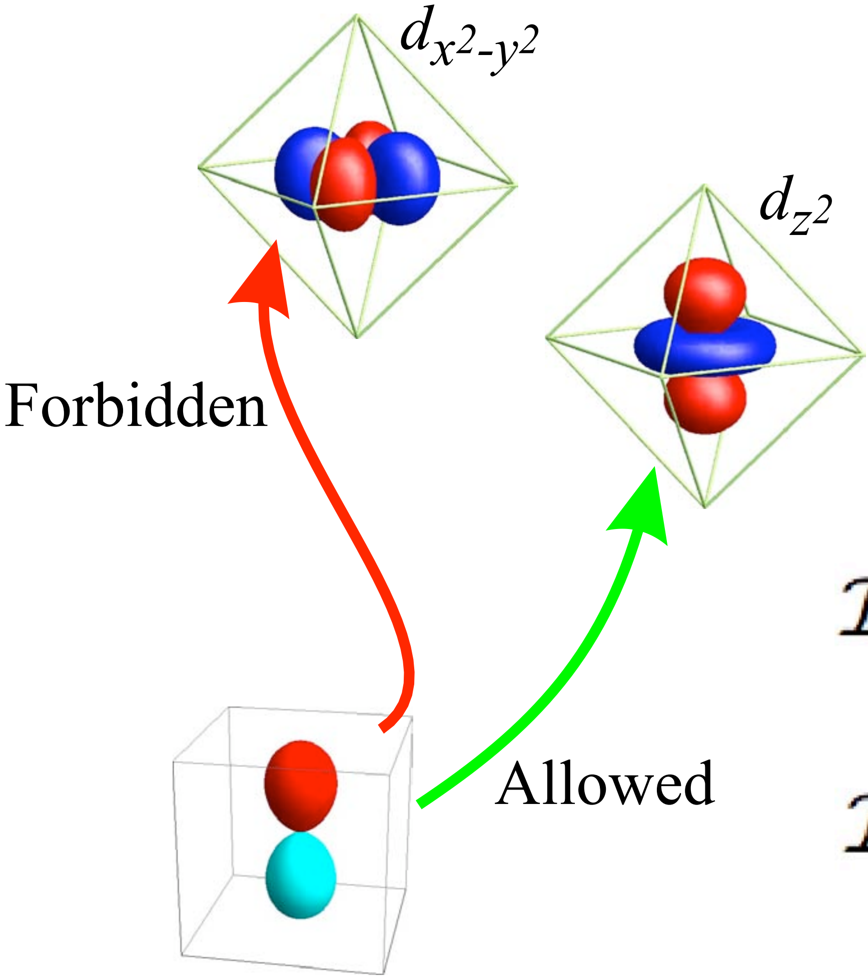


Orbital and spin resolved magnetic susceptibility ($LaCoO_3$)

XAS: Sum rules for linear dichroism orbital occupation

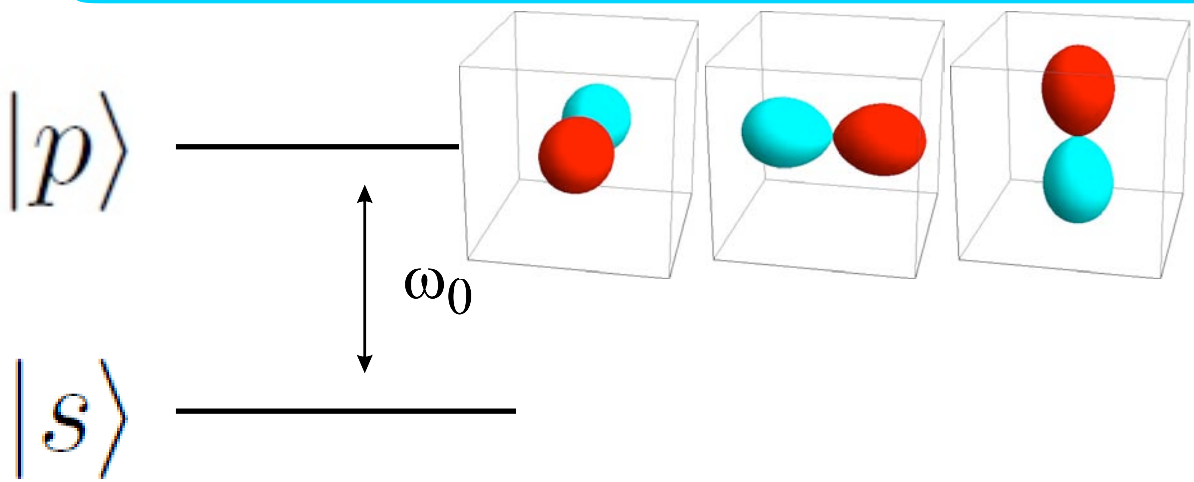


$$\mathcal{I}_x = \frac{1}{\underline{n}}\left(\frac{1}{2}\underline{n}_{xy} + \frac{1}{2}\underline{n}_{xz} + \frac{2}{3}\underline{n}_{x^2}\right)$$

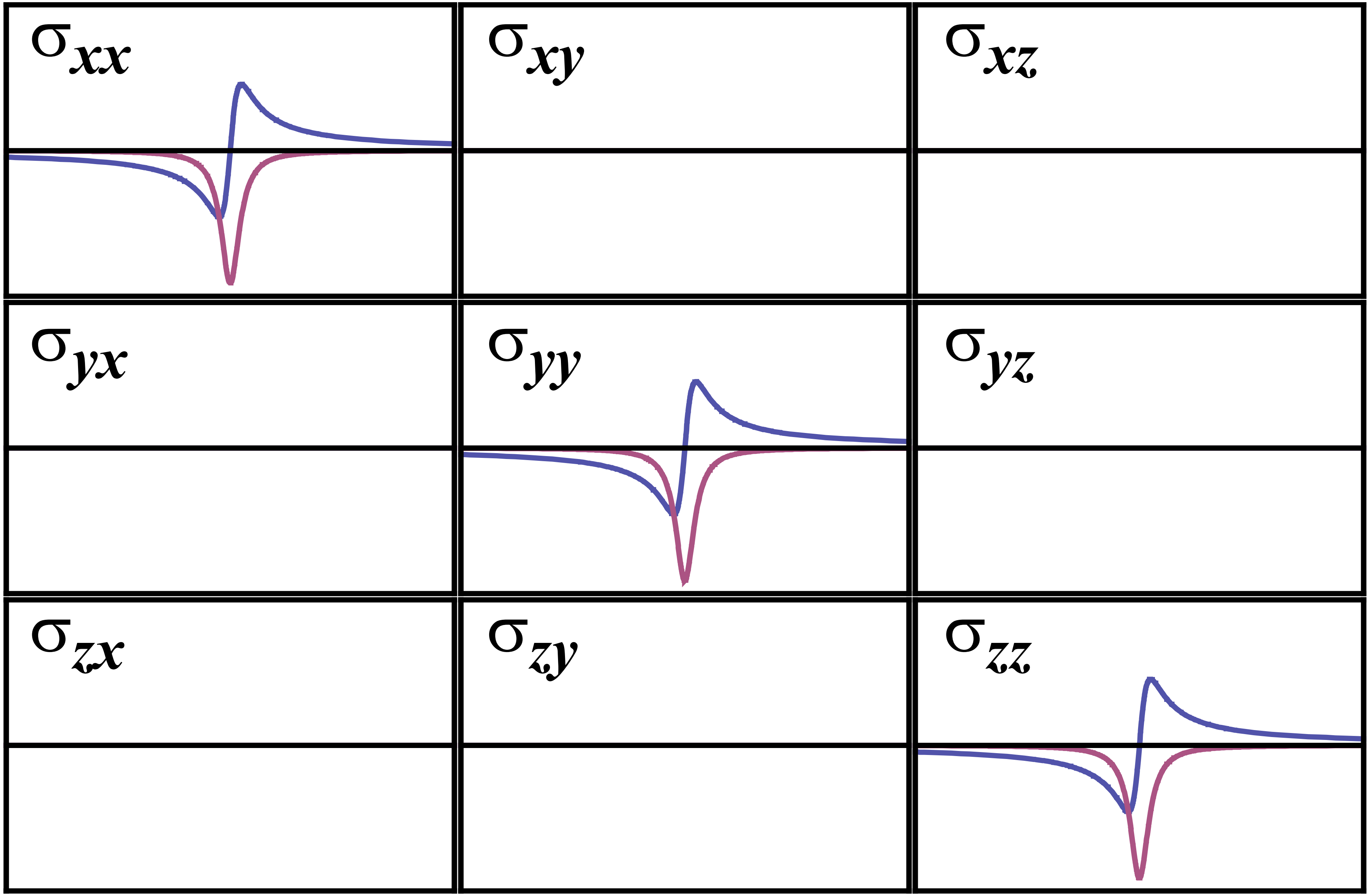
$$\mathcal{I}_y = \frac{1}{\underline{n}}\left(\frac{1}{2}\underline{n}_{xy} + \frac{1}{2}\underline{n}_{yz} + \frac{2}{3}\underline{n}_{y^2}\right)$$

$$\mathcal{I}_z = \frac{1}{\underline{n}}\left(\frac{1}{2}\underline{n}_{xz} + \frac{1}{2}\underline{n}_{yz} + \frac{2}{3}\underline{n}_{z^2}\right)$$

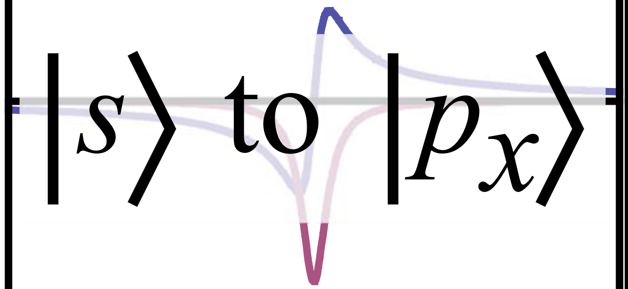
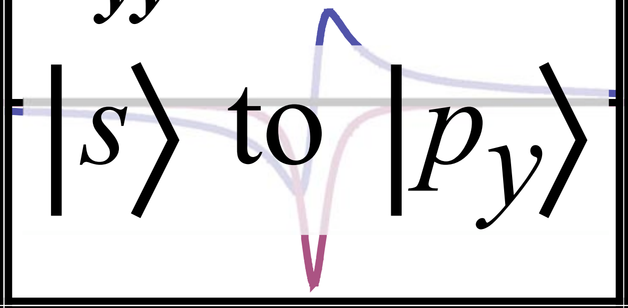
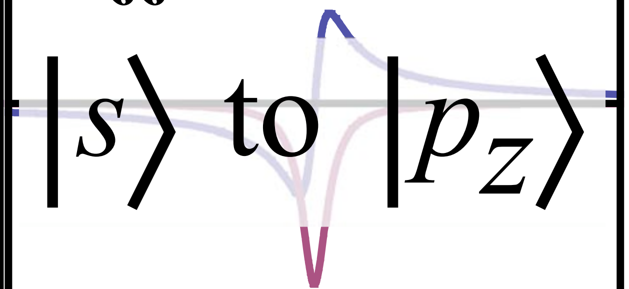
XAS and the conductivity tensor (σ)



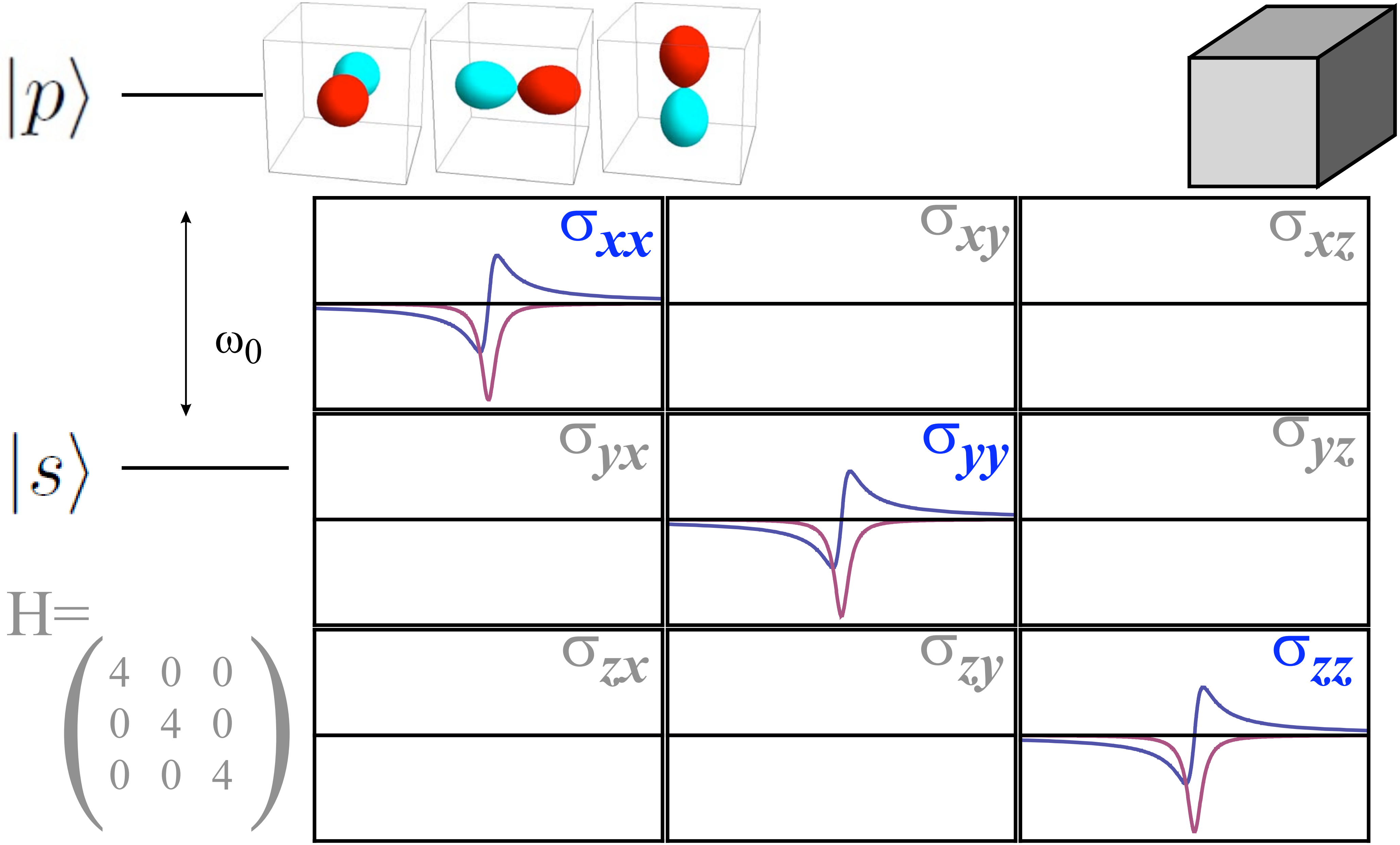
But the conductivity tensor (σ) is a TENSOR



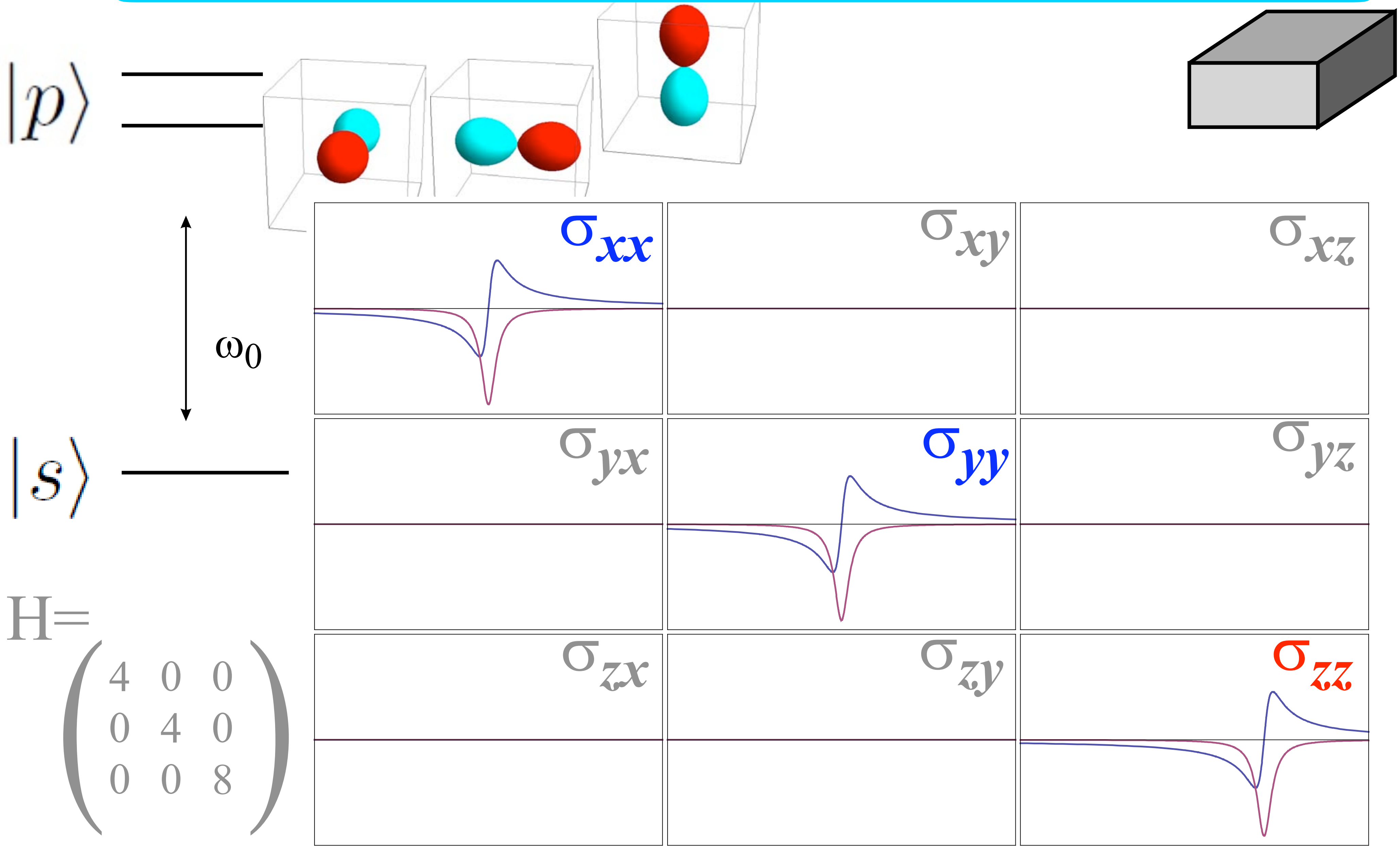
But the conductivity tensor (σ) is a TENSOR

σ_{xx}  $\lvert s\rangle$ to $\lvert p_x\rangle$	σ_{xy}	σ_{xz}
σ_{yx}	σ_{yy}  $\lvert s\rangle$ to $\lvert p_y\rangle$	σ_{yz}
σ_{zx}	σ_{zy}	σ_{zz}  $\lvert s\rangle$ to $\lvert p_z\rangle$

the conductivity tensor (σ) in Cubic symmetry

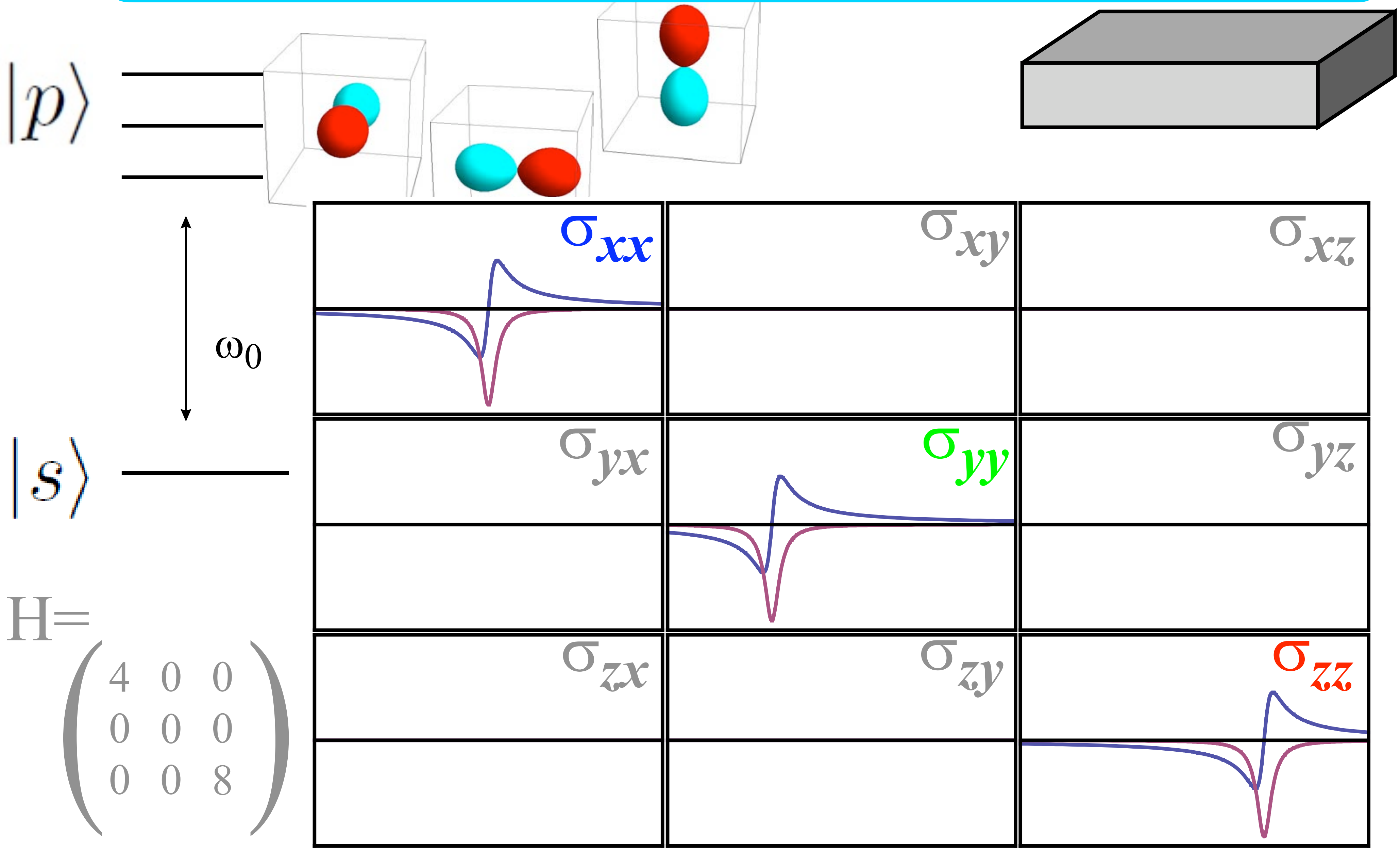


the conductivity tensor (σ) in Tetragonal symmetry

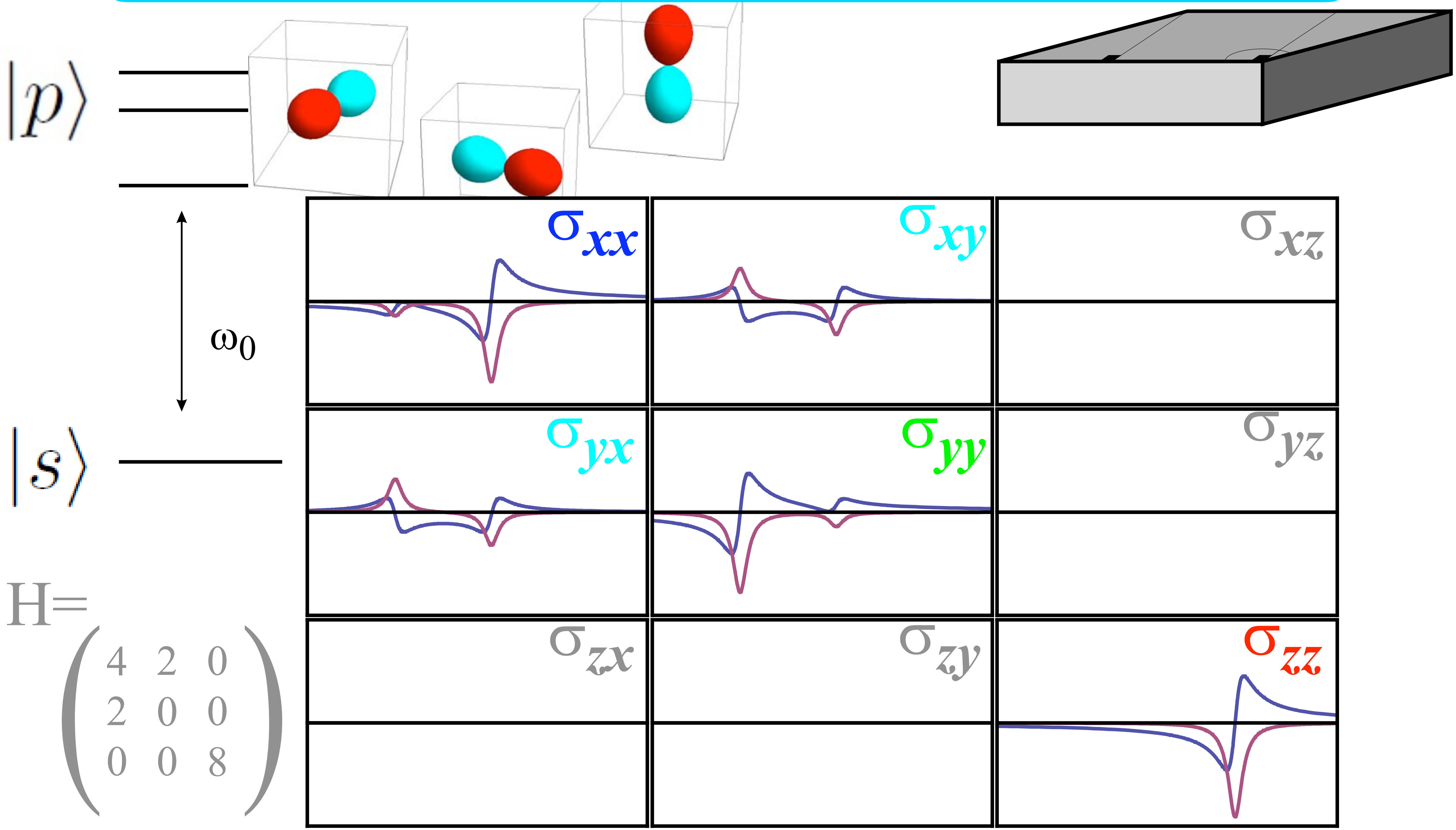


$$H=\begin{pmatrix} 4 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 8 \end{pmatrix}$$

the conductivity tensor (σ) in Orthorombic symmetry

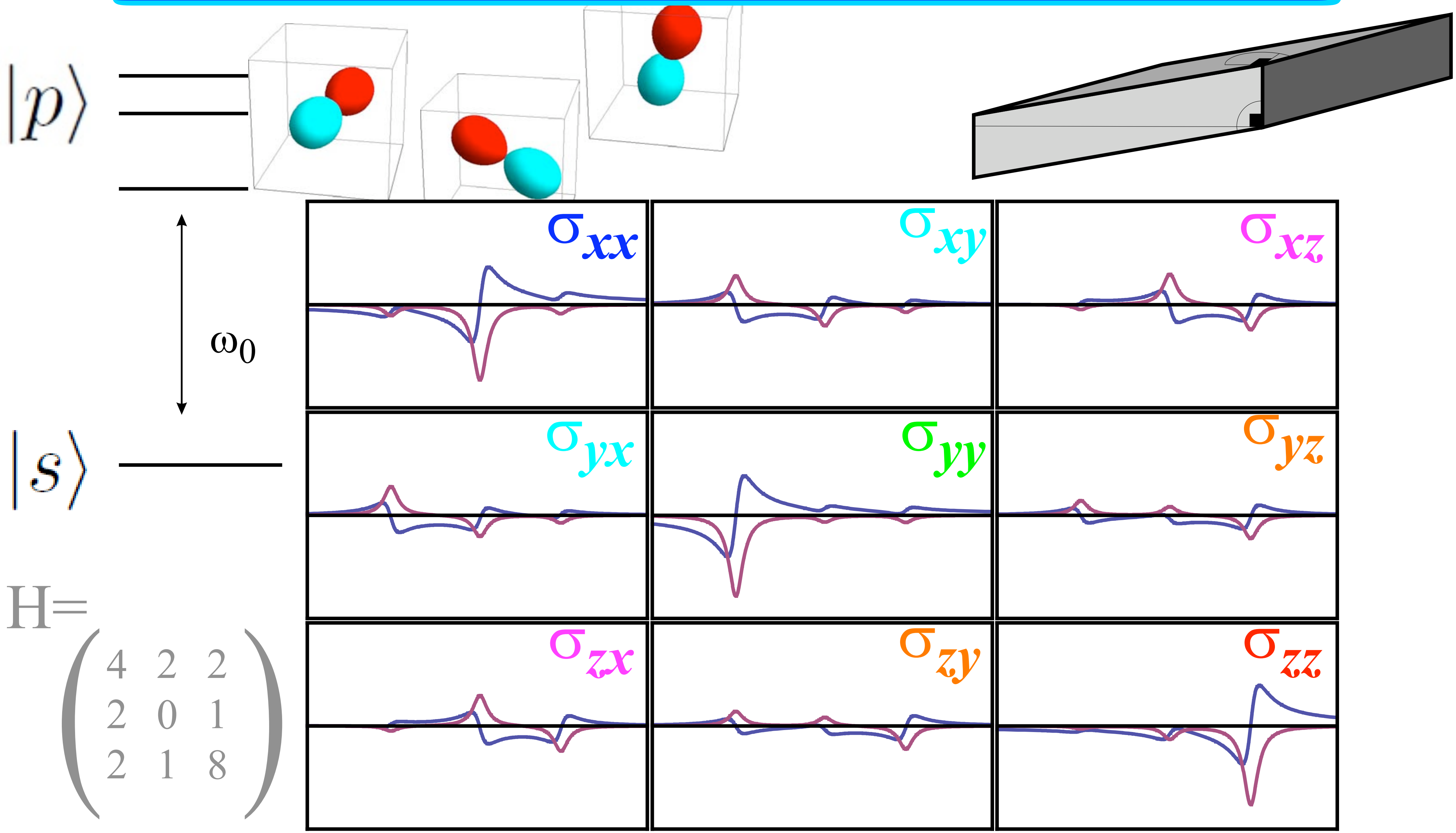


the conductivity tensor (σ) in Monoclinic symmetry



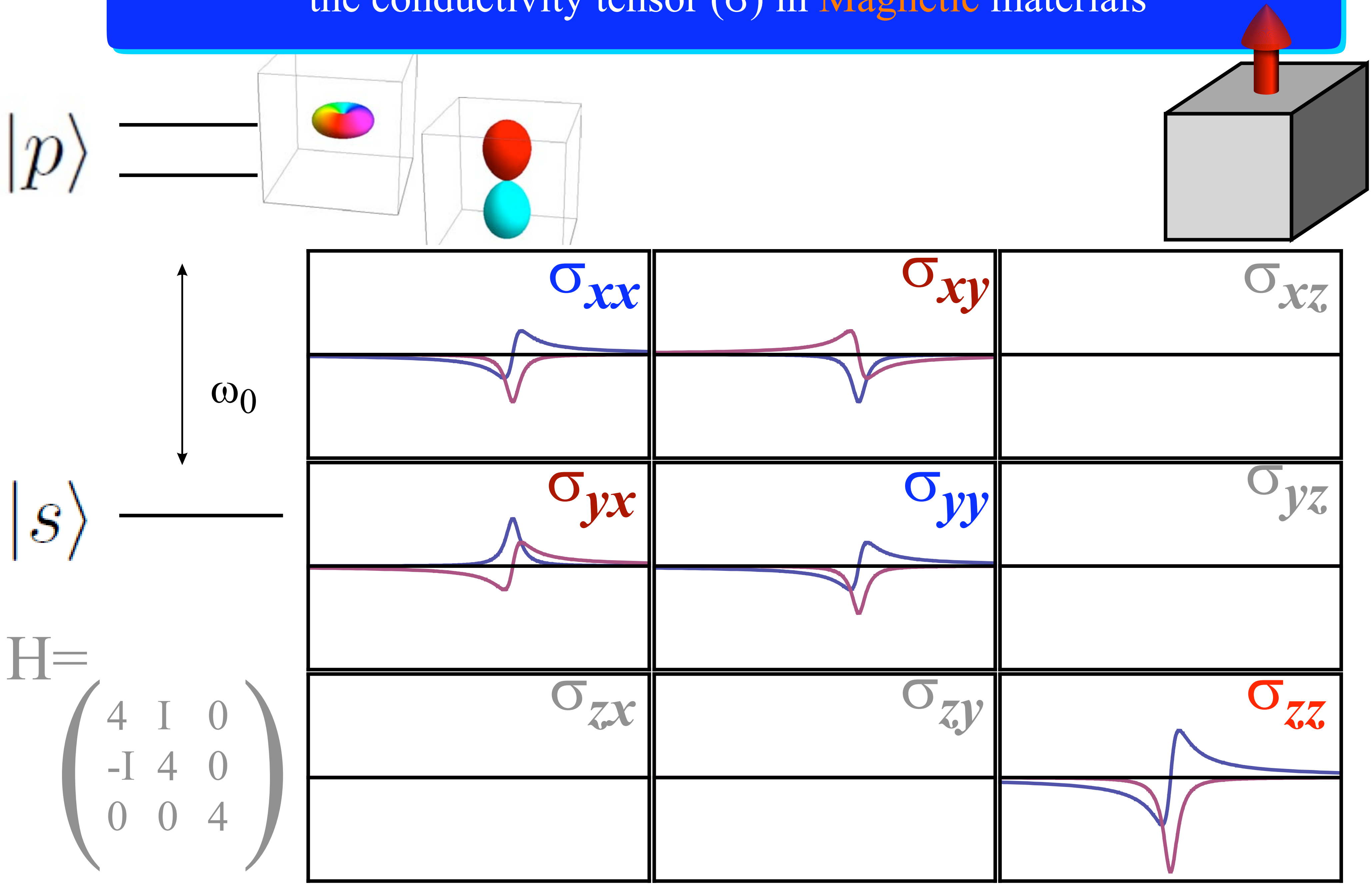
$$H = \begin{pmatrix} 4 & 2 & 0 \\ 2 & 0 & 0 \\ 0 & 0 & 8 \end{pmatrix}$$

the conductivity tensor (σ) in Triclinic symmetry

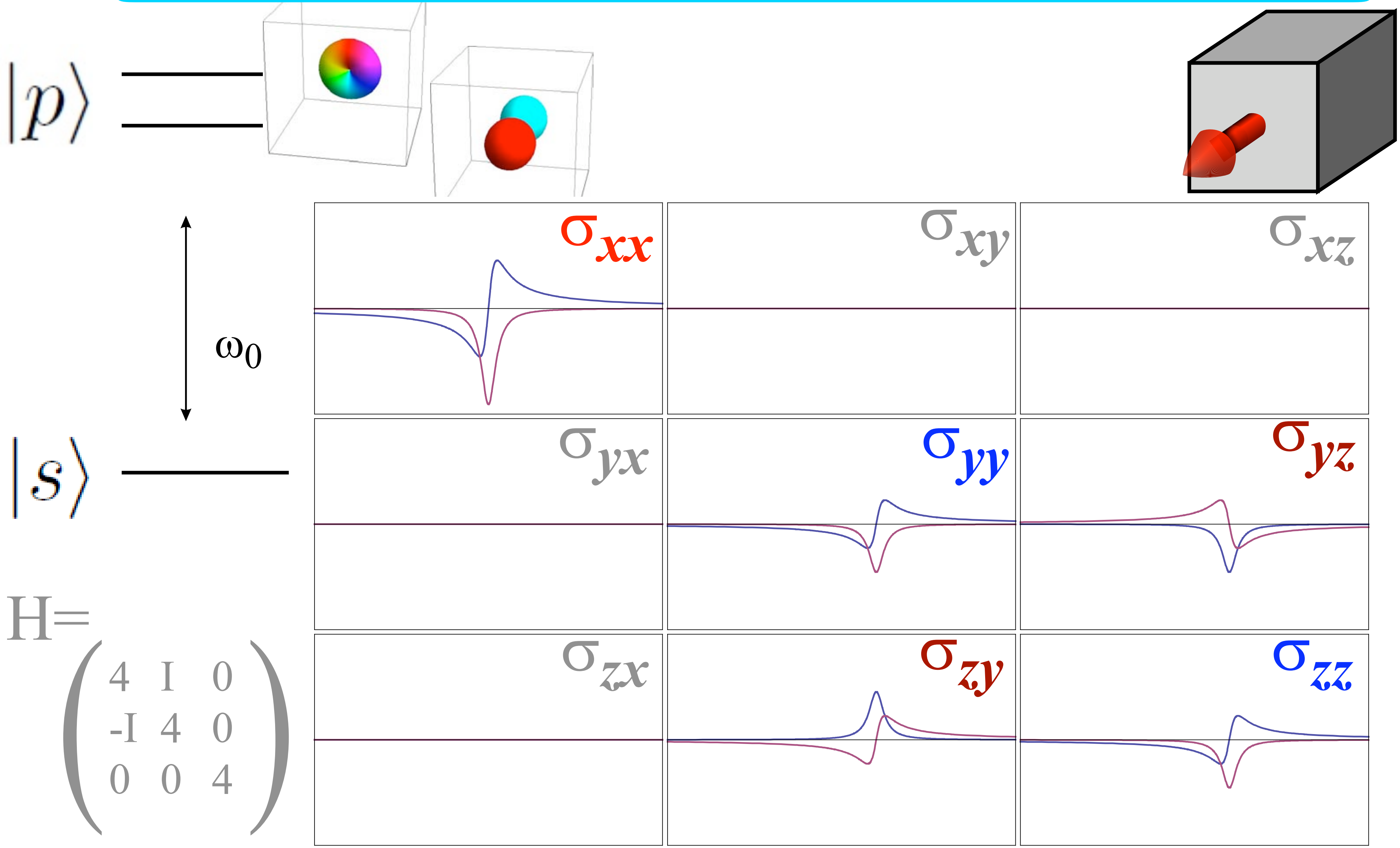


$$H = \begin{pmatrix} 4 & 2 & 2 \\ 2 & 0 & 1 \\ 2 & 1 & 8 \end{pmatrix}$$

the conductivity tensor (σ) in Magnetic materials



the conductivity tensor (σ) in Magnetic materials



XAS: Sum rules for circular dichroism orbital and spin moment

VOLUME 68, NUMBER 12 PHYSICAL REVIEW LETTERS 23 MARCH 1992

X-Ray Circular Dichroism as a Probe of Orbital Magnetization

B. T. Thole,[1] Paolo Carra,[2] F. Sette,[2] and G. van der Laan[3]

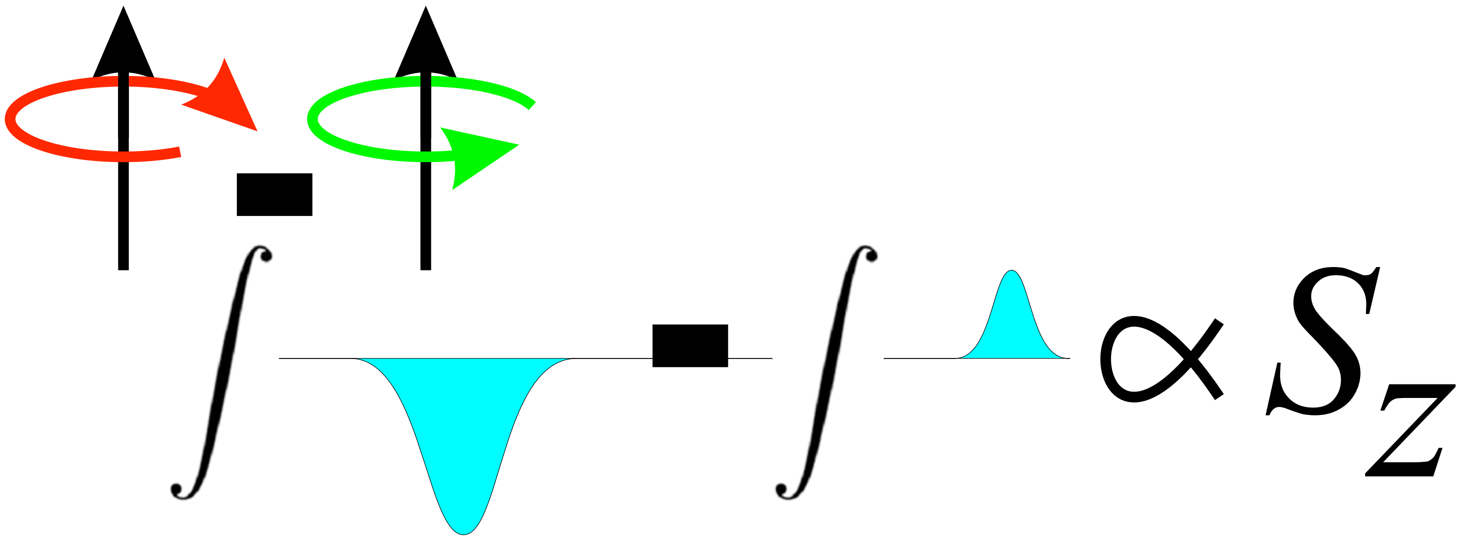
VOLUME 70, NUMBER 5 PHYSICAL REVIEW LETTERS 1 FEBRUARY 1993

X-Ray Circular Dichroism and Local Magnetic Fields

Paolo Carra,[1] B. T. Thole,[1],[2] Massimo Altarelli,[1] and Xindong Wang[3]

$$(\mathcal{I}_{-1}^{c+\frac{1}{2}} - \mathcal{I}_{1}^{c+\frac{1}{2}}) - \frac{l}{l-1}(\mathcal{I}_{-1}^{c-\frac{1}{2}} - \mathcal{I}_{1}^{c-\frac{1}{2}}) = \frac{2}{3\underline{n}}\mathbf{S}_z + \frac{2(2l+3)}{3l\underline{n}}\mathbf{T}_z$$

$$\mathcal{I}_{-1} - \mathcal{I}_1 = \frac{1}{\underline{n}}\sum_{m,\sigma}\underline{n}_{m\sigma}\frac{-m}{l} = \frac{\mathbf{L_z}}{l\underline{n}}$$

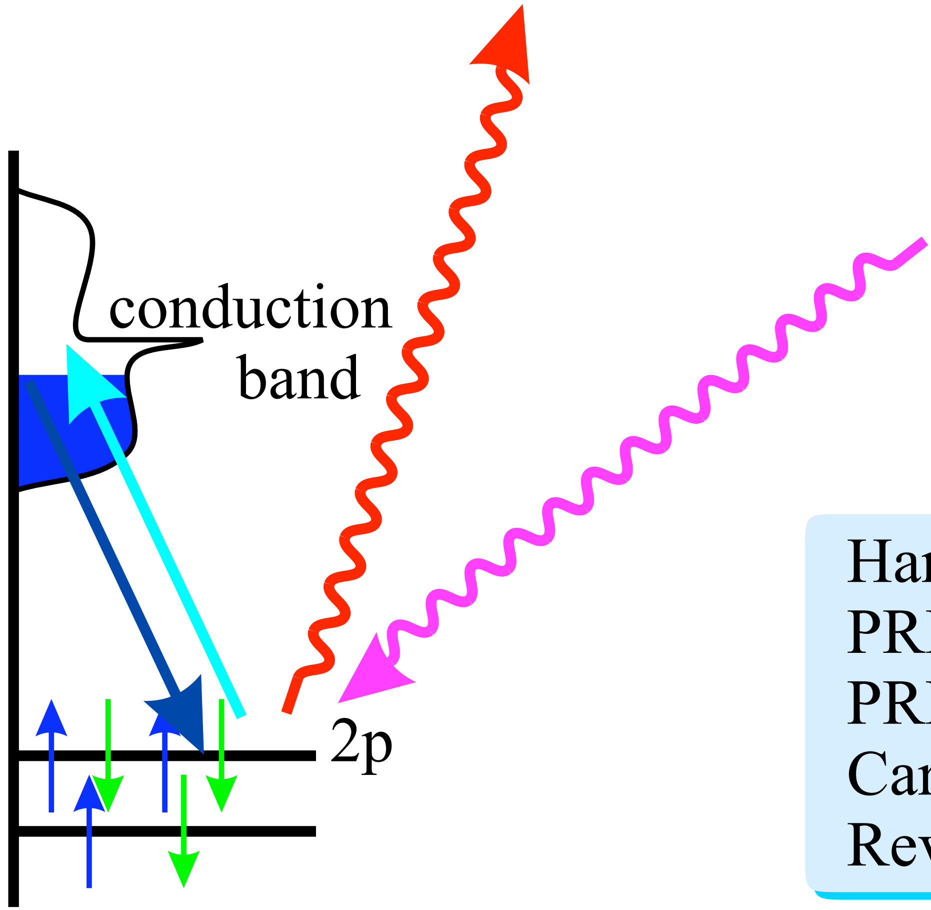


Thole *et al.*'s sum-rules in tensor form: s to p excitations

$$\int_{K} \sigma = \mathrm{i}\,\overline{\rho_{p}}$$

And now momentum, i.e. spatial resolved, from XAS to RXD

- X-ray Absorption Spectroscopy (XAS) at the TM *2p* to *3d* edge
- Resonant X-ray Diffraction (RXD)



Hannon, Trammel, Bloom, Gibbs
PRL **61**, 1245 (1988)
PRB **43**, 5663 (1991)
Carra, Thole
Rev. Mod. Phys. 66, 1509 (1994).

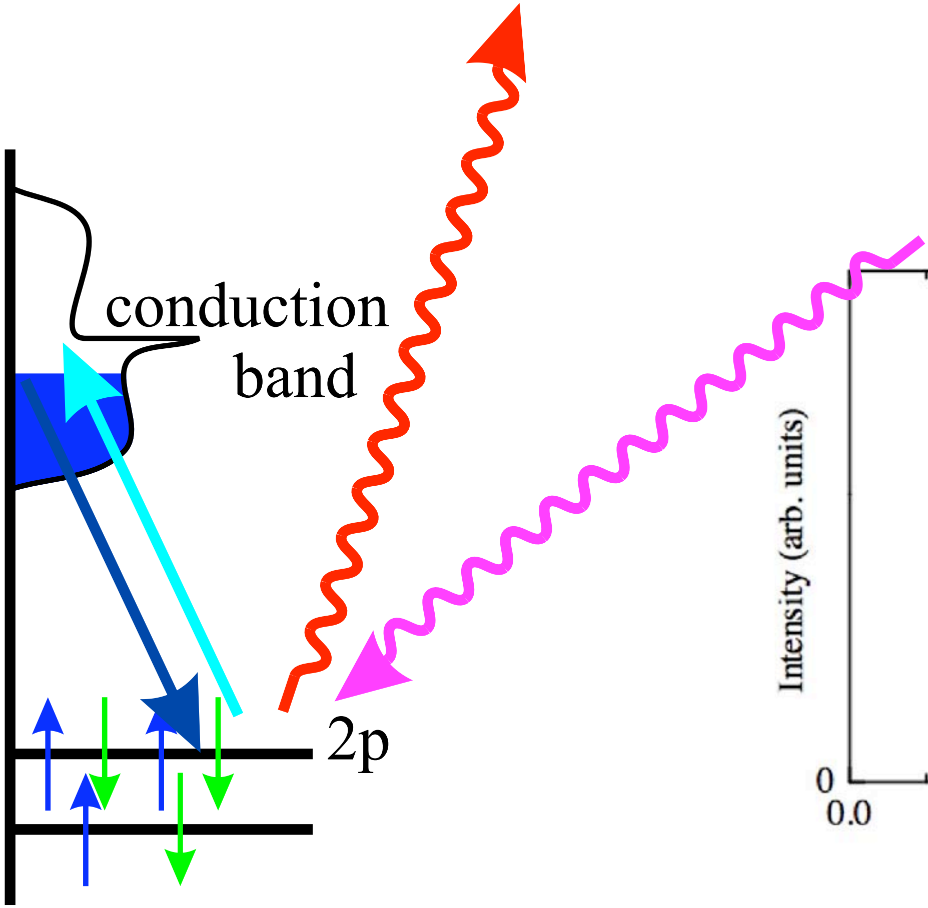
RXD: Magnetic Bragg reflection

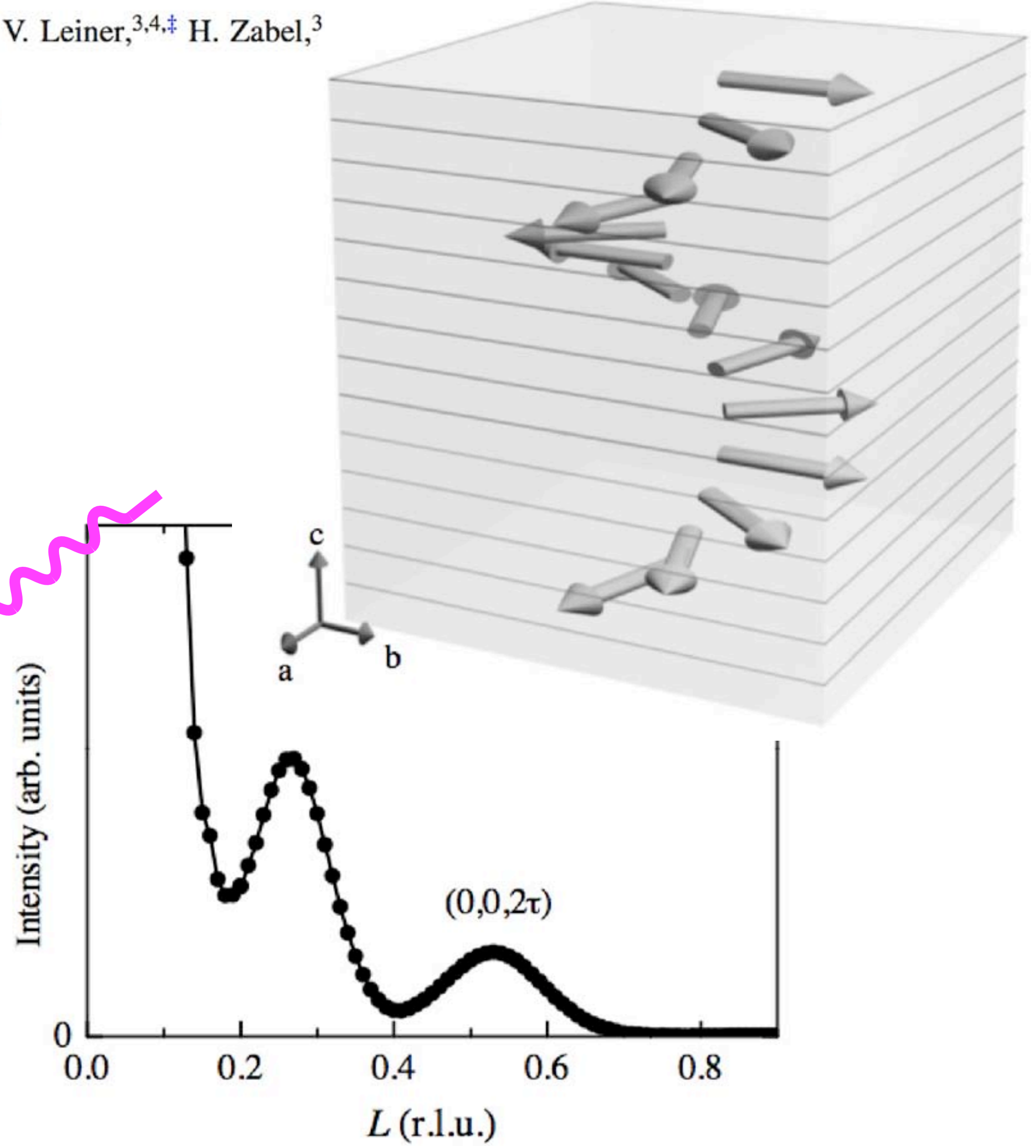
Magnetic x-ray scattering at the M_5 absorption edge of Ho

H. Ott,[1,*] C. Schüßler-Langeheine,[1,2] E. Schierle,[1] A. Yu. Grigoriev,[1,†] V. Leiner,[3,4,‡] H. Zabel,[3]
G. Kaindl,[1] and E. Weschke[1]

PHYSICAL REVIEW B **74**, 094412 (2006)

Ho metal film





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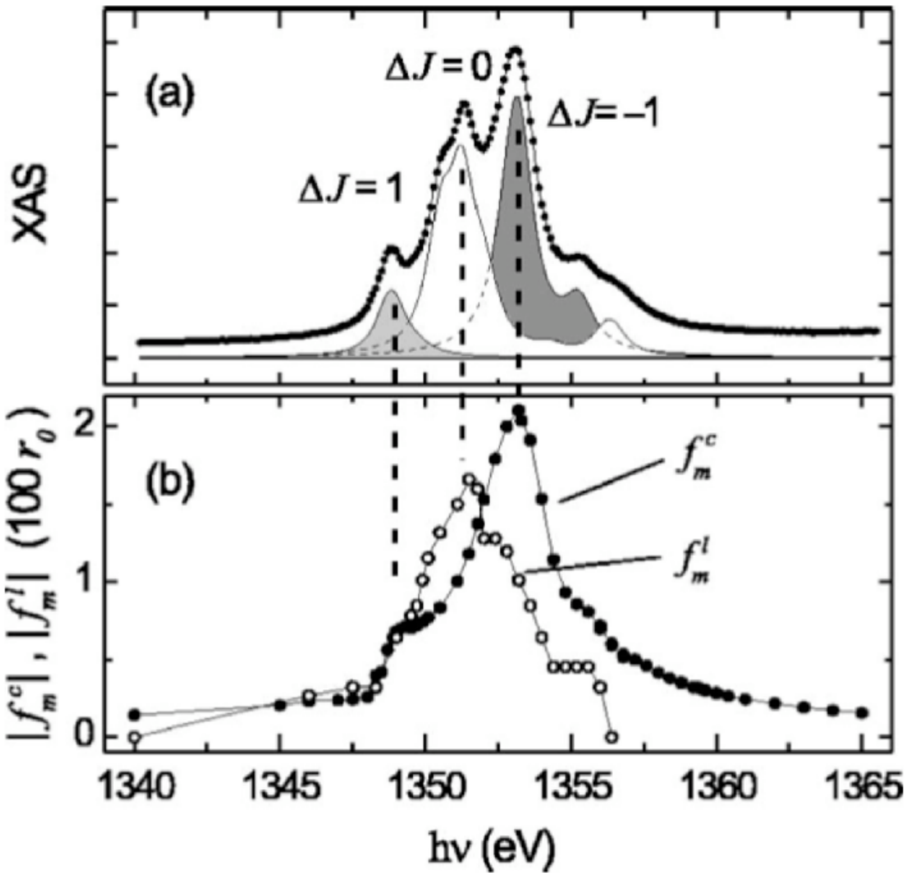
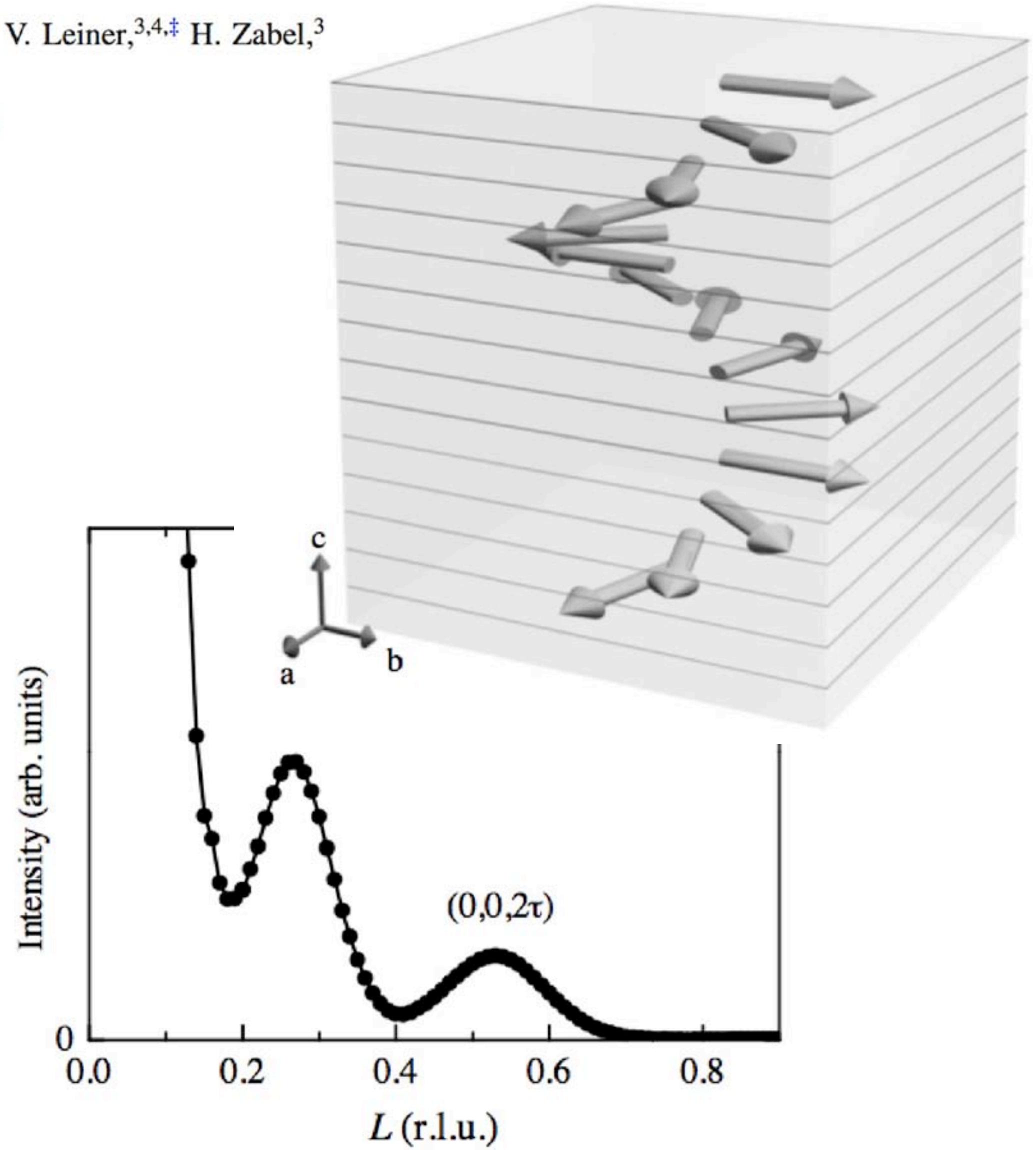
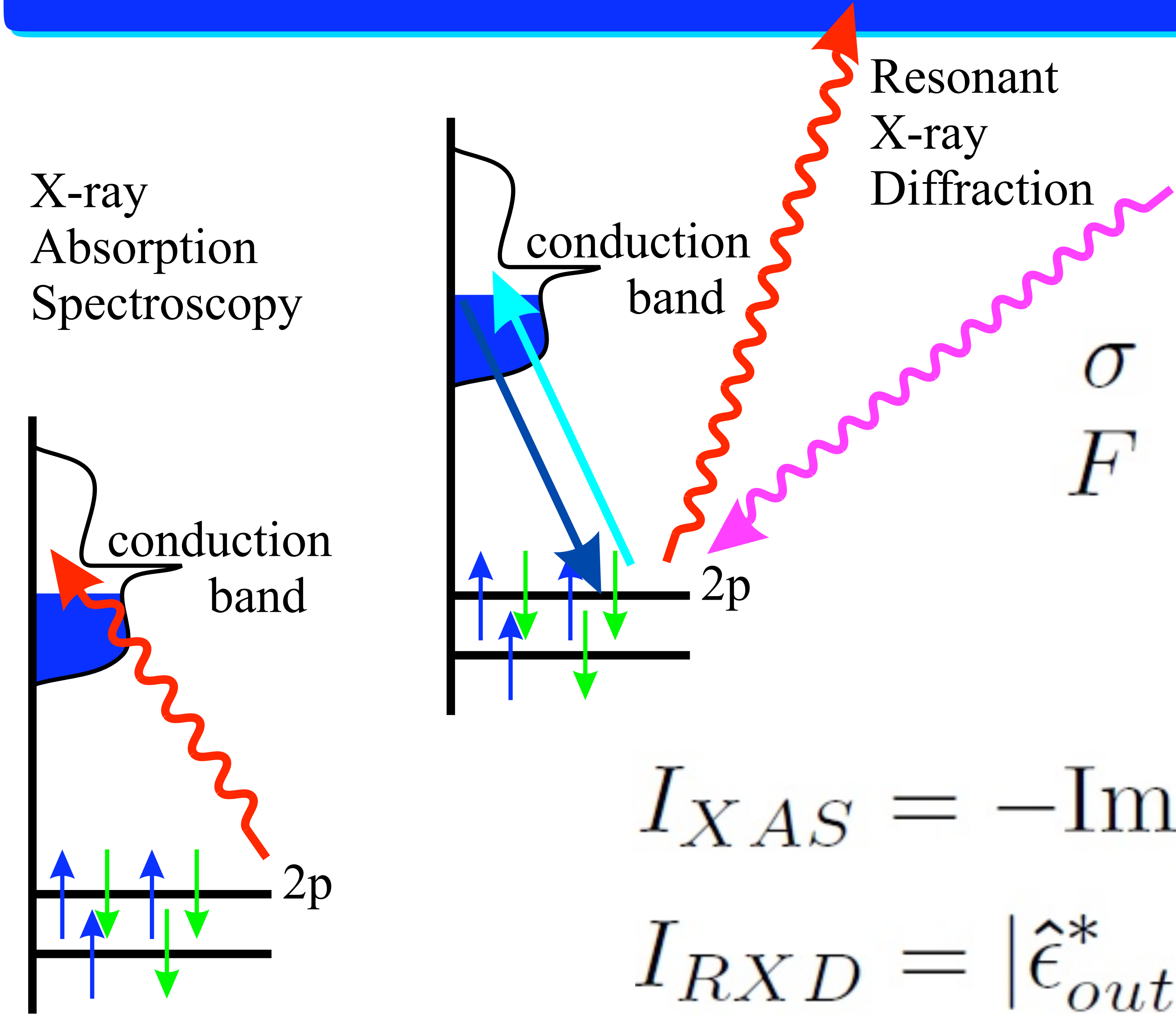




Relation between resonant x-ray diffraction and absorption



$$\sigma = \omega\chi$$
$$F = \omega\sigma$$

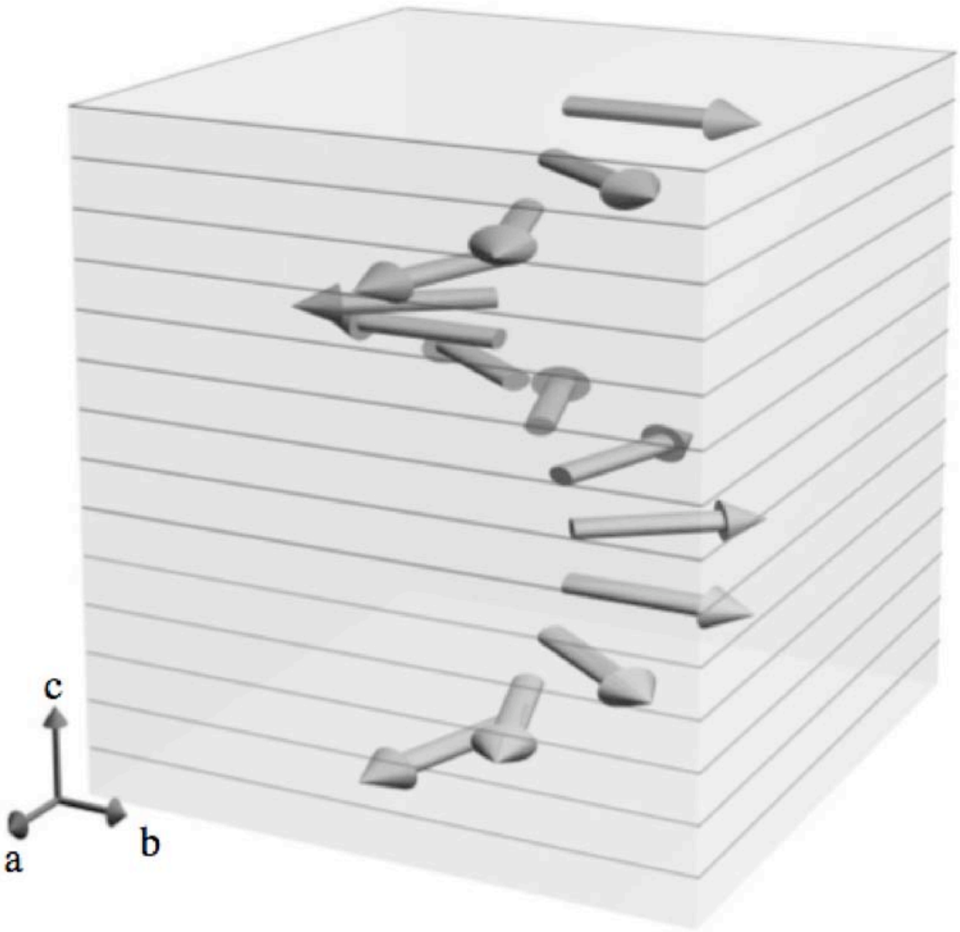
$$I_{XAS} = -\mathrm{Im}[\hat{\epsilon}^* \cdot \sigma \cdot \hat{\epsilon}]$$

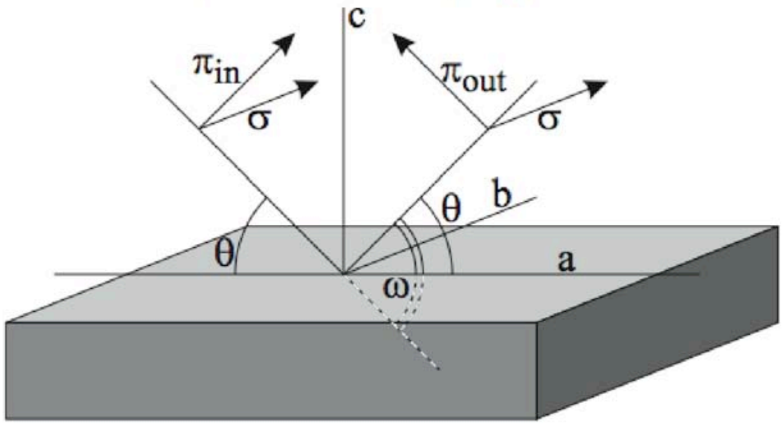
$$I_{RXD} = |\hat{\epsilon}^*_{out} \cdot F \cdot \hat{\epsilon}_{in}|^2$$

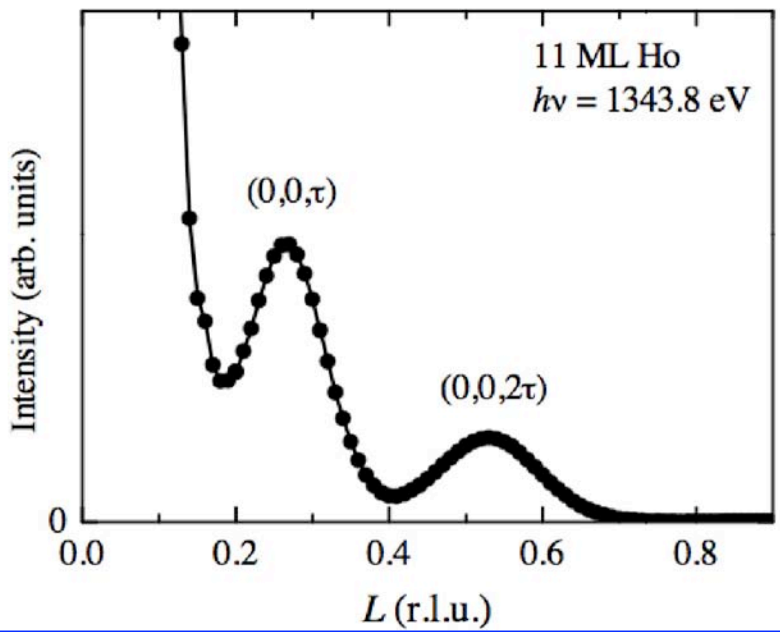
Example on Ho

Atomic multiplet calculation of $3d_{5/2} \rightarrow 4f$ resonant x-ray diffraction from Ho metal

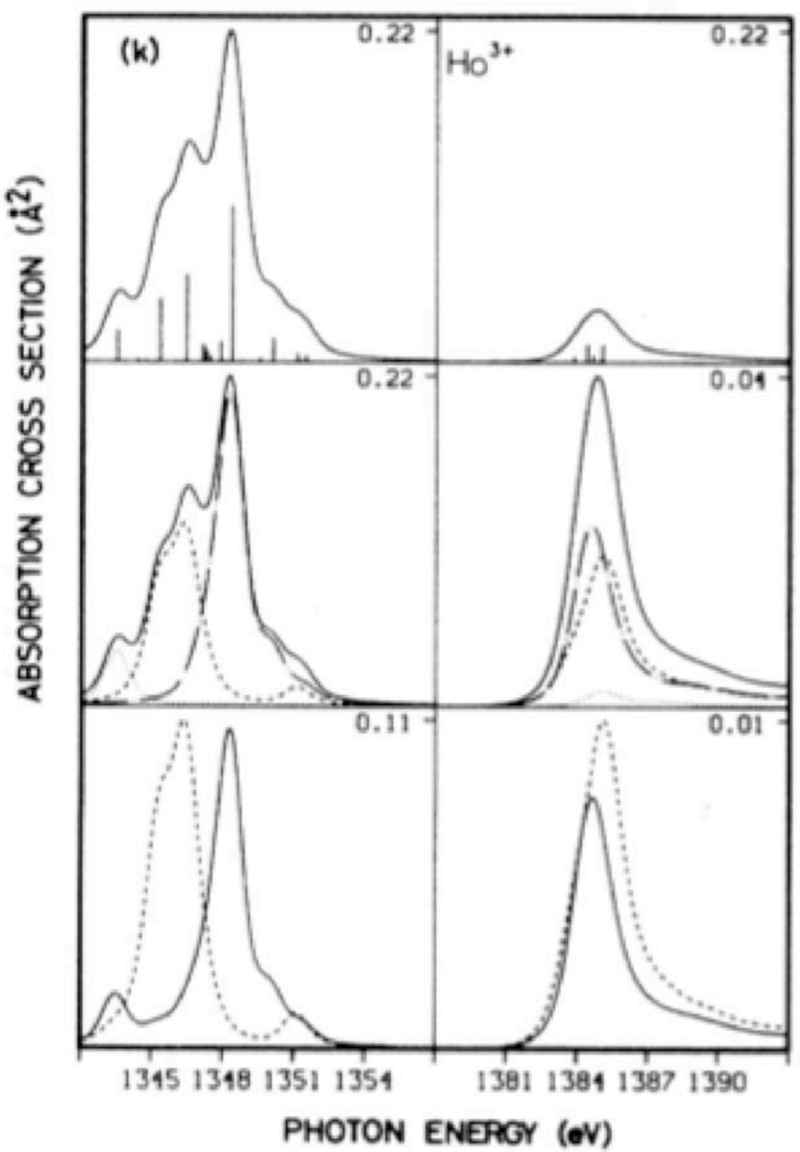
M. W. Haverkort,[1,2] C. Schüßler-Langeheine,[1] C. F. Chang,[1] M. Buchholz,[1]
H.-H. Wu,[1] H. Ott,[1] E. Schierle,[3] D. Schmitz,[3] A. Tanaka,[4] and L. H. Tjeng[1]







Fundamental spectra from the literature



PHYSICAL REVIEW B VOLUME 37, NUMBER 4 1 FEBRUARY 1988

Calculations of magnetic x-ray dichroism in the 3*d* absorption spectra of rare-earth compounds

J. B. Goedkoop
Research Institute of Materials, Faculty of Science, University of Nijmegen, Toernooiveld, 6525 ED Nijmegen, The Netherlands

B. T. Thole, G. van der Laan, and G. A. Sawatzky
Department of Applied and Solid State Physics, Materials Science Center, University of Groningen, Nijenborgh 18, 9747 AG Groningen, The Netherlands

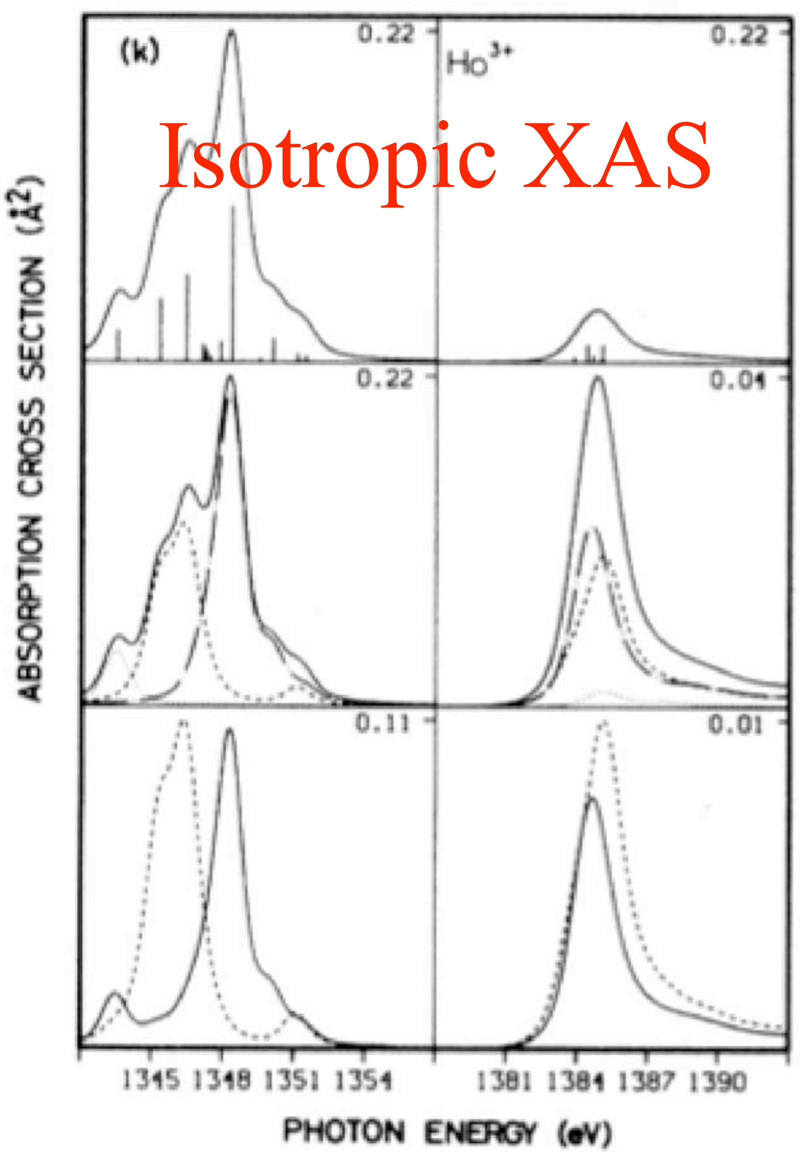
F. M. F. de Groot and J. C. Fuggle
Research Institute of Materials, Faculty of Science, University of Nijmegen, Toernooiveld, 6525 ED Nijmegen, The Netherlands

(Received 13 April 1987)

Plotted is -Im[σ]

top: $\sigma^{(0)}$
middle $\sigma^{(1)}$ (difference between the two spectra)
bottom $\sigma^{(2)}$ (difference between the two spectra)

Fundamental spectra from the literature



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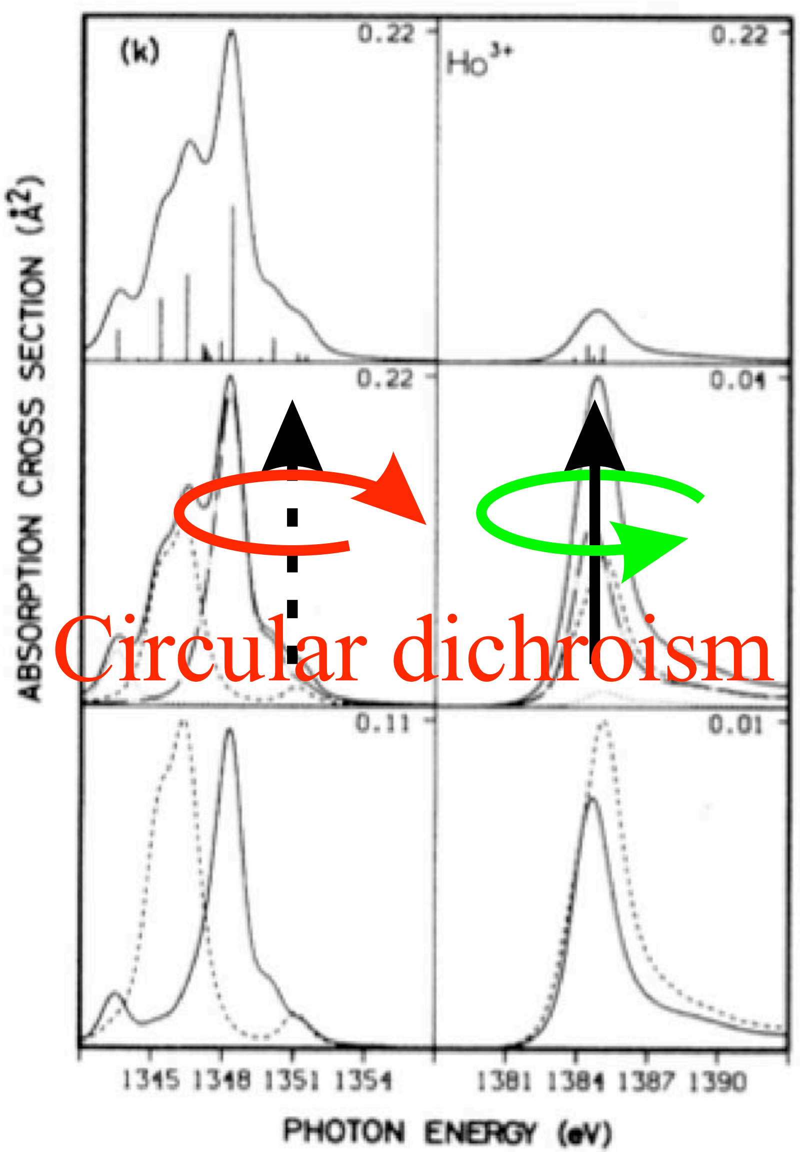

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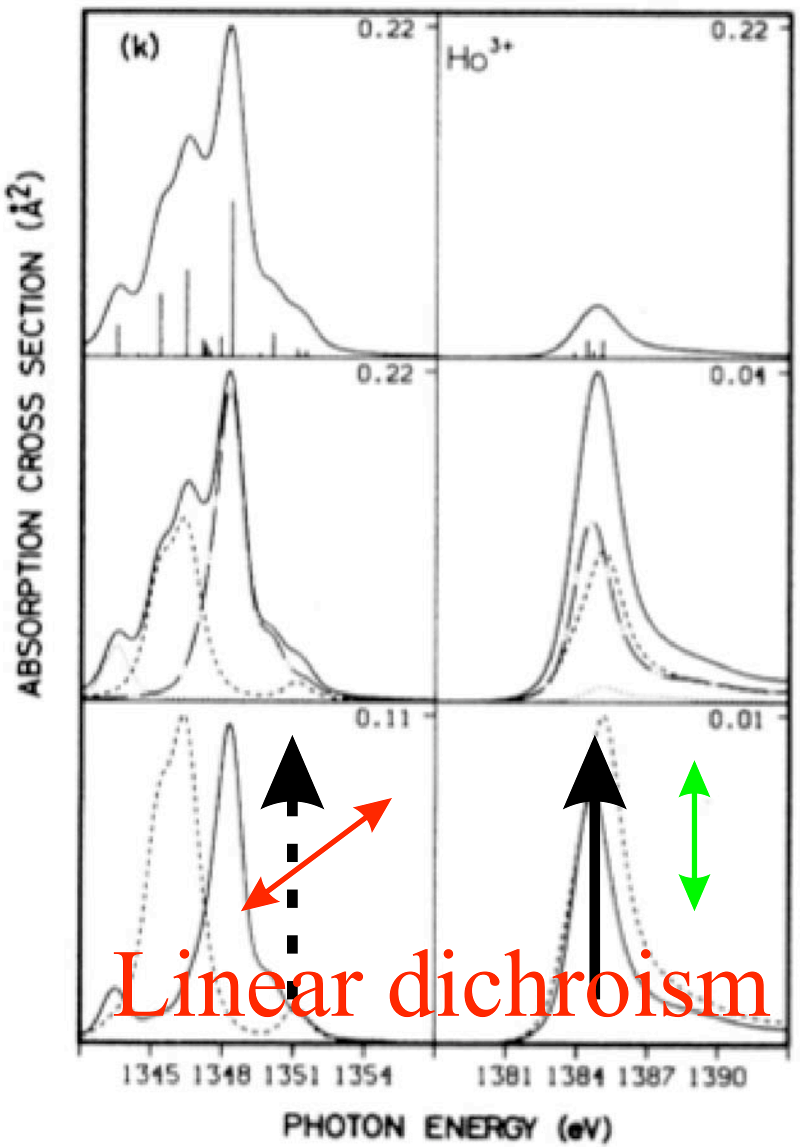
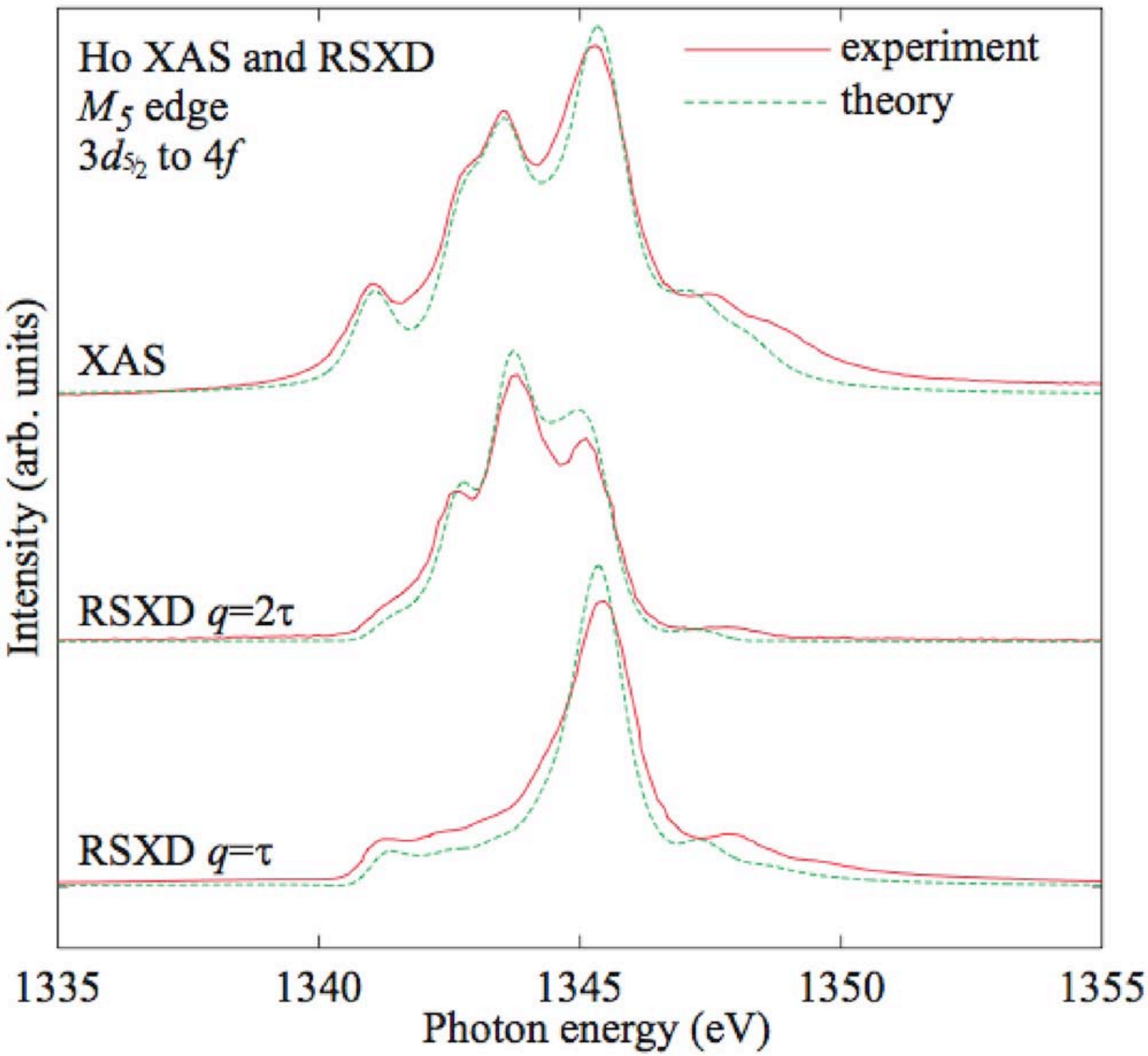


Plotted is -Im[σ]

top: $\sigma^{(0)}$
middle $\sigma^{(1)}$ (difference between the two spectra)
bottom $\sigma^{(2)}$ (difference between the two spectra)

Example on Ho: Elastic diffraction



top: $-\mathrm{Im}[\sigma^{(0)}]$

middle $|\omega\ \sigma^{(2)}|^2$

bottom $|\omega\ \sigma^{(1)}|^2$

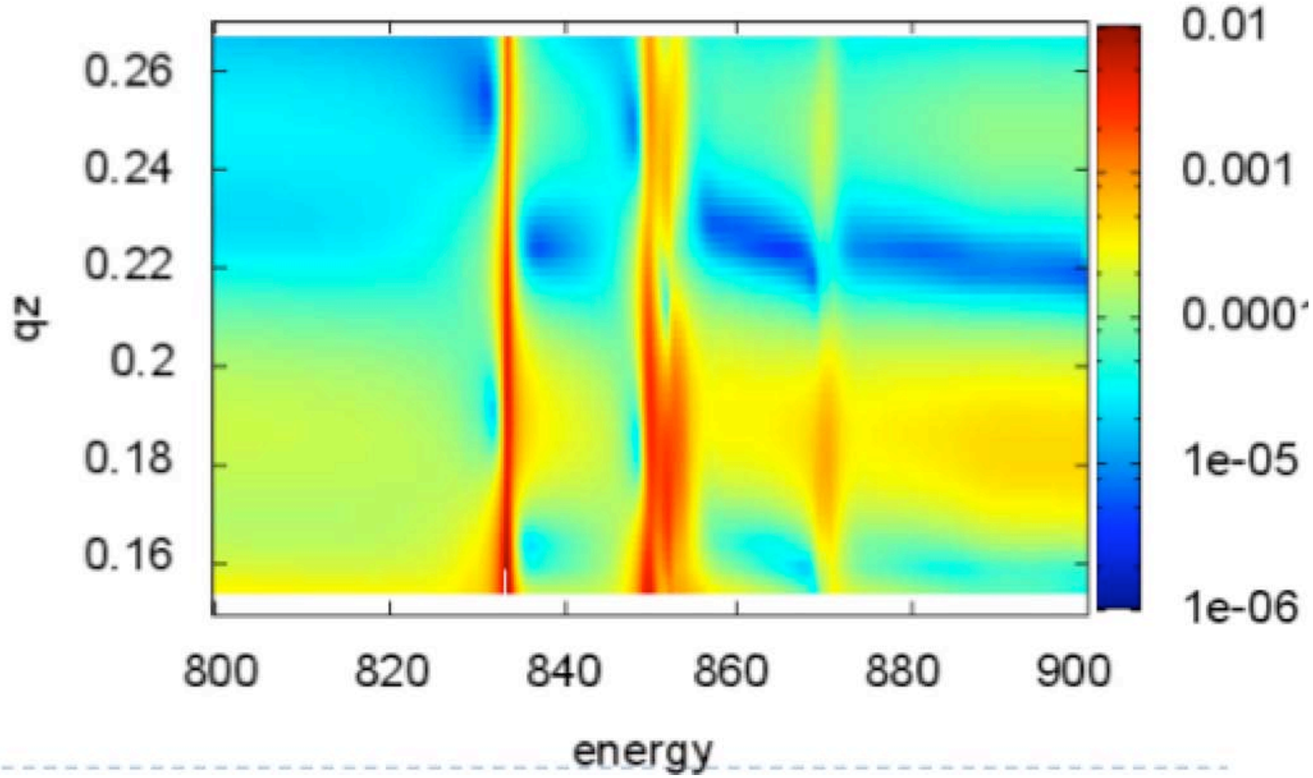
Can we use sum-rules to get quantitative information?

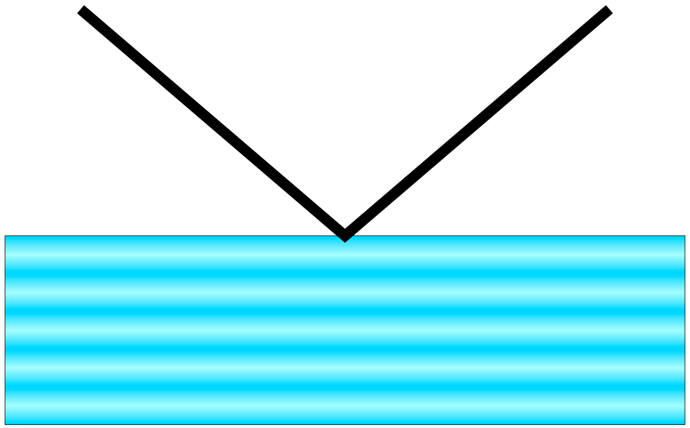
- Measure intensity for different ***q*** and polarizations
- Find F_q from the measured values of $|F_q|^2$
- Use that $F_i = \omega\,\sigma_i$

$$\int_K \sigma = i\,\overline{\rho}_p$$

Can we use sum-rules to get quantitative information?

- Yes, but one needs to include dynamical scattering effects





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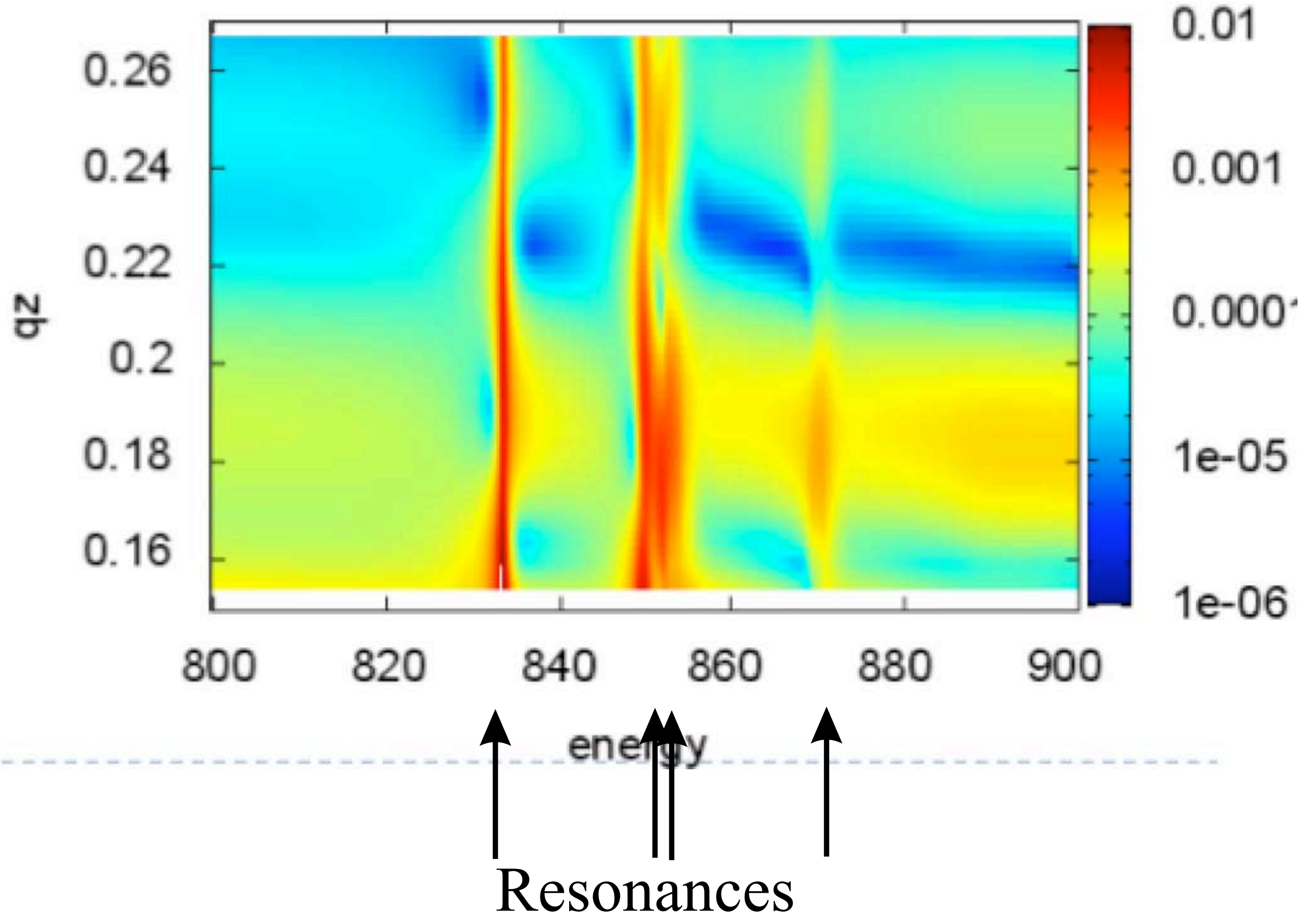

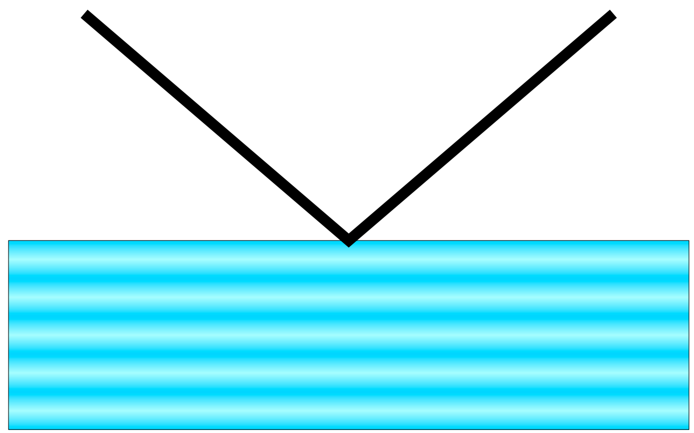

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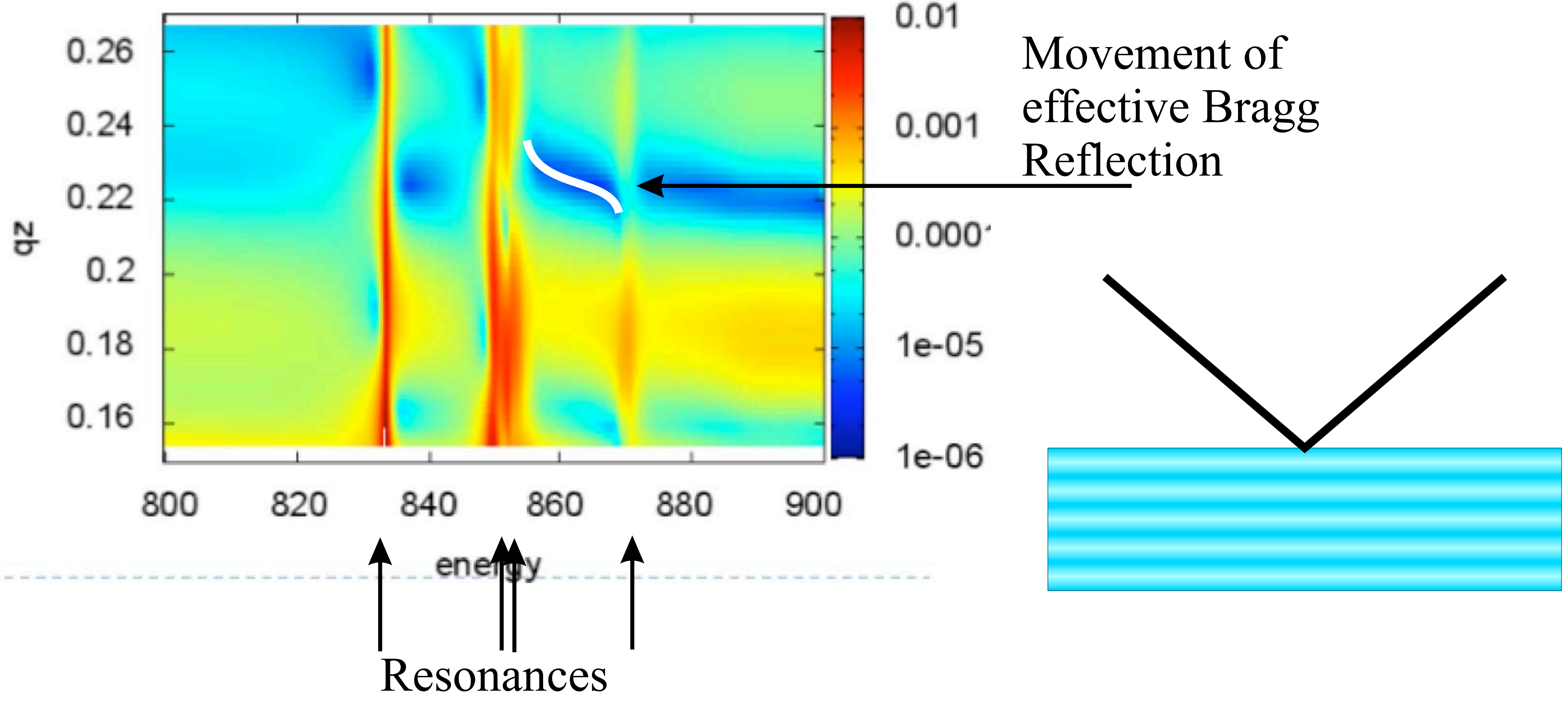

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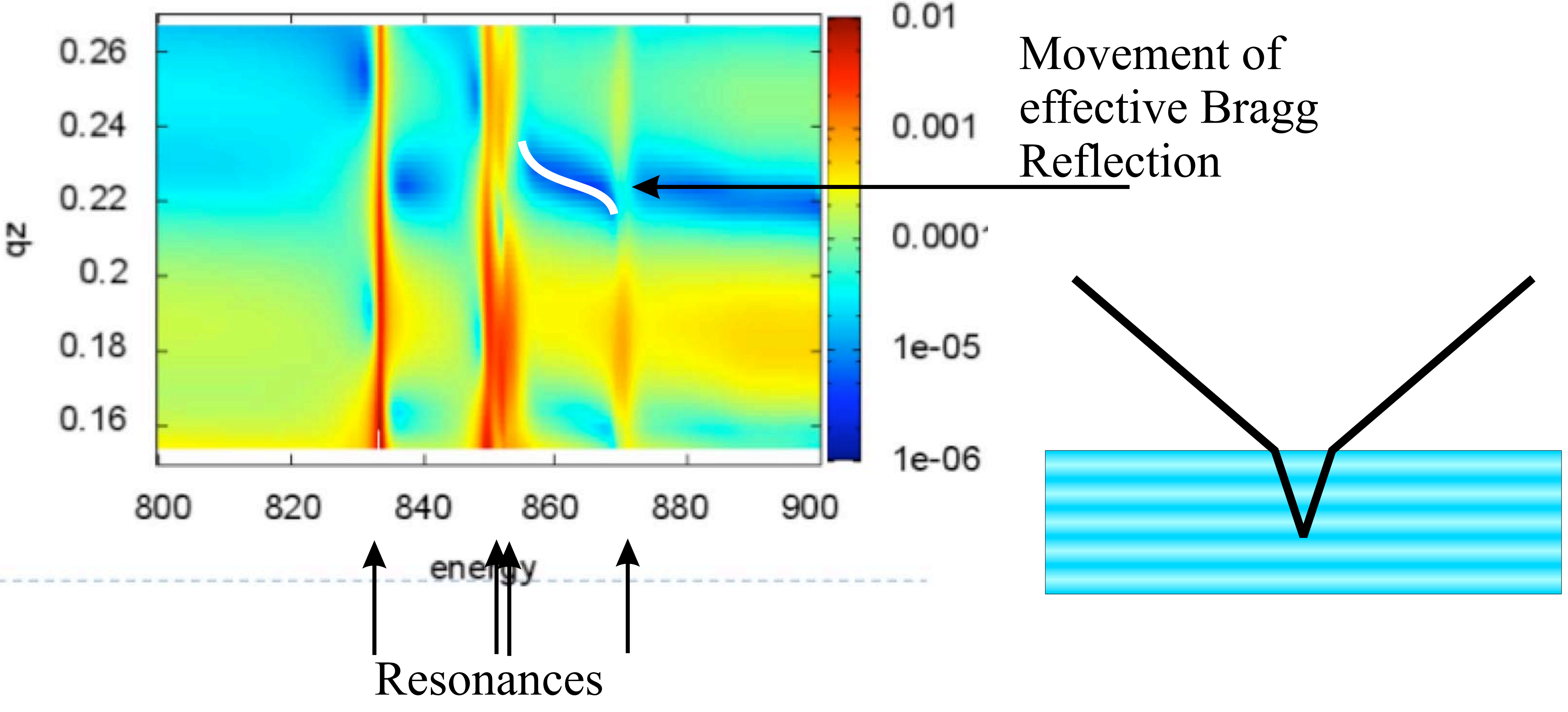


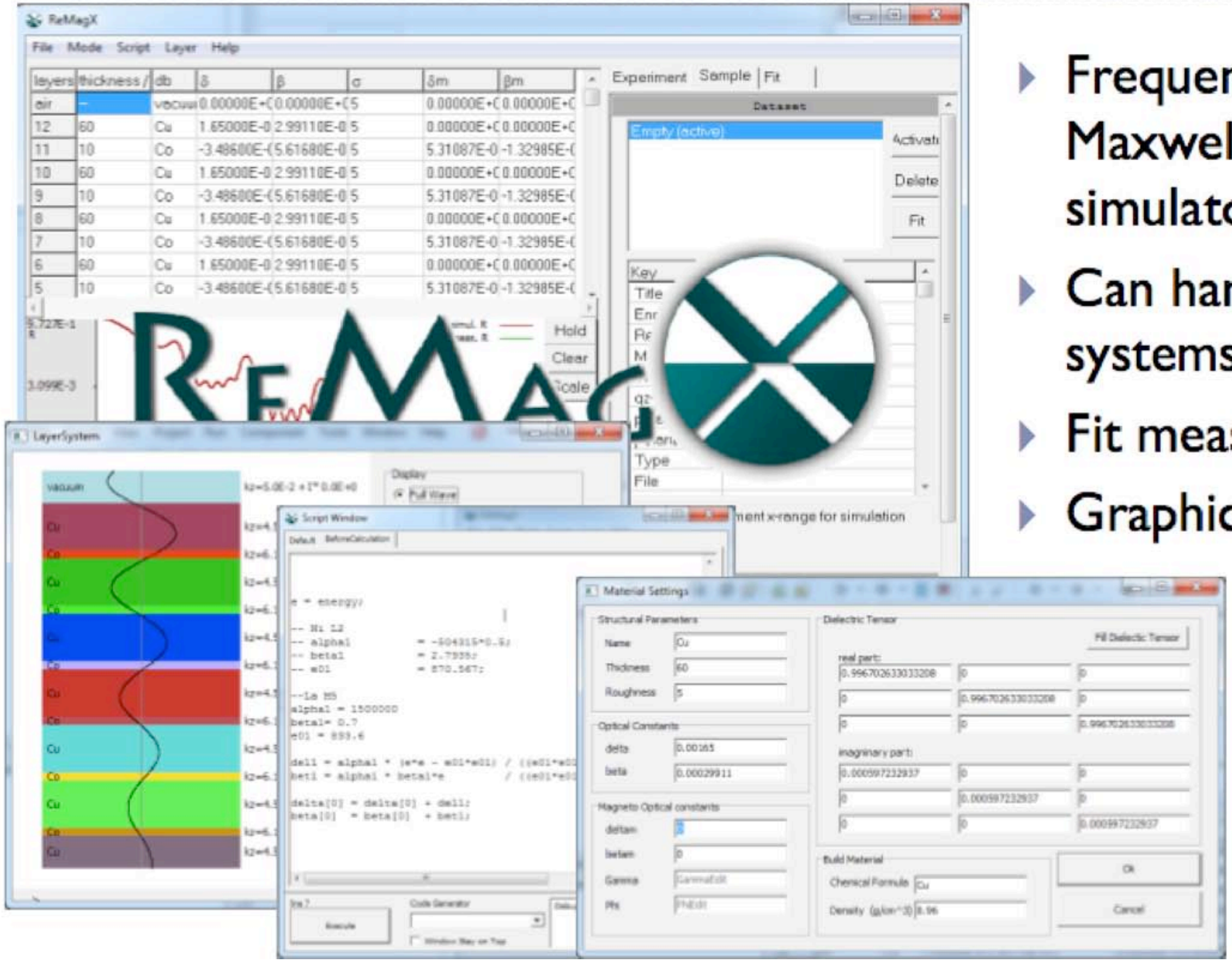
Can we use sum-rules to get quantitative information?

- Measure intensity for different ***q*** and polarizations
- Starting from $|F_q|^2$ reversely solve Maxwell equations to obtain F_i
- Use that $F_i = \omega\, \sigma_i$

$$\int_K \sigma = i\, \overline{\rho_p}$$

Solve Maxwell equations (with side conditions)

Analysis tool ReMagX



- Frequency-domain Maxwell-equation simulator
- Can handle dichroic systems
- Fit measurements
- Graphical user interface

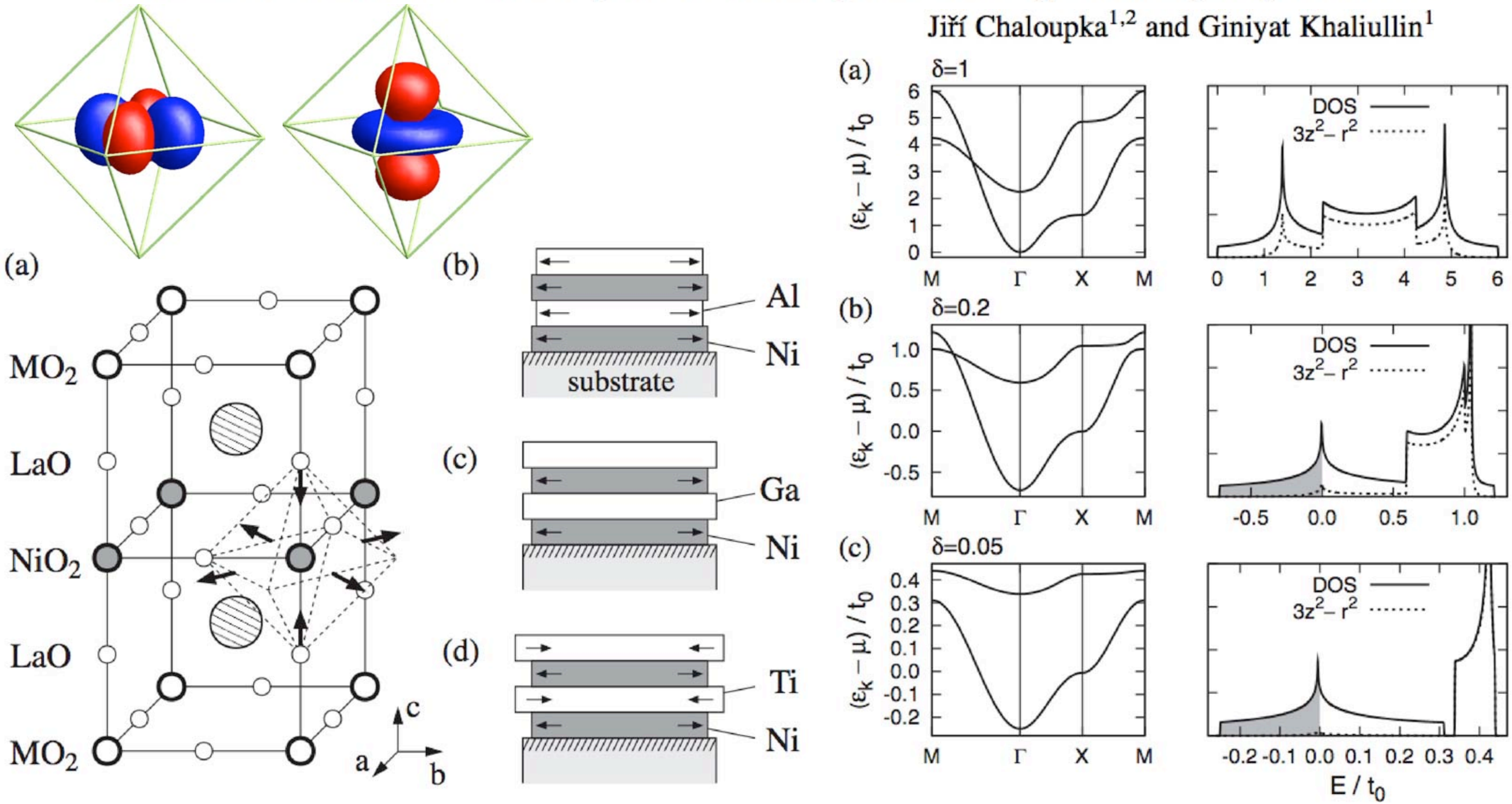
Developed at MPI Stuttgart
and now at UBC
by S. Macke

Creating a High-Tc Cuprate like fermi-surface in Nickelates

PRL **100**, 016404 (2008) PHYSICAL REVIEW LETTERS week ending 11 JANUARY 2008

Orbital Order and Possible Superconductivity in $LaNiO_3/LaMO_3$ Superlattices

Jiří Chaloupka[1,2] and Giniyat Khaliullin[1]

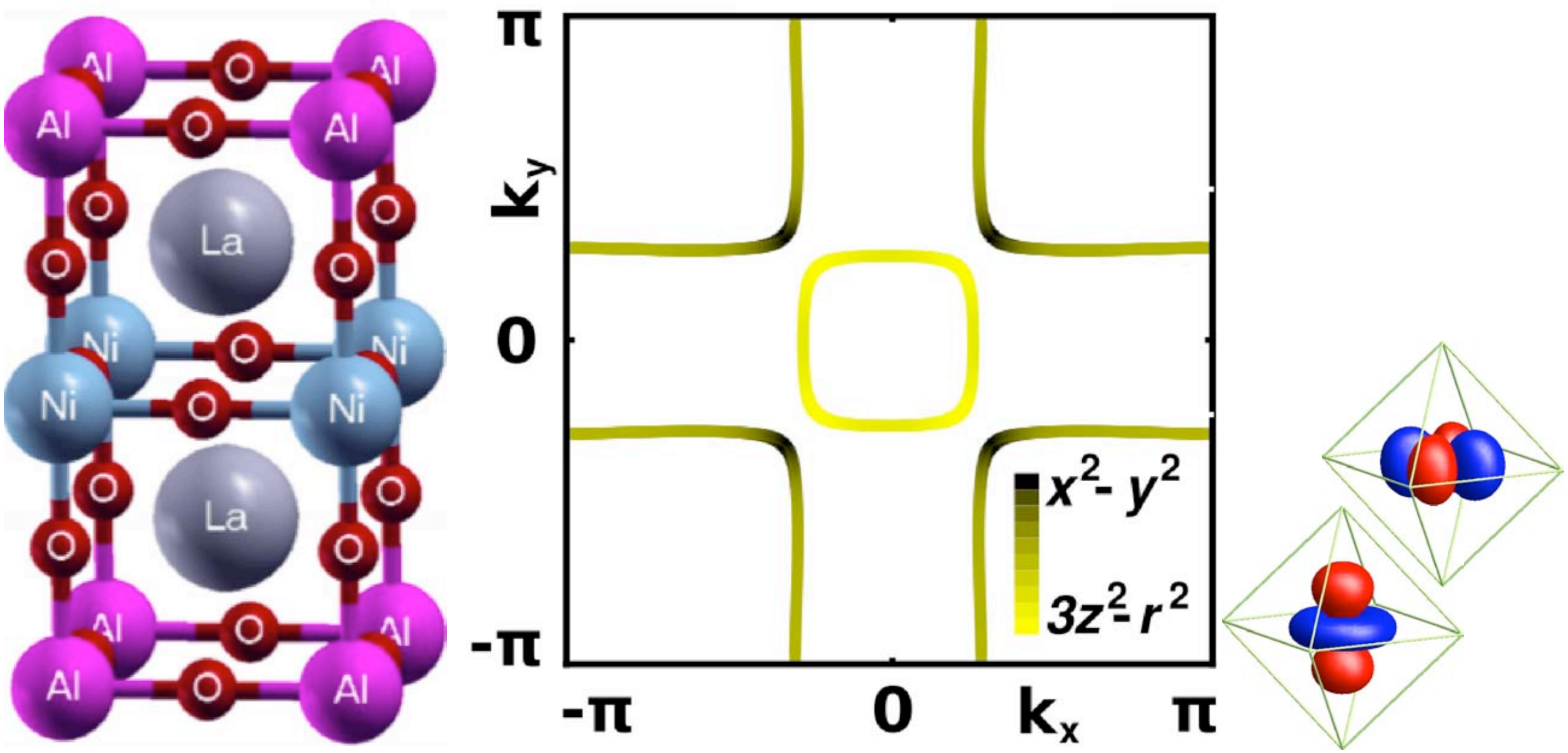


Creating a High-Tc Cuprate like fermi-surface in Nickelates

PRL **103,** 016401 (2009) PHYSICAL REVIEW LETTERS week ending 3 JULY 2009

Turning a Nickelate Fermi Surface into a Cupratelike One through Heterostructuring

P. Hansmann,[1,2] Xiaoping Yang,[1] A. Toschi,[1,2] G. Khaliullin,[1] O. K. Andersen,[1] and K. Held[2]
[1]*Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany*
[2]*Institute for Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria*



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PRL 103, 016401 (2009) PHYSICAL REVIEW LETTERS week ending 3 JULY 2009

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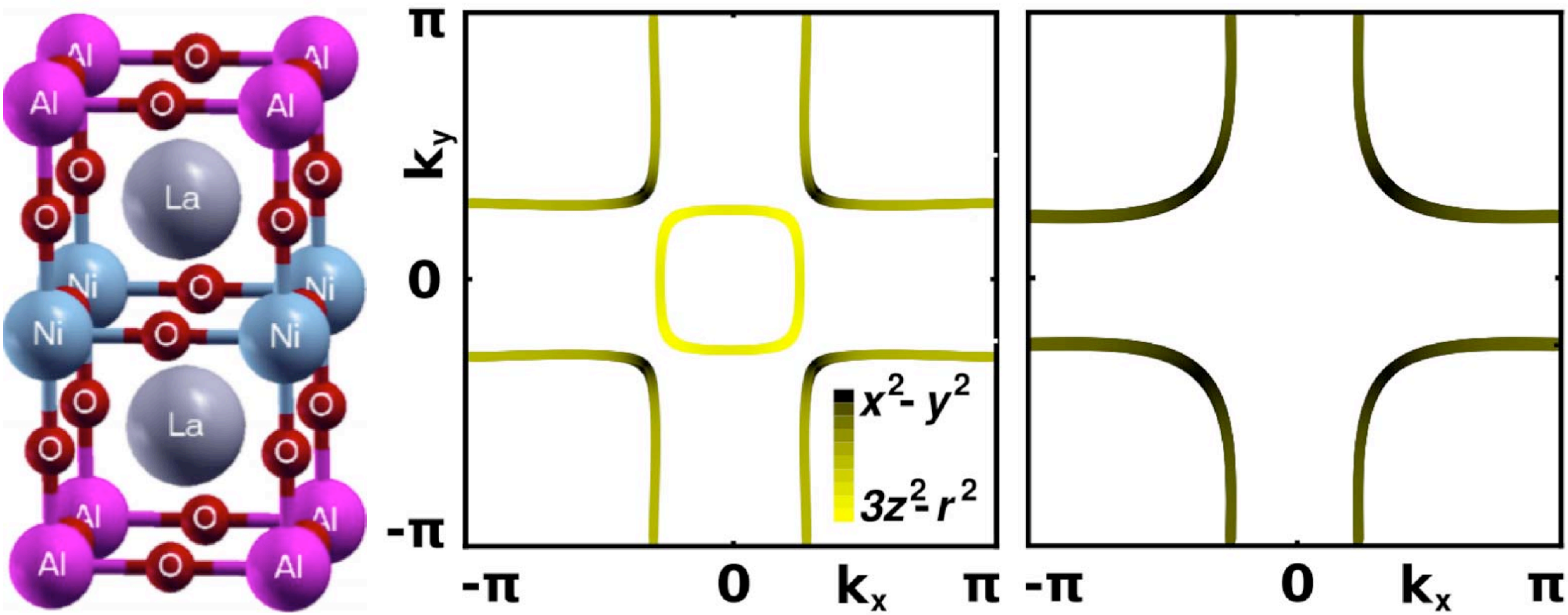


Do we have an orbitally polarized Ni Film

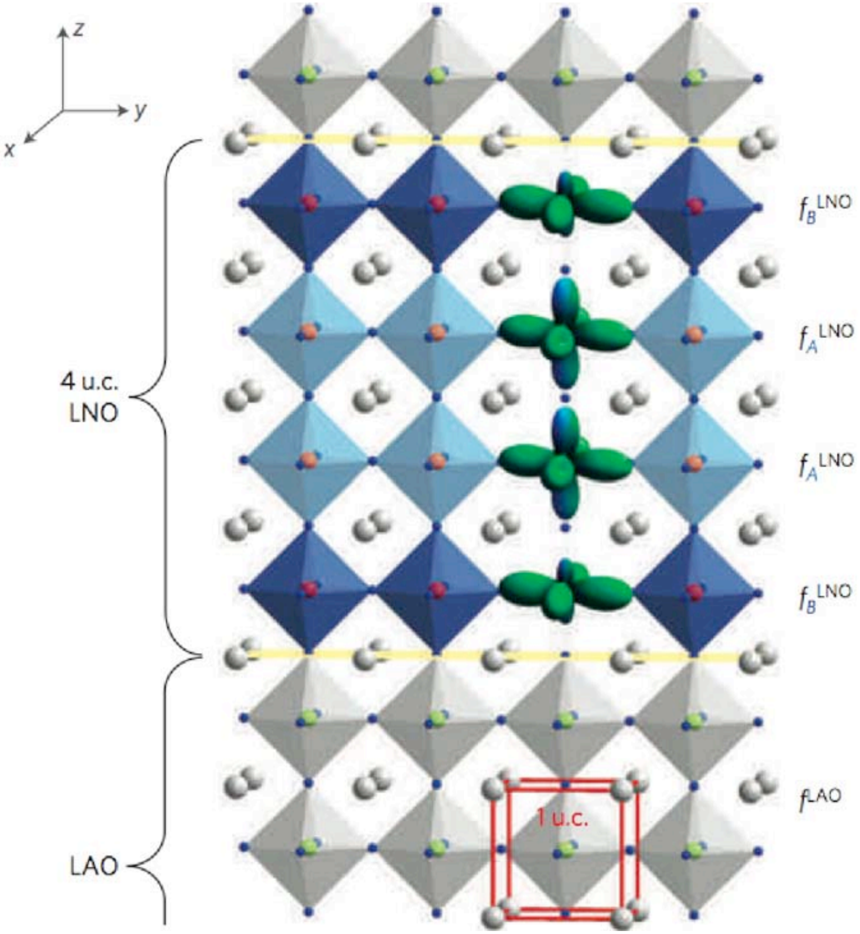
nature materials

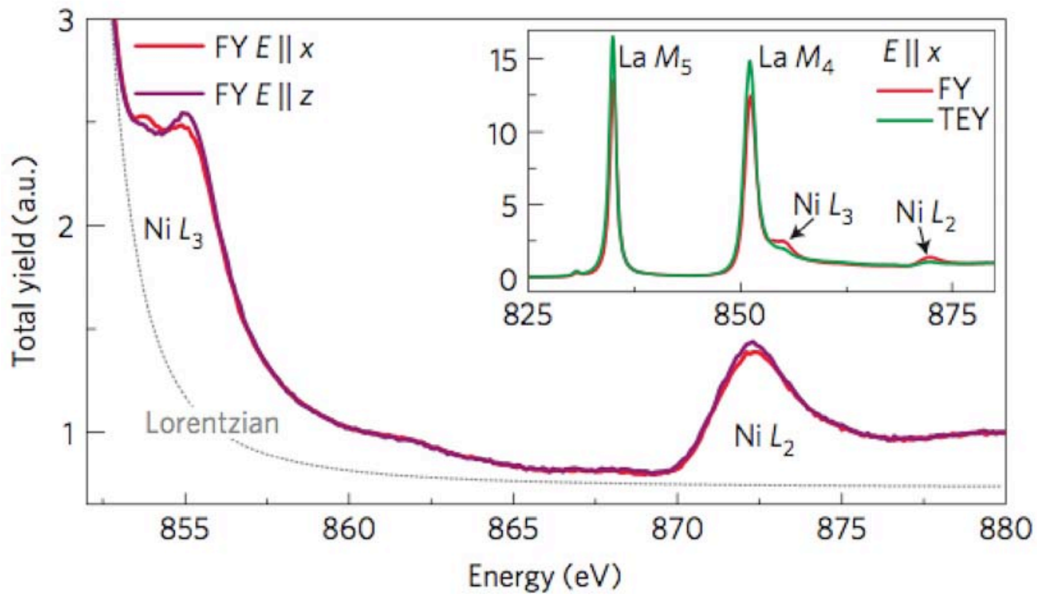
LETTERS

PUBLISHED ONLINE: 6 FEBRUARY 2011 | DOI: 10.1038/NMAT2958

Orbital reflectometry of oxide heterostructures

Eva Benckiser[1], Maurits W. Haverkort[1], Sebastian Brück[2,3], Eberhard Goering[2], Sebastian Macke[2], Alex Frañó[1], Xiaoping Yang[1,4], Ole K. Andersen[1], Georg Cristiani[1], Hanns-Ulrich Habermeier[1], Alexander V. Boris[1], Ioannis Zegkinoglou[1], Peter Wochner[2], Heon-Jung Kim[1,5], Vladimir Hinkov[1]* and Bernhard Keimer[1]*





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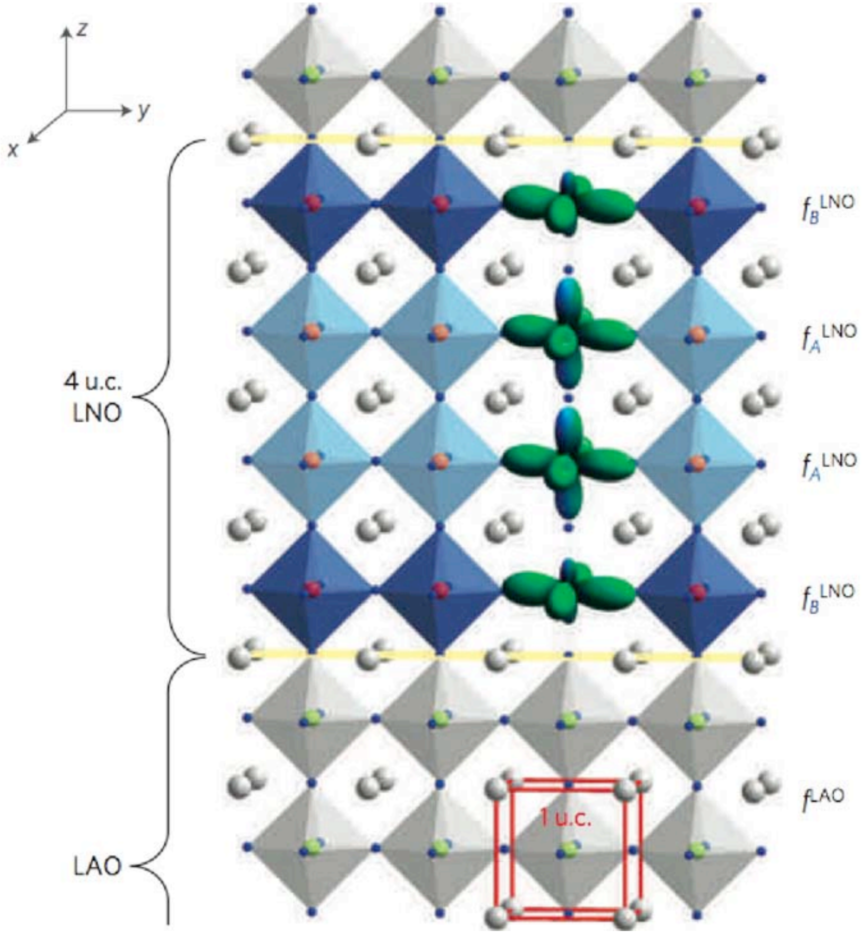

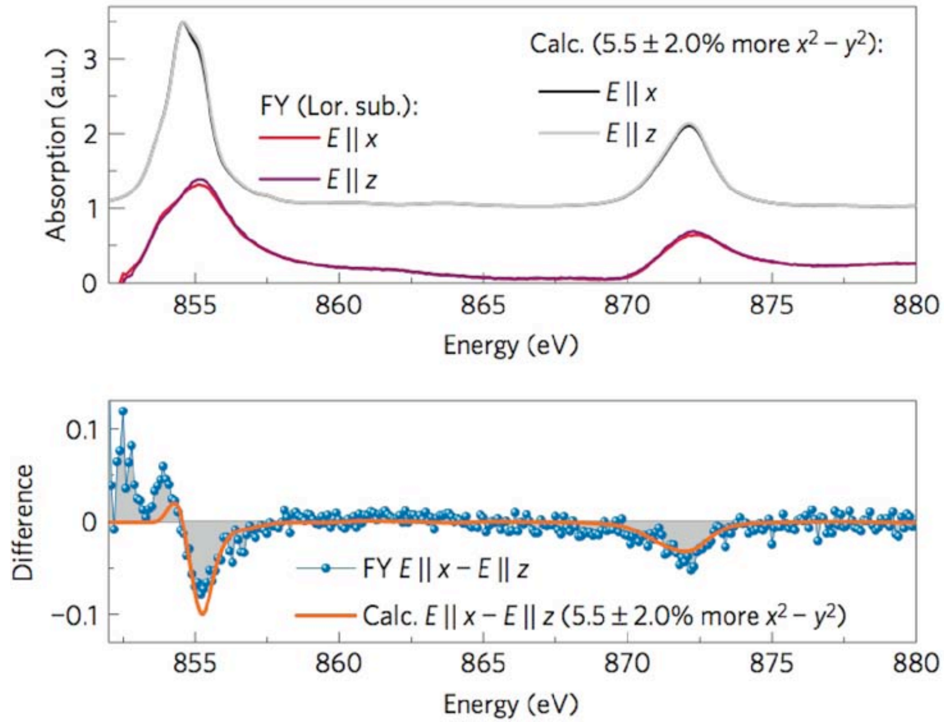

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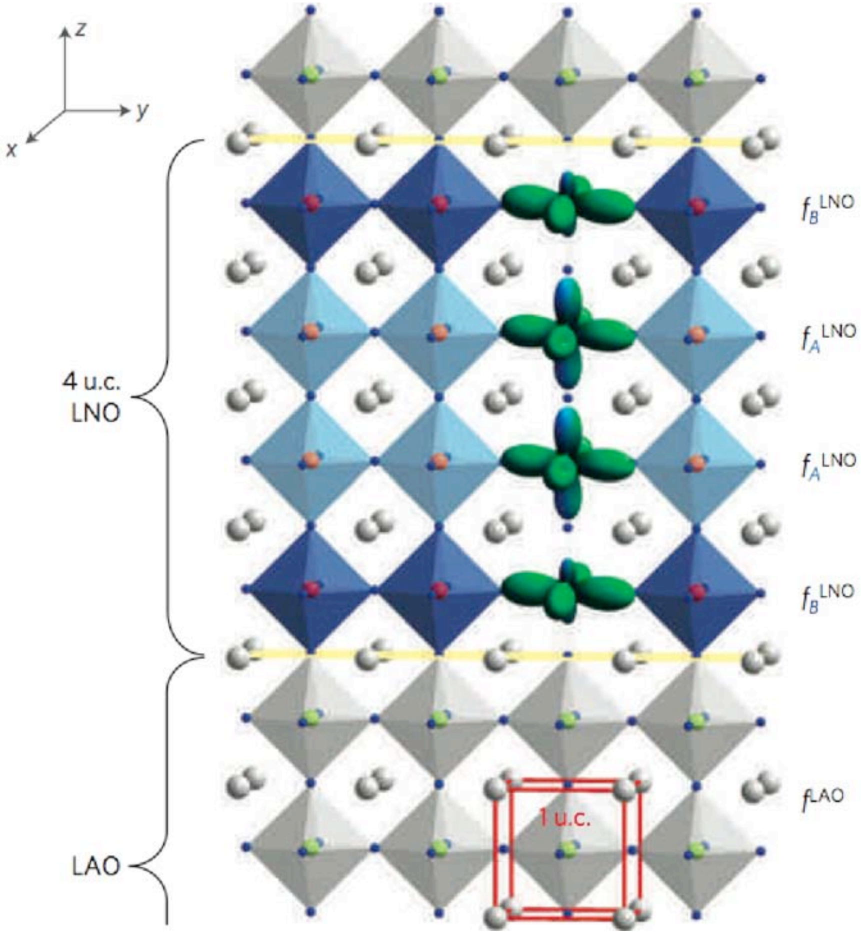
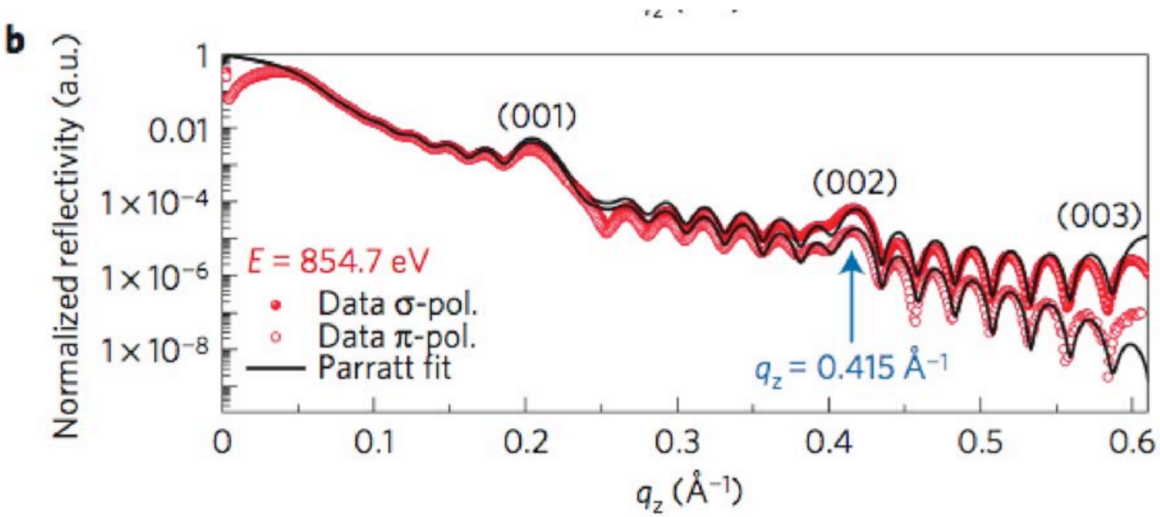




Do we have an orbitally polarized Ni Film

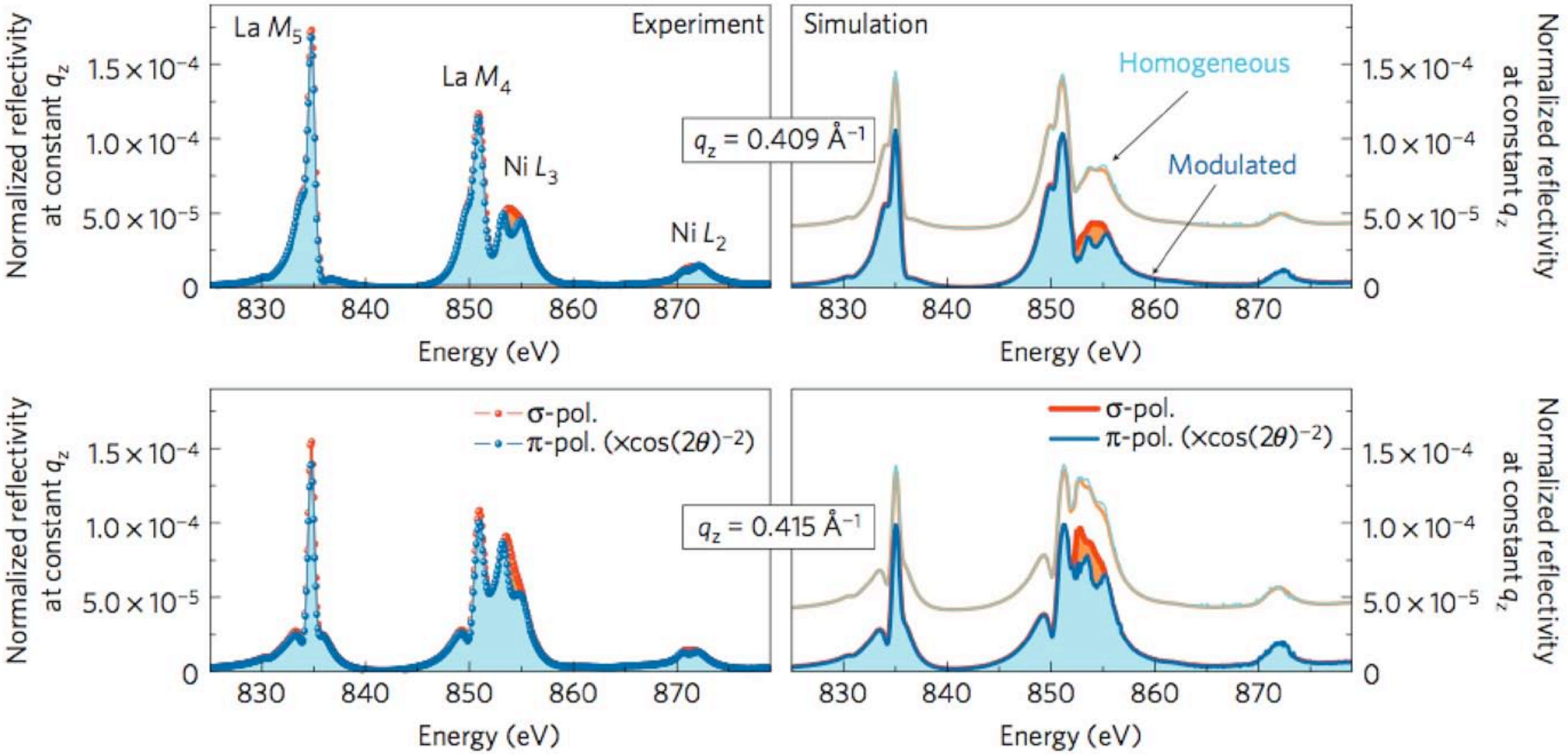
nature materials

LETTERS

PUBLISHED ONLINE: 6 FEBRUARY 2011 | DOI: 10.1038/NMAT2958

Orbital reflectometry of oxide heterostructures

Eva Benckiser[1], Maurits W. Haverkort[1], Sebastian Brück[2,3], Eberhard Goering[2], Sebastian Macke[2], Alex Frañó[1], Xiaoping Yang[1,4], Ole K. Andersen[1], Georg Cristiani[1], Hanns-Ulrich Habermeier[1], Alexander V. Boris[1], Ioannis Zegkinoglou[1], Peter Wochner[2], Heon-Jung Kim[1,5], Vladimir Hinkov[1]* and Bernhard Keimer[1]*



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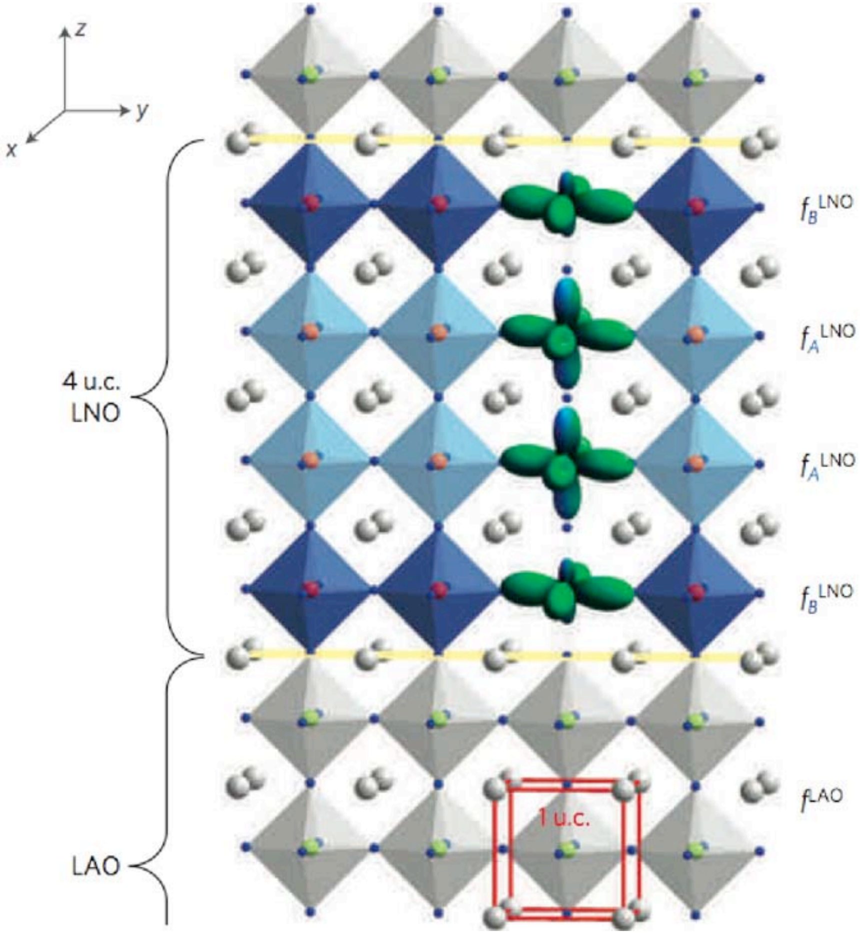

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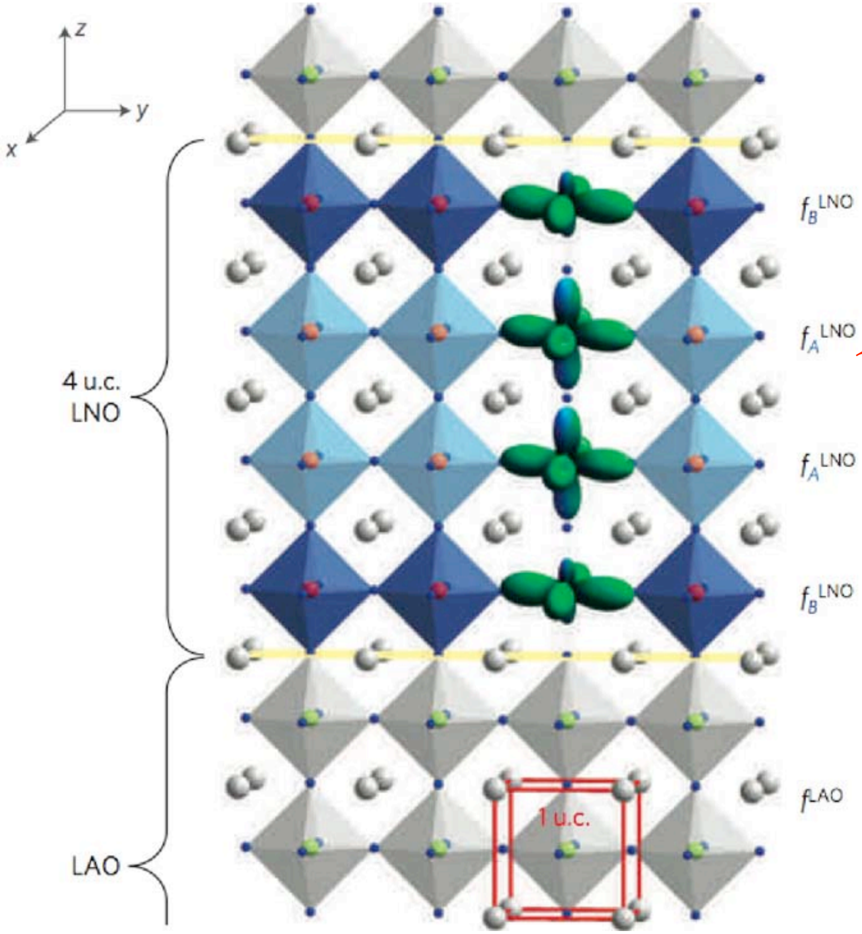
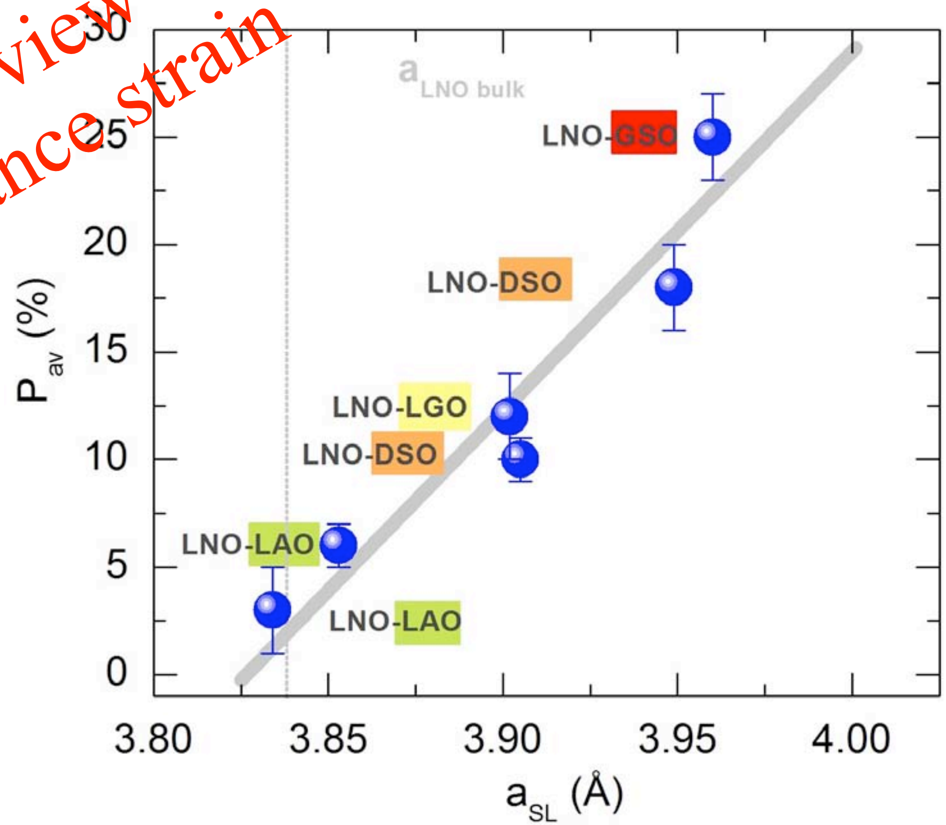
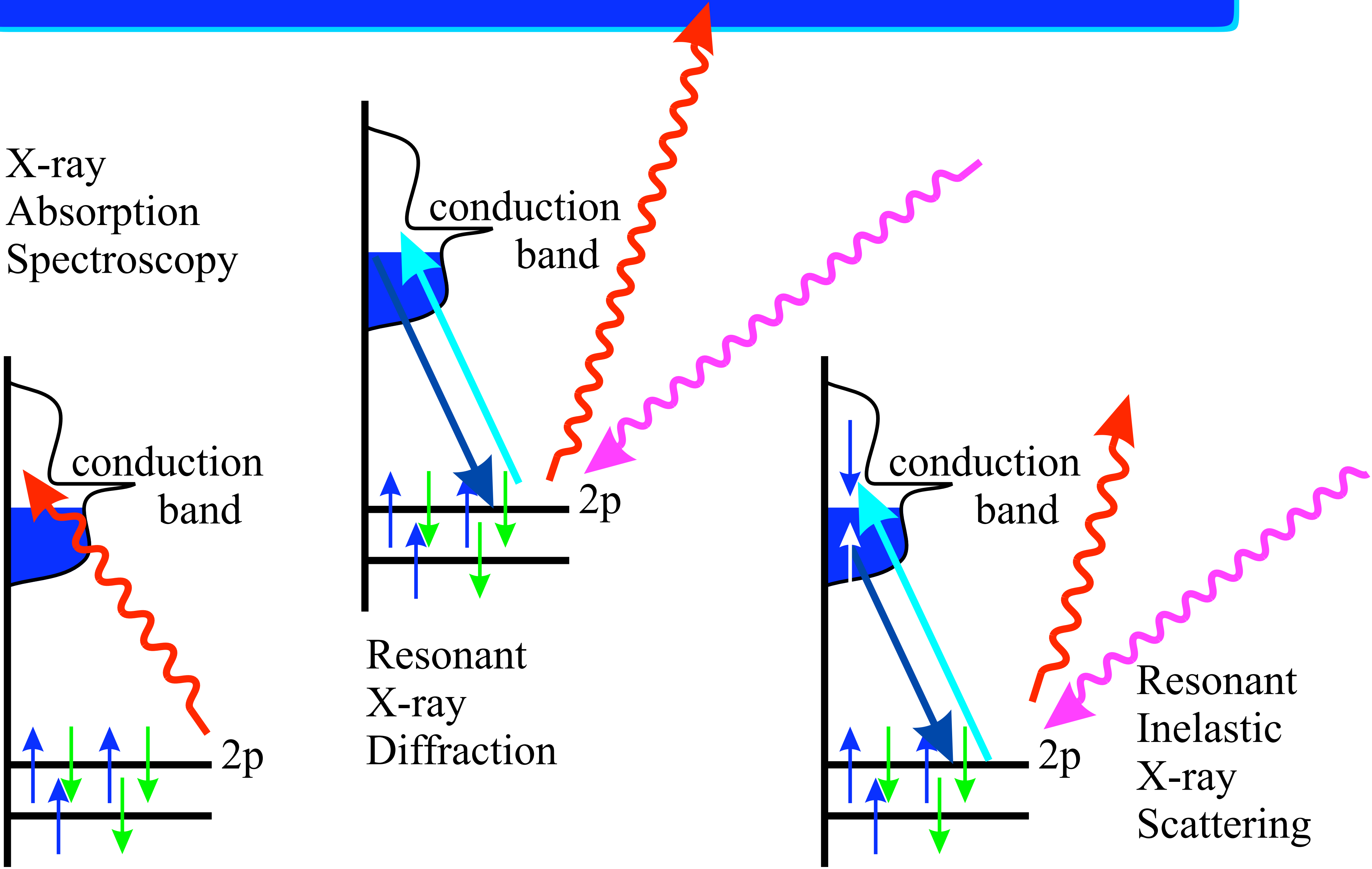


preview
Enhance strain



Theory of XAS, RXD, and **RIXS**



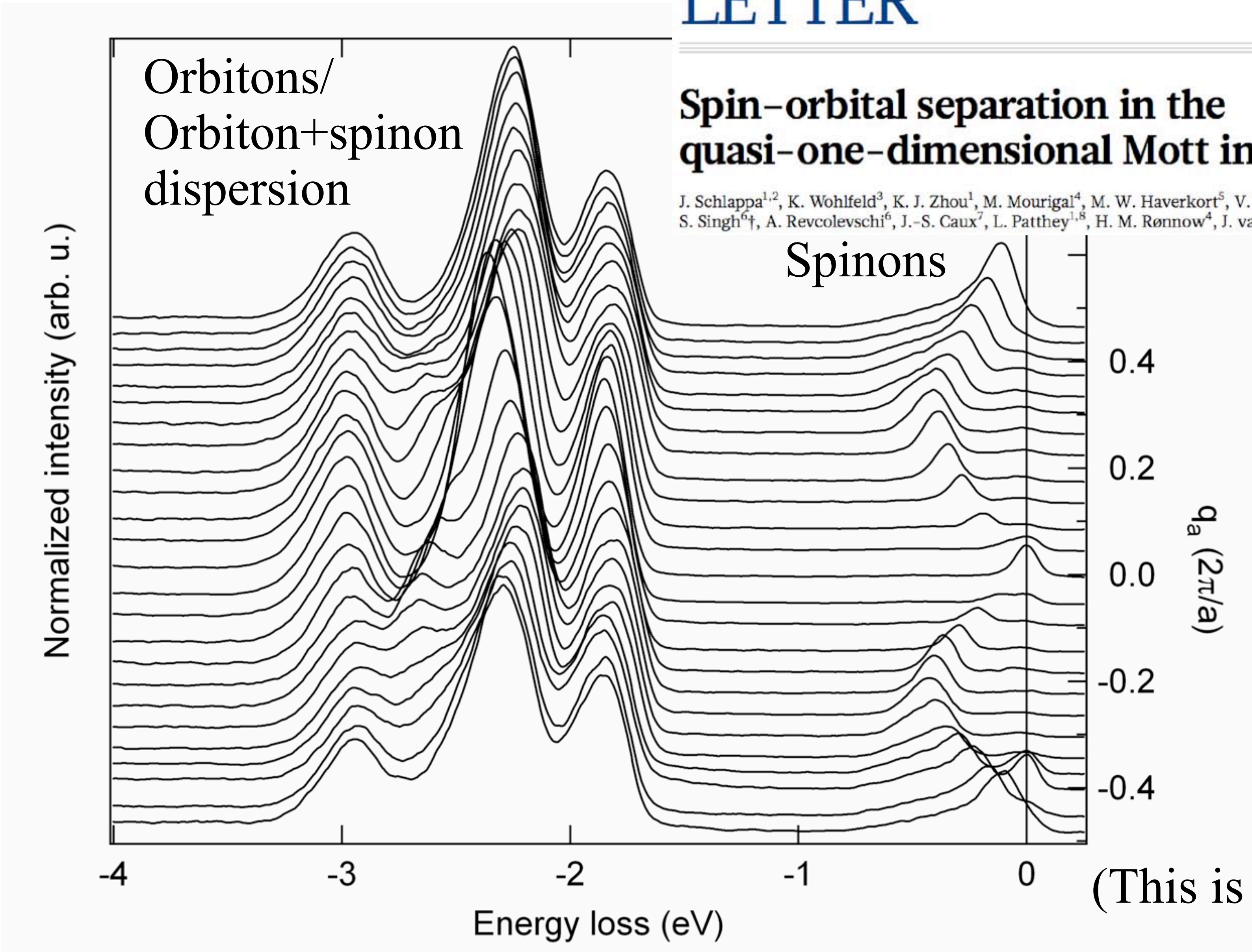
RIXS: Spin and Orbital (dispersing) excitations

LETTER

doi:10.1038/nature10974

Spin–orbital separation in the quasi-one-dimensional Mott insulator Sr_2CuO_3

J. Schlappa[1,2], K. Wohlfeld[3], K. J. Zhou[1], M. Mourigal[4], M. W. Haverkort[5], V. N. Strocov[1], L. Hozoi[3], C. Monney[1], S. Nishimoto[3], S. Singh[6]†, A. Revcolevschi[6], J.-S. Caux[7], L. Patthey[1,8], H. M. Rønnow[4], J. van den Brink[3] & T. Schmitt[1]

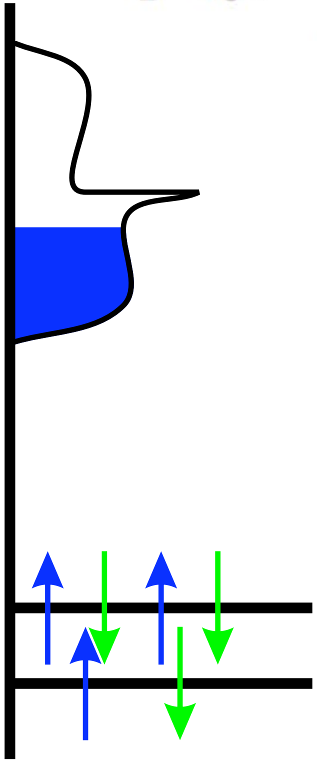


(This is raw data!!)

Spin excitations with resonant x-rays: Theory

- Interaction of Neutrons with matter is easy (magnetic dipole) but for resonant x-ray scattering nothing is obvious.
  A lot is known though...

$$\frac{\delta^2\sigma}{\delta\Omega\delta\omega} \propto \lim_{\Gamma\to 0^+} \sum_f \left| \langle f | T^\dagger_{\varepsilon_o} \frac{1}{\omega_i + E_i + \imath\Gamma/2 - H} T_{\varepsilon_i} | i \rangle \right|^2 \delta(\omega_i - \omega_o + E_i - E_f)$$



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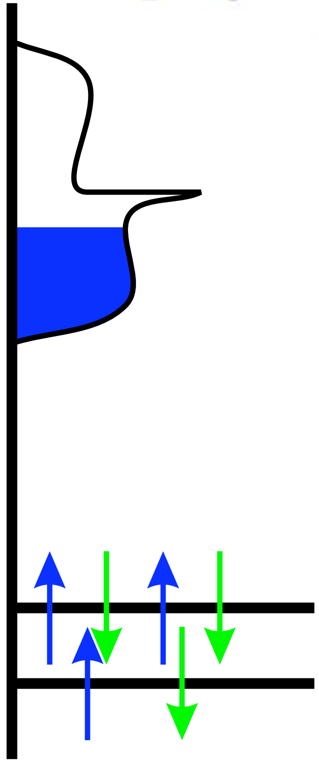

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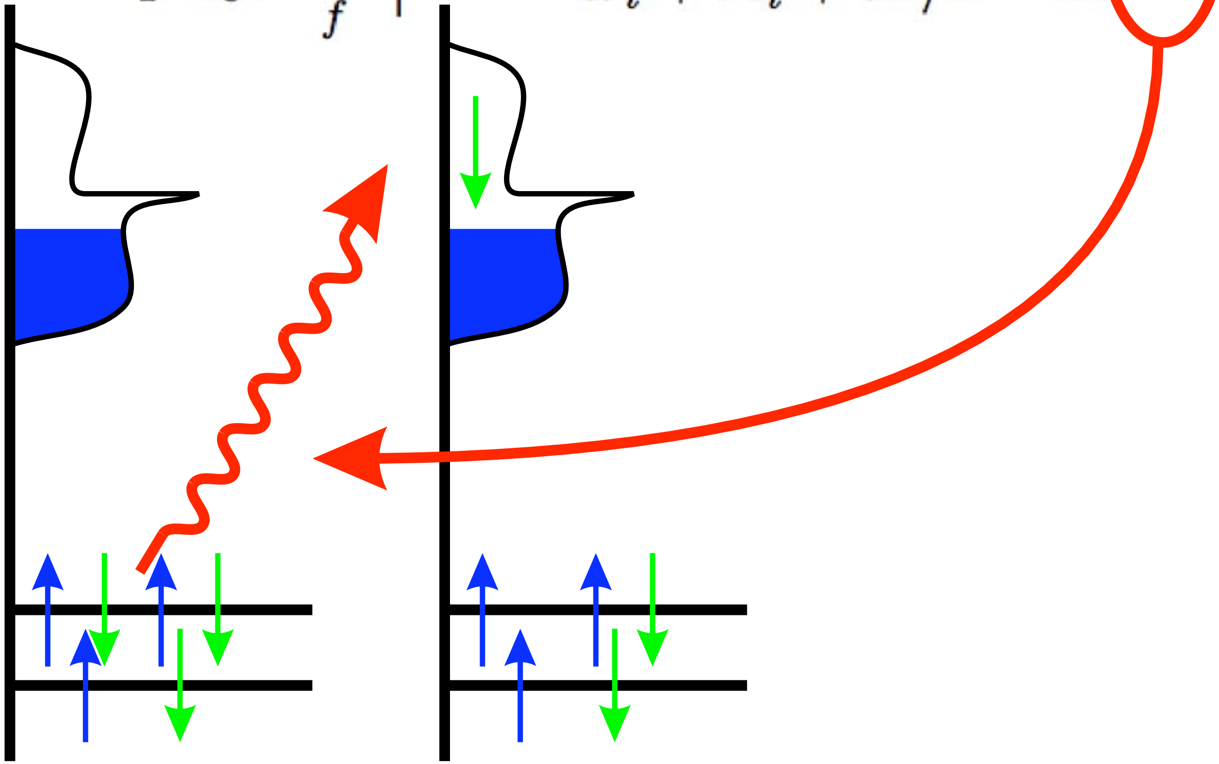

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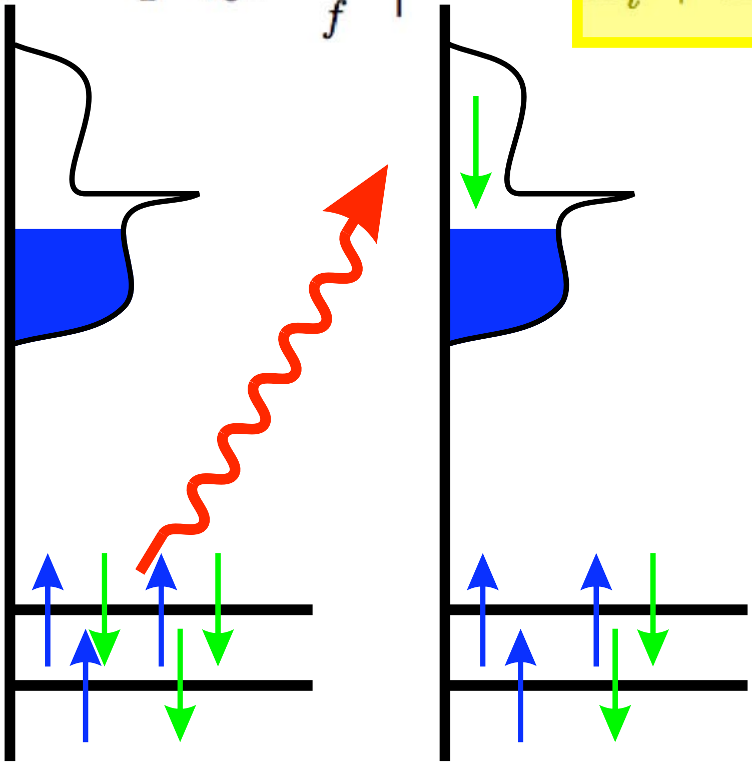

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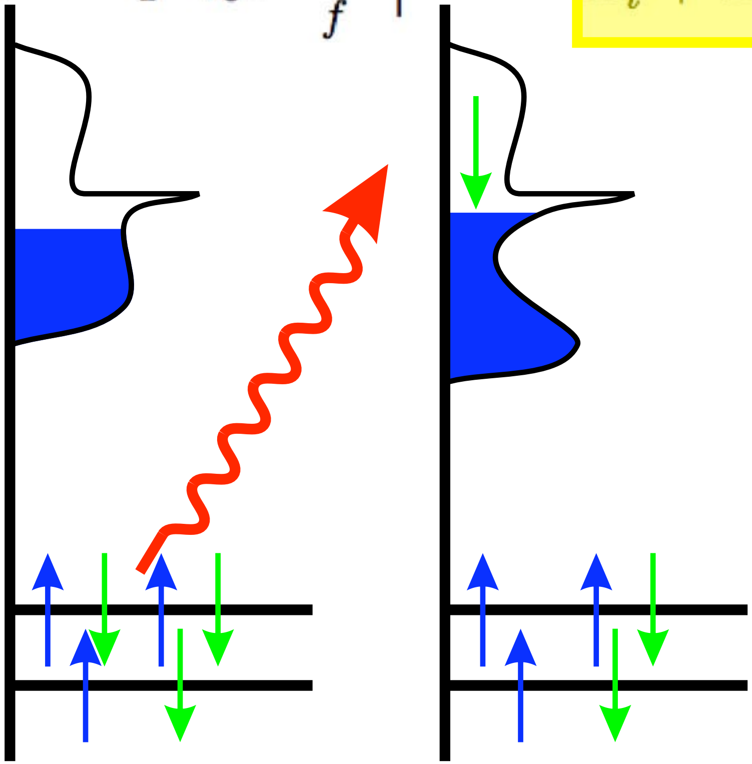

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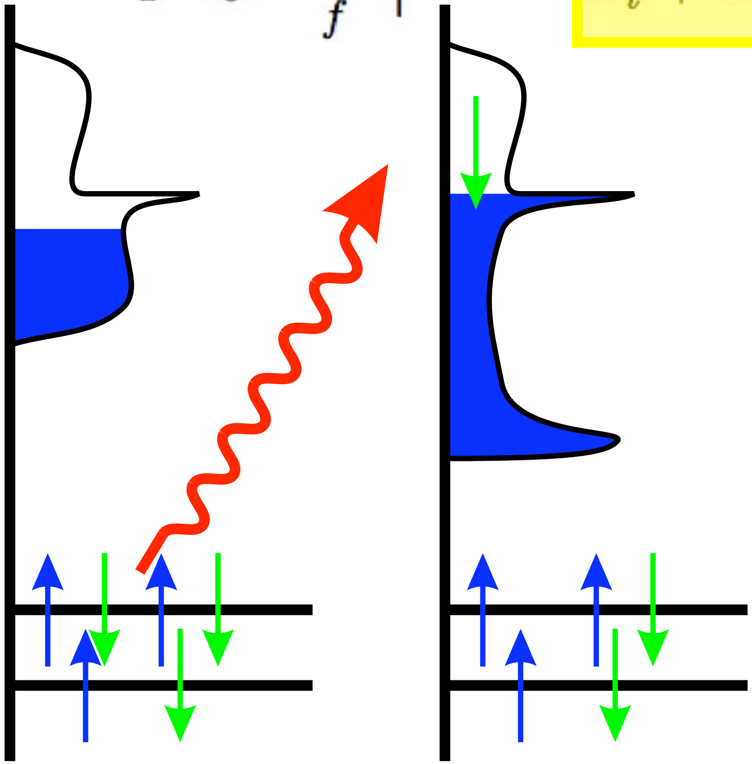

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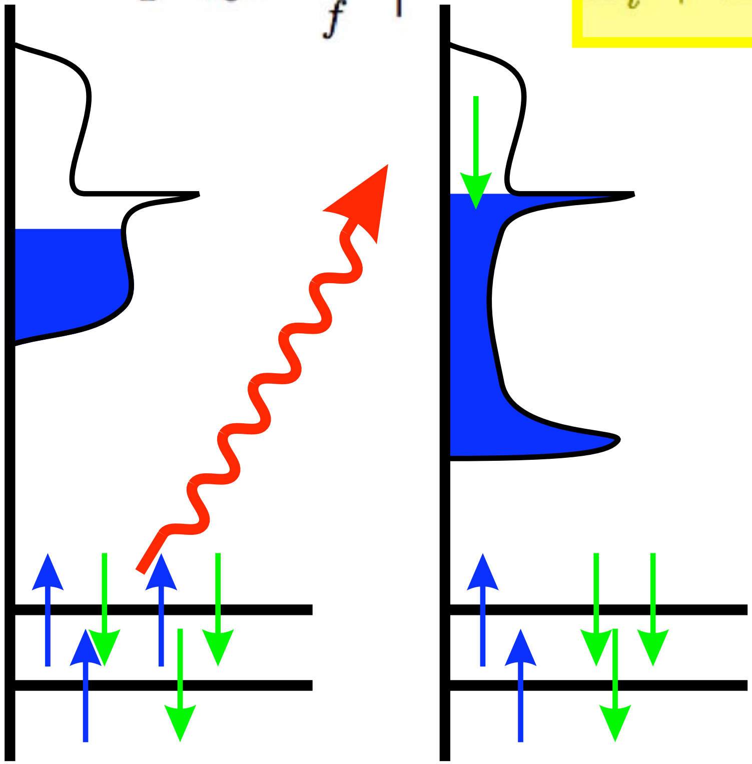

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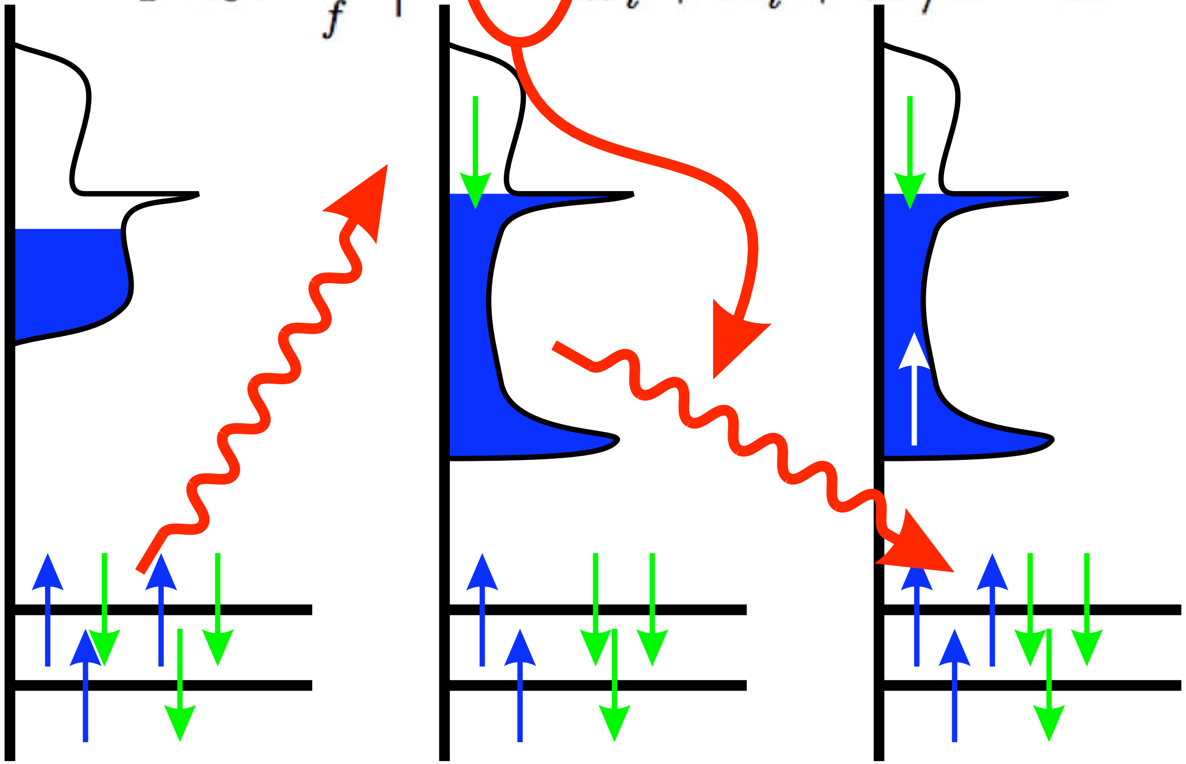

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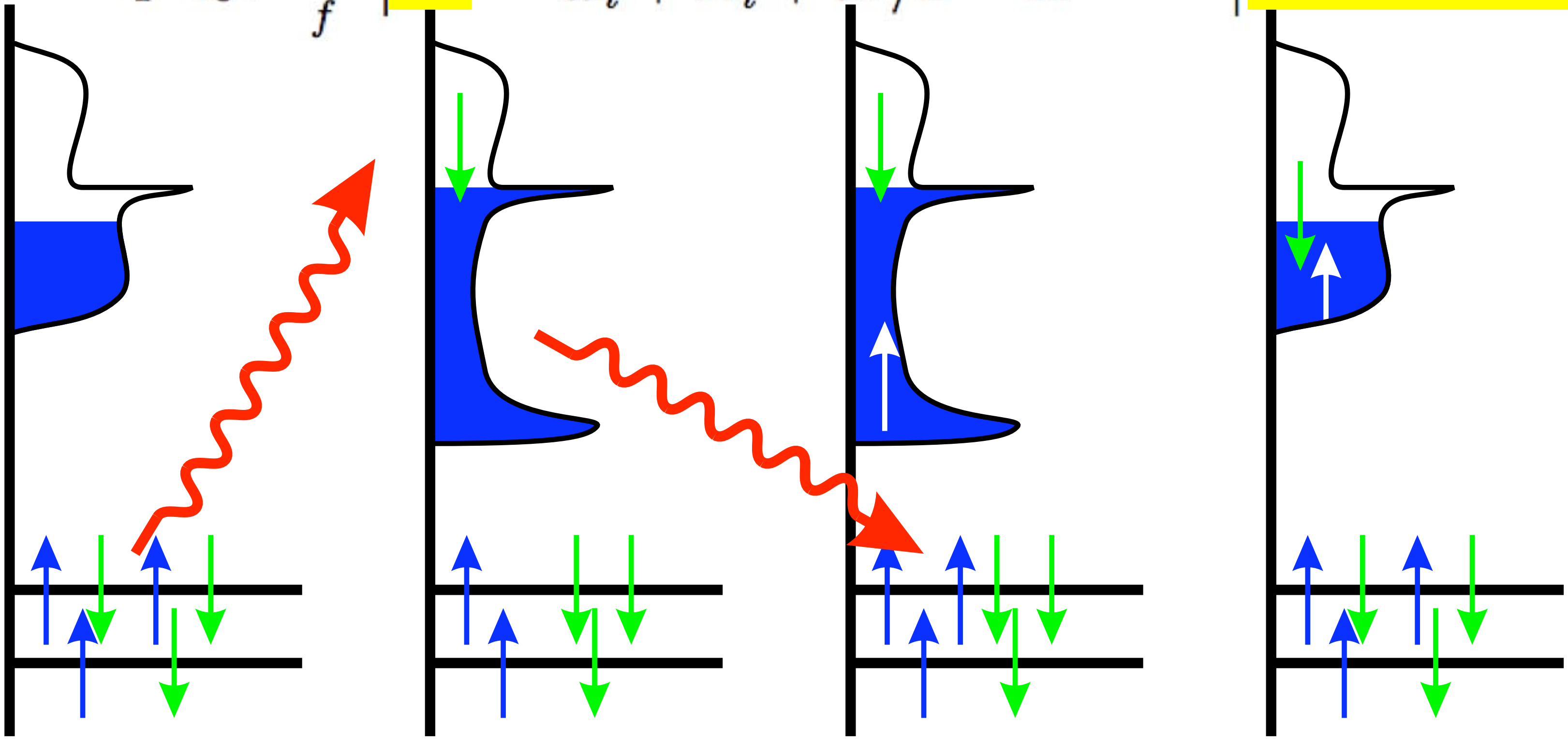

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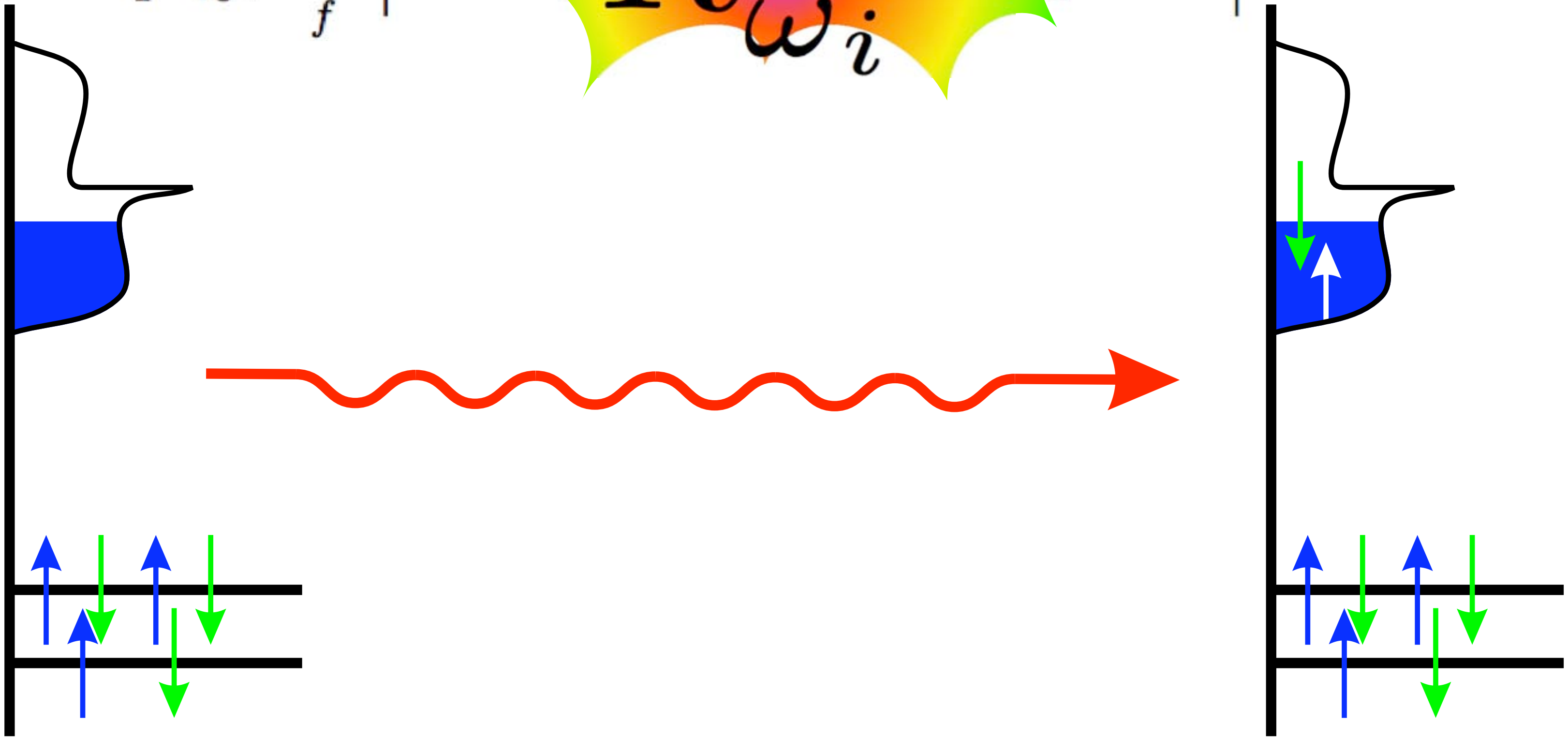
$$R^{\varepsilon_i \varepsilon_o}_{\omega_i}$$



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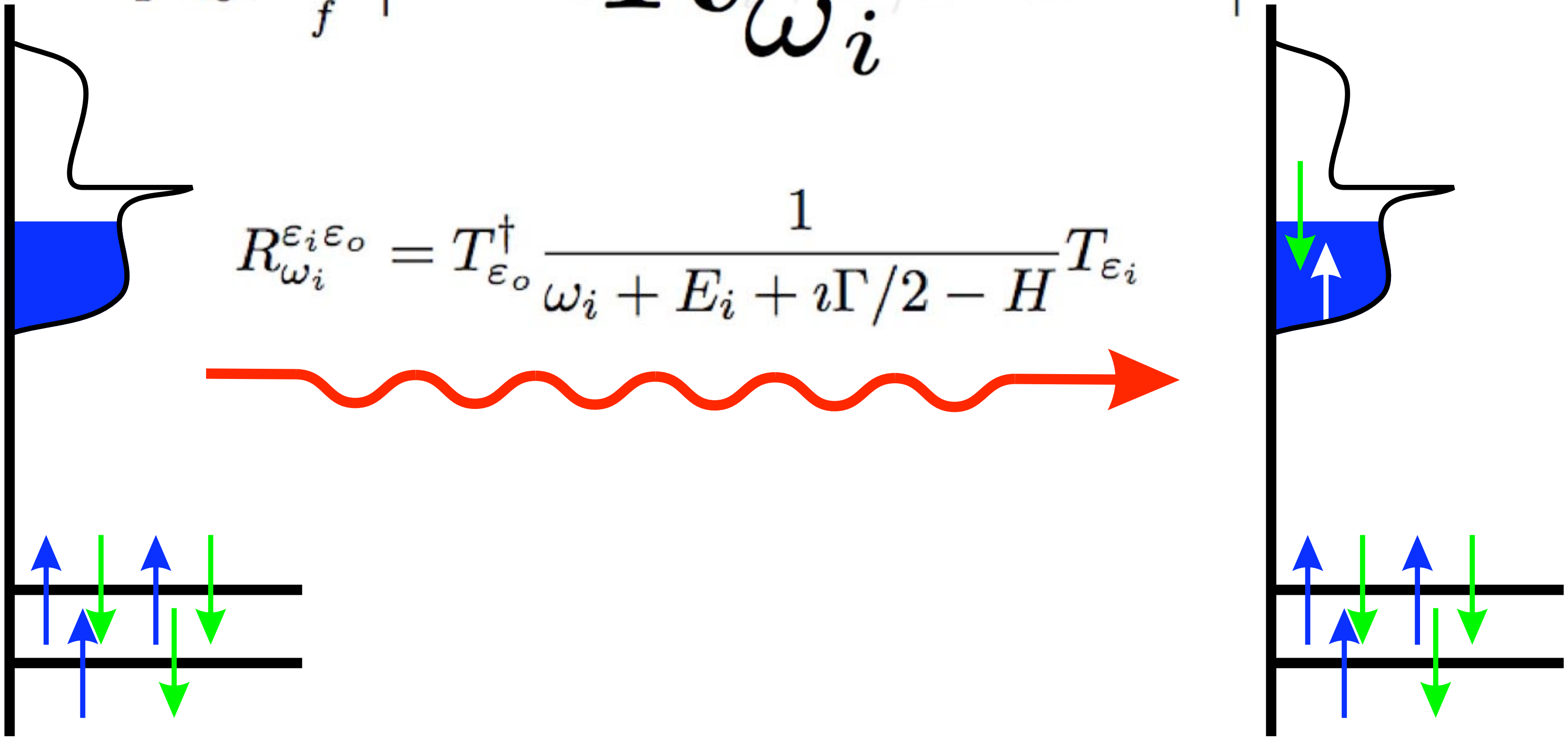
$$R^{\varepsilon_i\varepsilon_o}_{\omega_i} = T^\dagger_{\varepsilon_o}\frac{1}{\omega_i+E_i+\imath\Gamma/2-H}T_{\varepsilon_i}$$



Spin excitations with resonant x-rays: Theory

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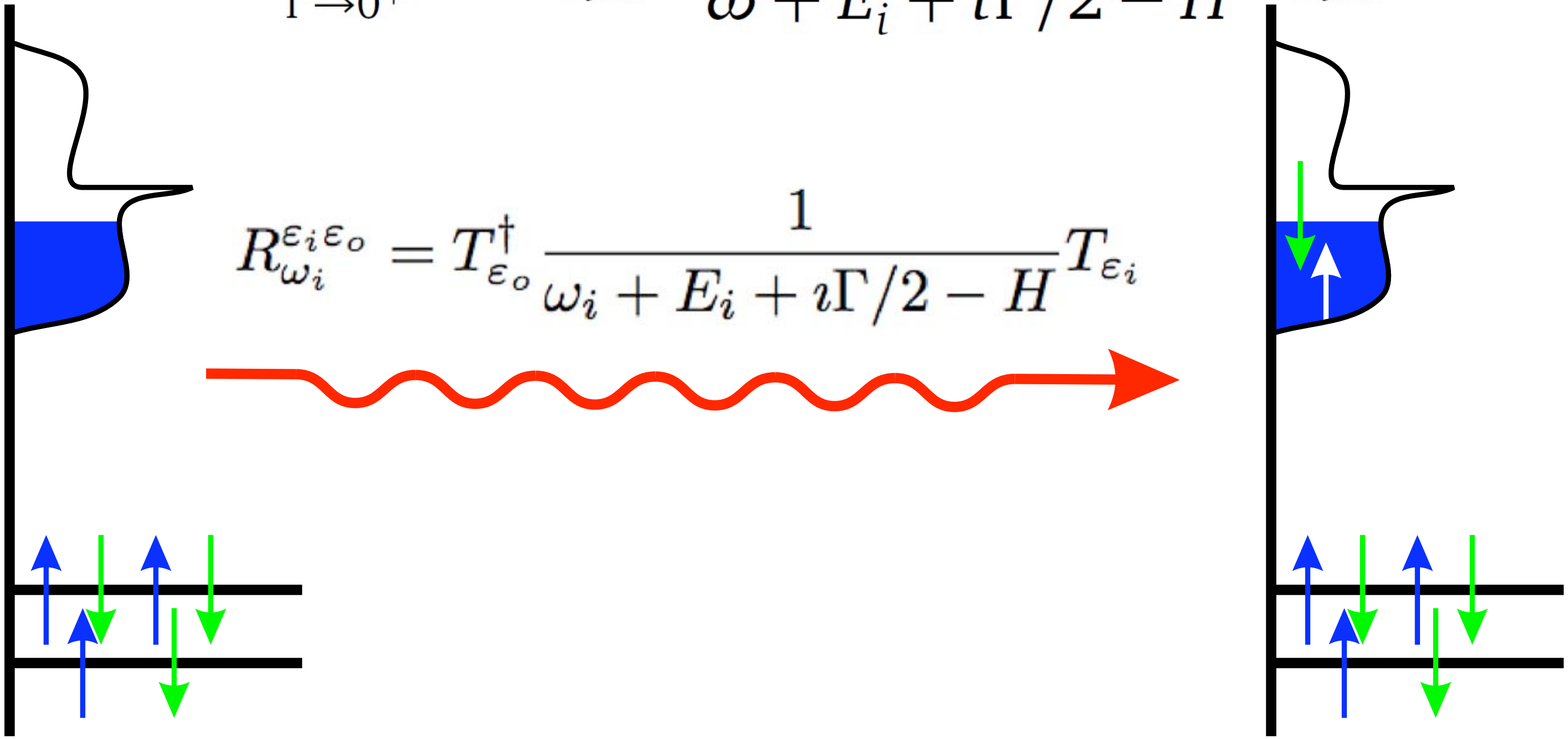
$$\frac{\delta^2\sigma}{\delta\Omega\delta\omega} \propto -\mathrm{Im} \lim_{\Gamma\to 0^+} \langle i|(R^{\varepsilon_i\varepsilon_o}_{\omega_i,\mathbf{Q}})^\dagger \frac{1}{\omega+E_i+\imath\Gamma/2-H} R^{\varepsilon_i\varepsilon_o}_{\omega_i,\mathbf{Q}}|i\rangle$$

$$R^{\varepsilon_i\varepsilon_o}_{\omega_i} = T^\dagger_{\varepsilon_o}\frac{1}{\omega_i+E_i+\imath\Gamma/2-H}T_{\varepsilon_i}$$



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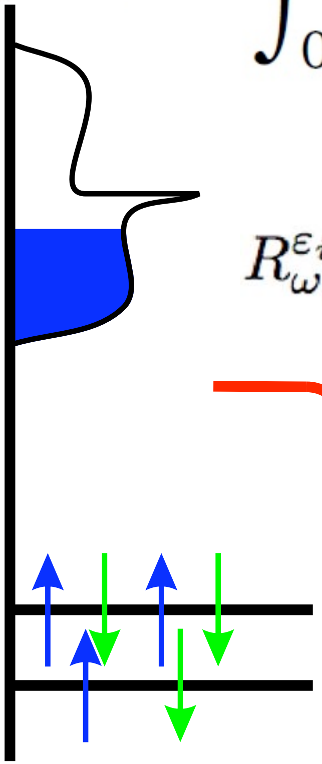
$$\frac{\delta^2\sigma}{\delta\Omega\delta\omega} \propto \mathrm{Re}\int_0^\infty e^{\imath\omega t}\langle i|R^{\varepsilon_i\varepsilon_o}_{\omega_i,\mathbf{Q}}(t)^\dagger R^{\varepsilon_i\varepsilon_o}_{\omega_i,\mathbf{Q}}(t=0)|i\rangle dt$$



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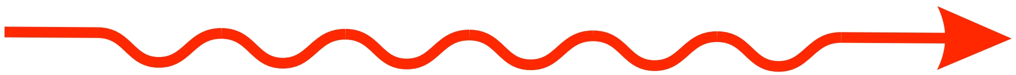

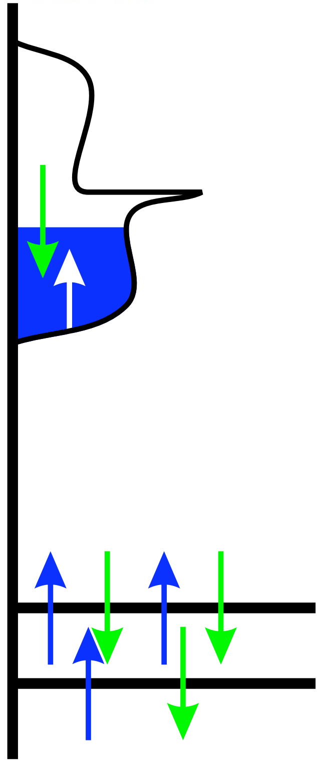

Relation to absorbtion

- Interaction of Neutrons with matter is easy (magnetic dipole) but for resonant x-ray scattering nothing is obvious.
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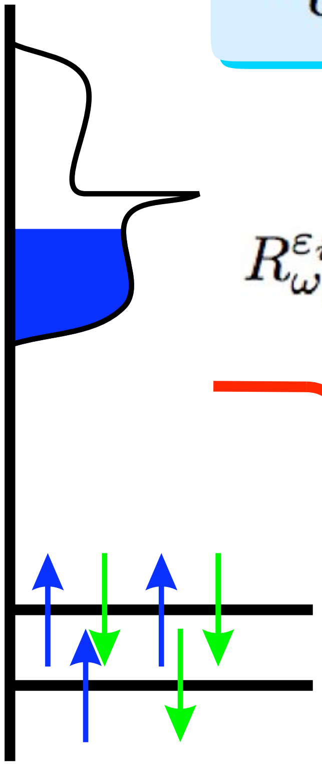
$$\epsilon_o^* \cdot \sigma \cdot \epsilon_i = \langle i | R^{\varepsilon_i \varepsilon_o}_{\omega_i, \boldsymbol{q}} | i \rangle$$



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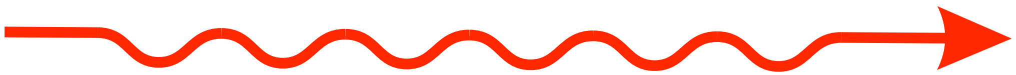
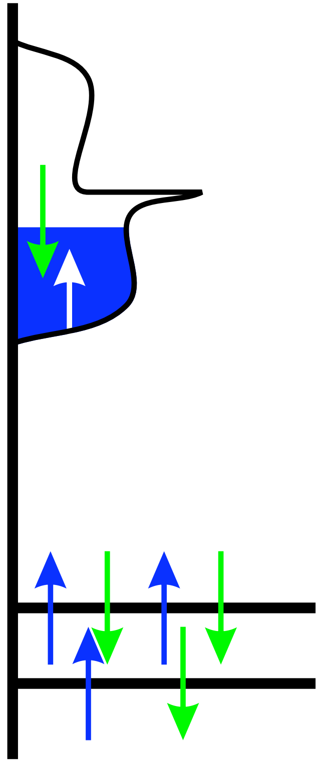




Effective scattering operator for magnetic spin excitations

M. W. Haverkort
Phys. Rev. Lett. **105**, 167404 (2010)

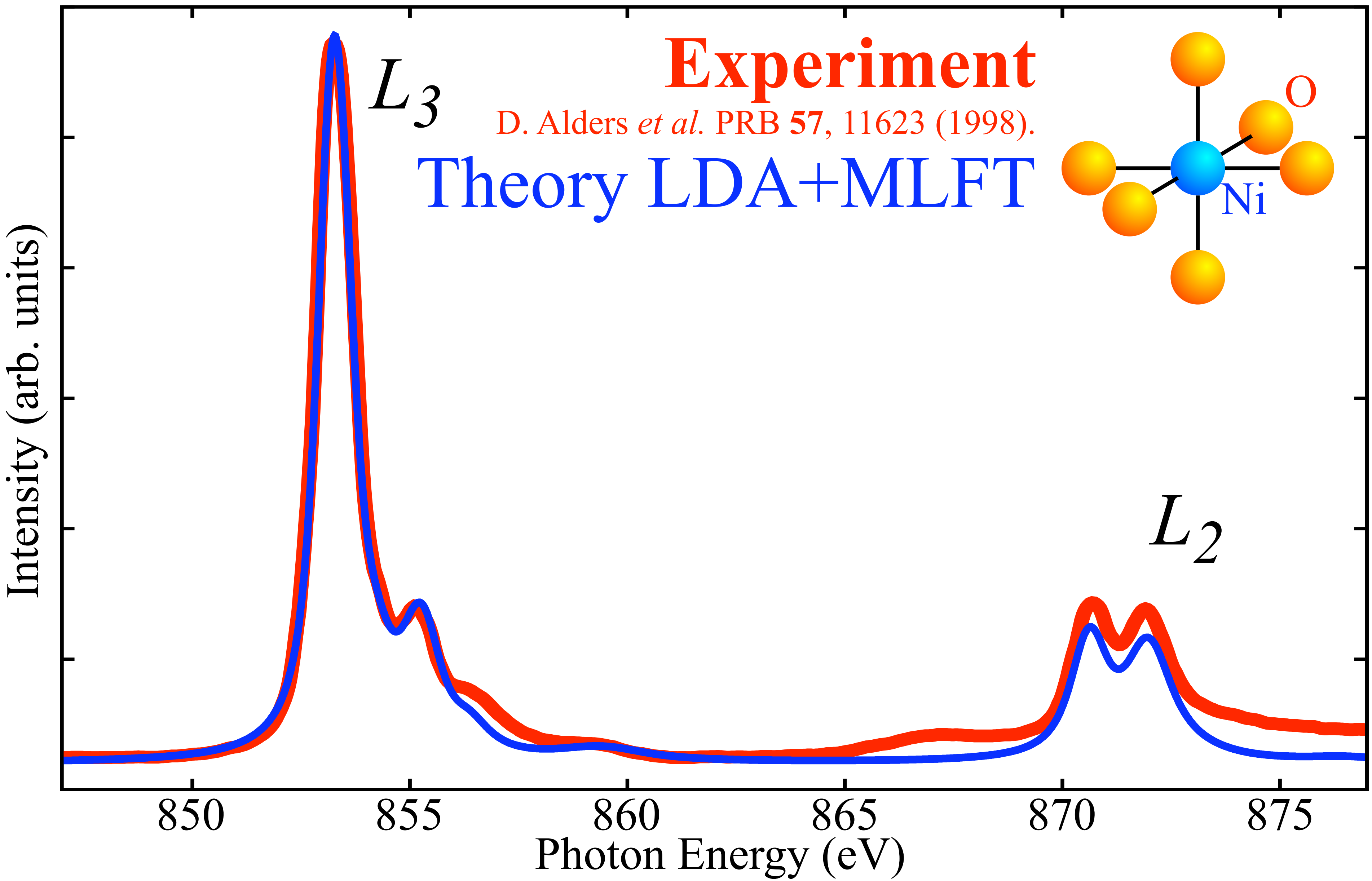
One needs to calculate x-ray absorption spectra

... and spin susceptibilities

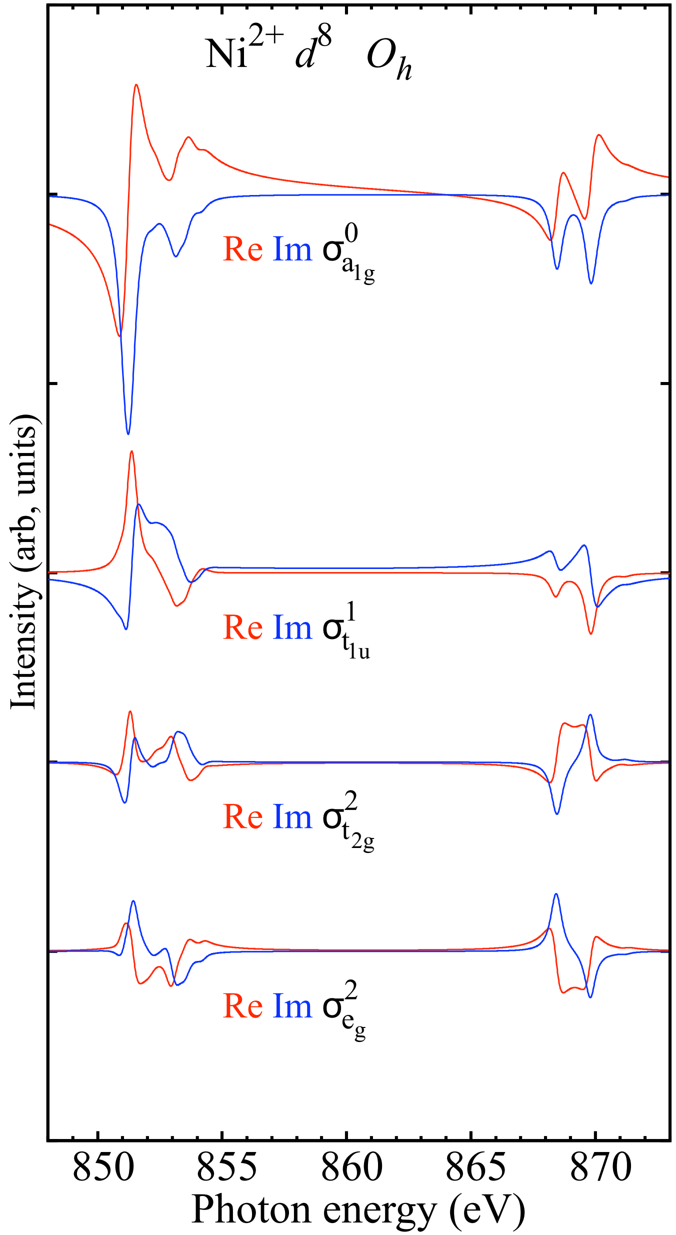
$$R^{\varepsilon_i \varepsilon_o}_{\omega_i, j} = \sigma^{(0)} \varepsilon_i \cdot \varepsilon_o^* + \frac{\sigma^{(1)}}{s} \varepsilon_o^* \times \varepsilon_i \cdot S_j$$

$$+ \frac{\sigma^{(2)}}{s(2s-1)} \left(\varepsilon_i \cdot S_j \; \varepsilon_o^* \cdot S_j + \varepsilon_o^* \cdot S_j \; \varepsilon_i \cdot S_j - \frac{2}{3} \varepsilon_i \cdot \varepsilon_o^* S_j^2 \right)$$

2p X-ray Absorption Spectroscopy of NiO



σ for Ni^{2+} in Oh



$$R_j^{\varepsilon_i \varepsilon_o} = \sigma^{(0)} \varepsilon_i \cdot \varepsilon_o^* + \frac{\sigma^{(1)}}{s} \varepsilon_i \times \varepsilon_o^* \cdot S$$

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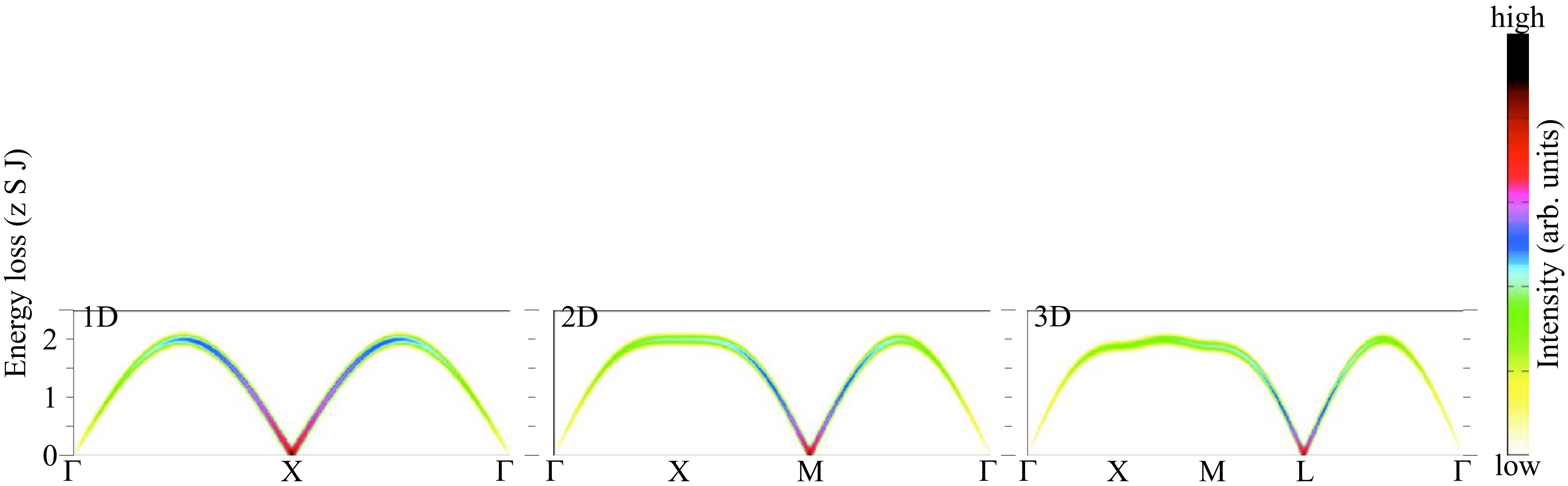
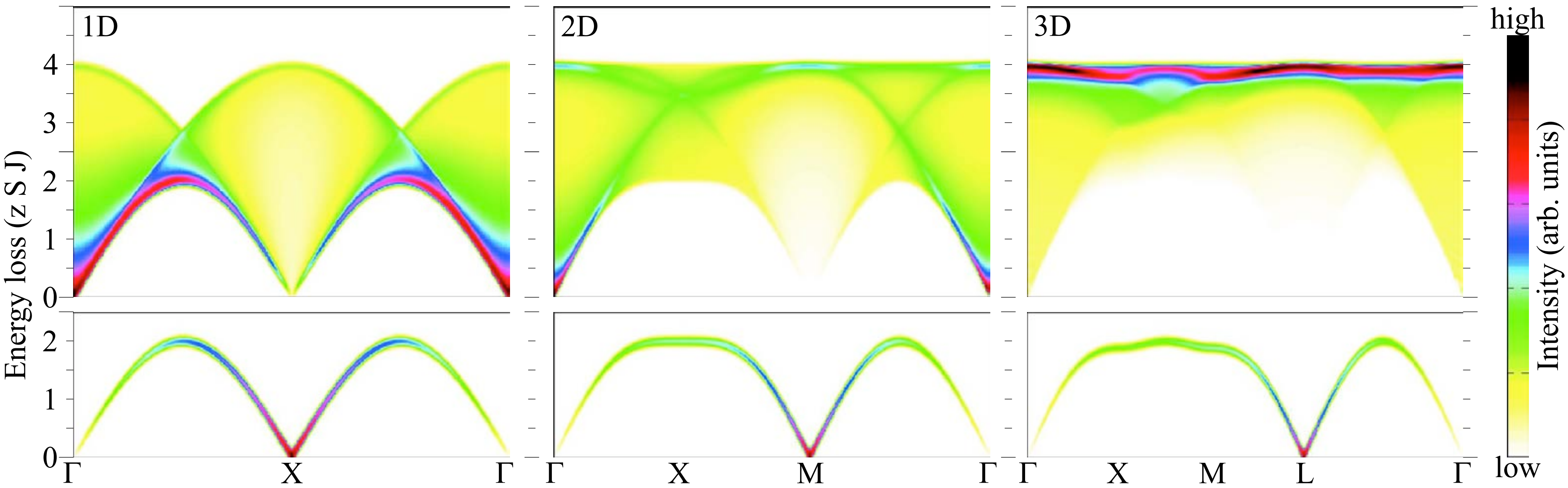
Single spin-flips resonant enhancement proportional to XMCD



Two spin-flips resonant enhancement proportional to XMLD



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Spin and orbital excitations in Sr_2CuO_3

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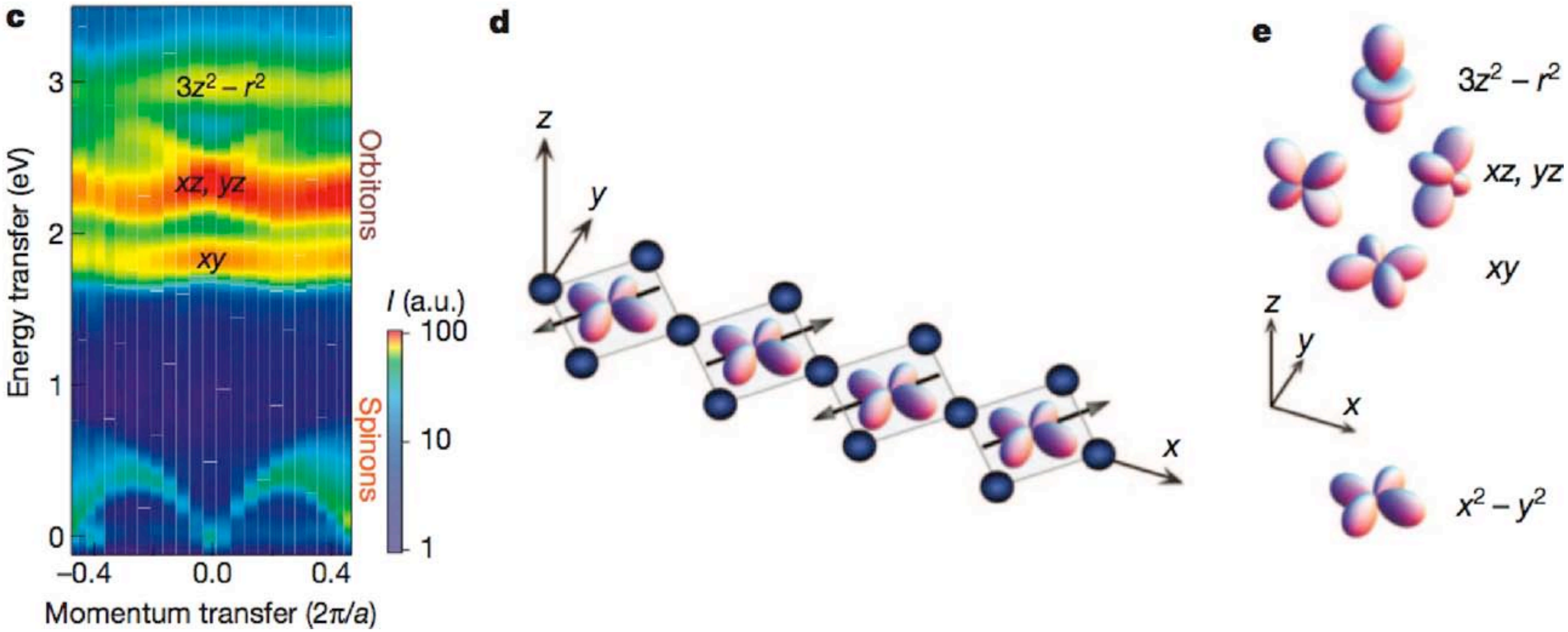
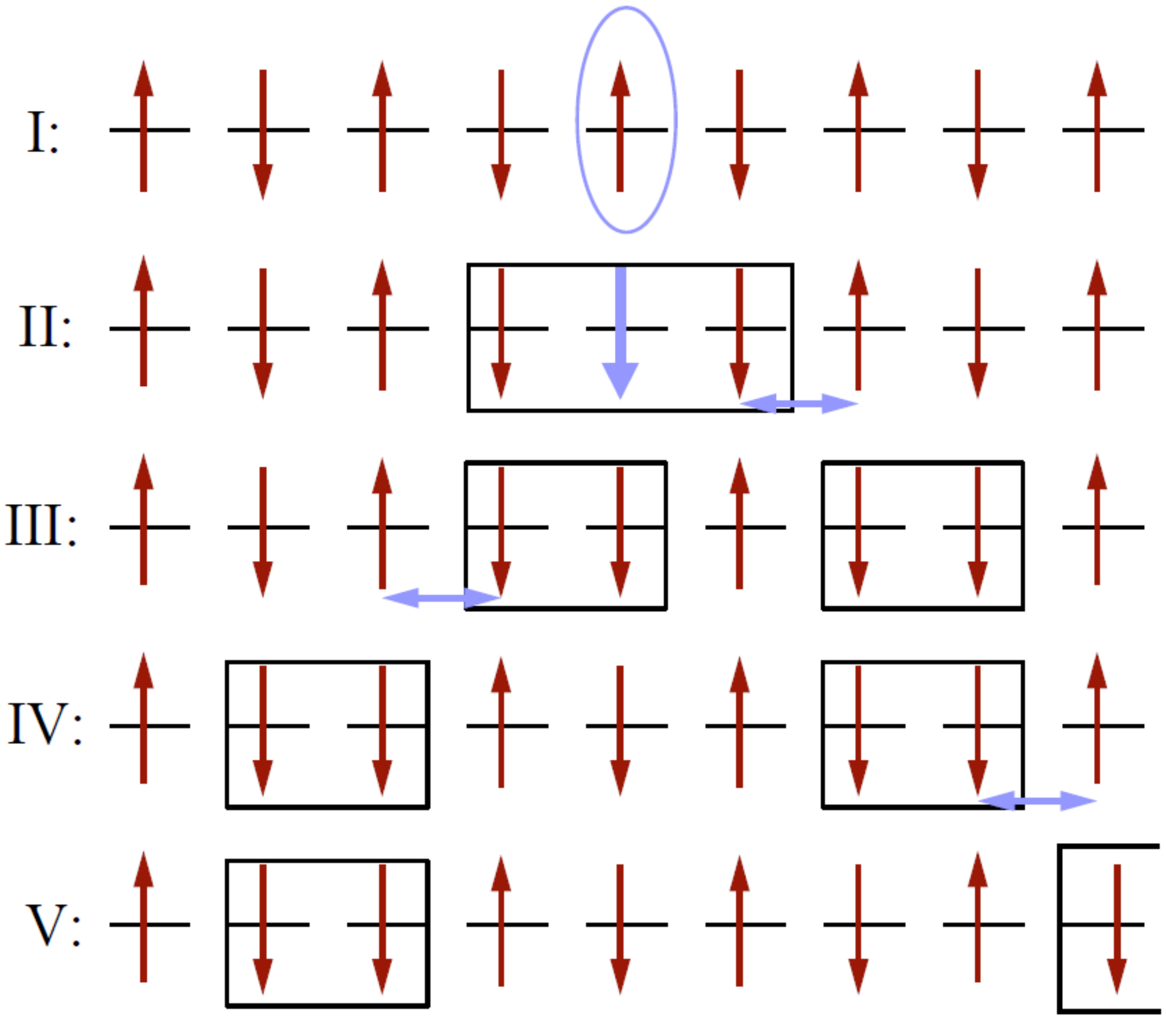


Spin and orbital excitations in Sr_2CuO_3

Dynamical spin structure factor

For a 1-dimensiona spin chain the fundamental excitations are 2 spinon excitations



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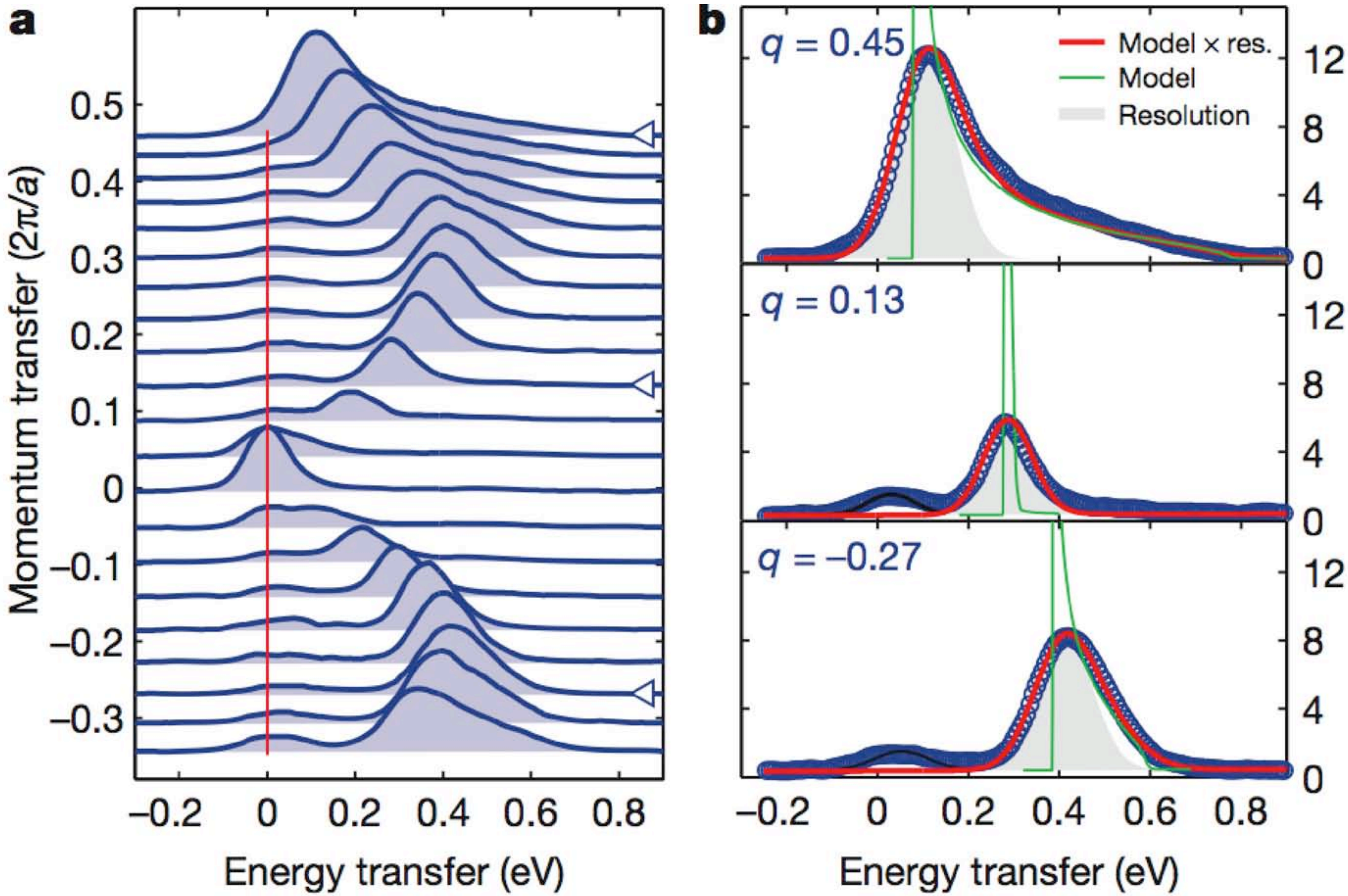

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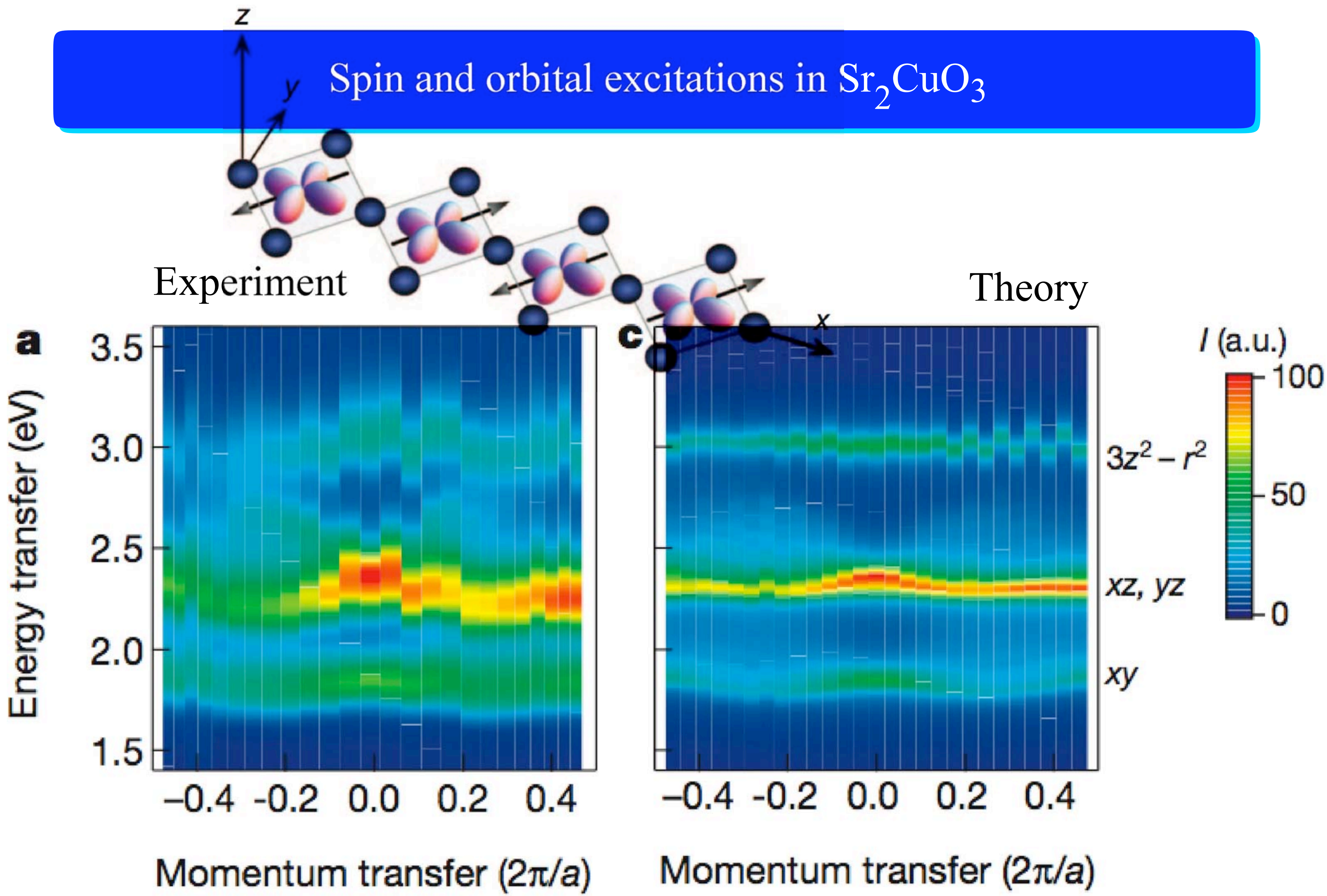

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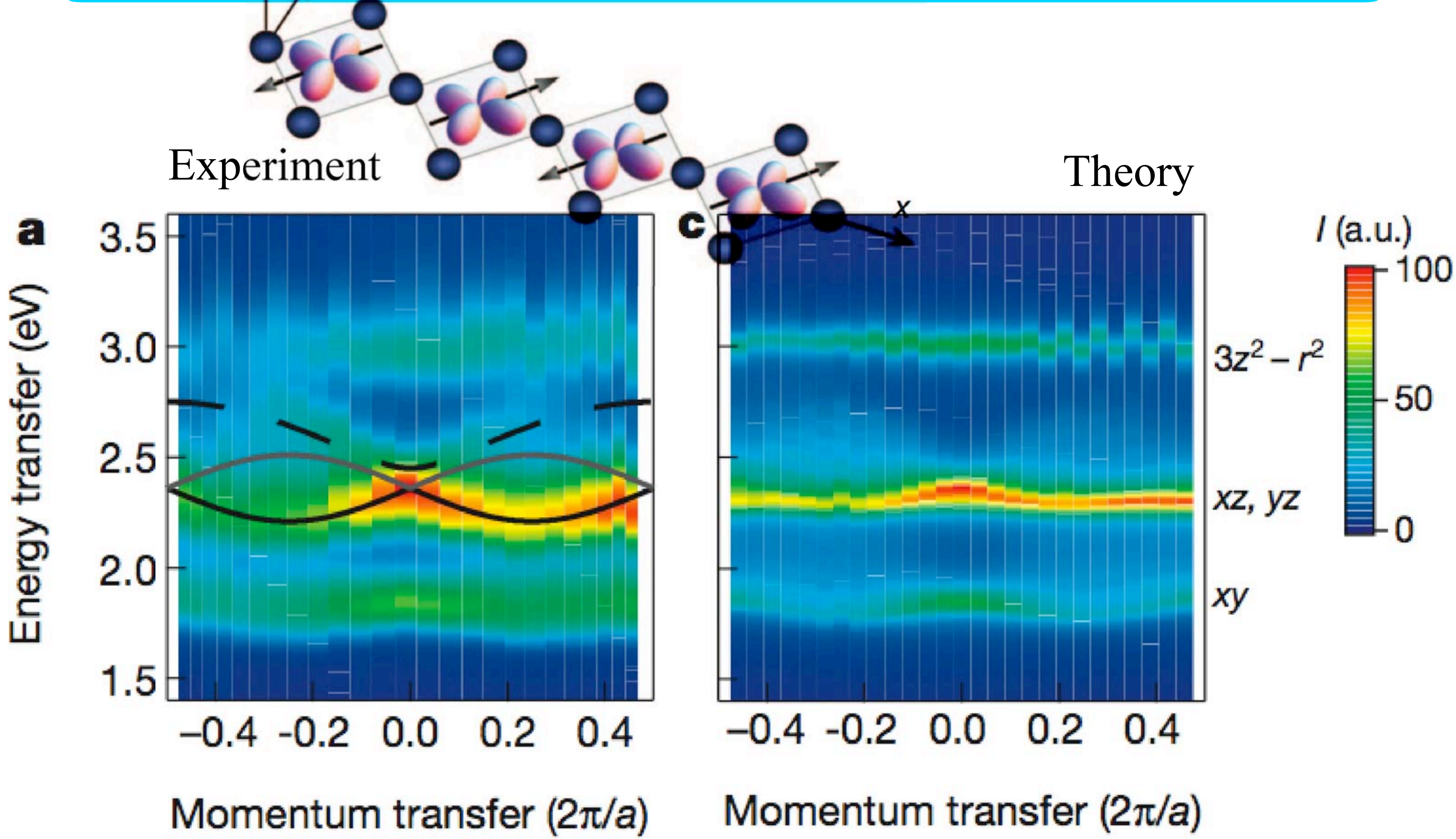

Additional literature

- *Core Level Spectroscopy of Solids*
  Frank de Groot and Akio Kotani

- *NEXAFS Spectroscopy*
  Joachim Stöhr

- Journal of Electron Spectroscopy and Related Phenomena
  Vol **86** (1997).

- *Introduction to ligand field theory*
  Carl Johan Ballhausen (1962)