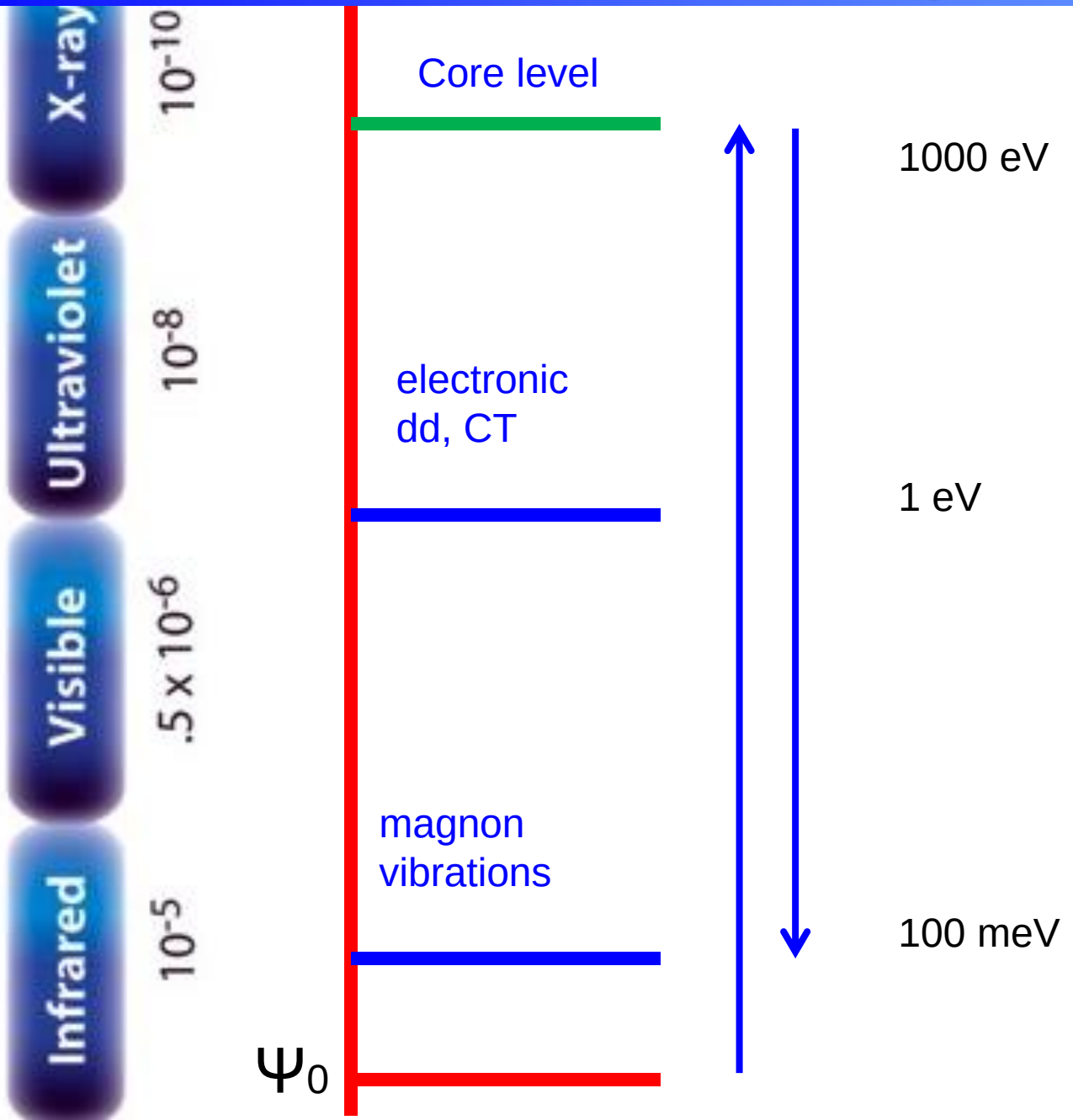
resonant inelastic x-ray scattering

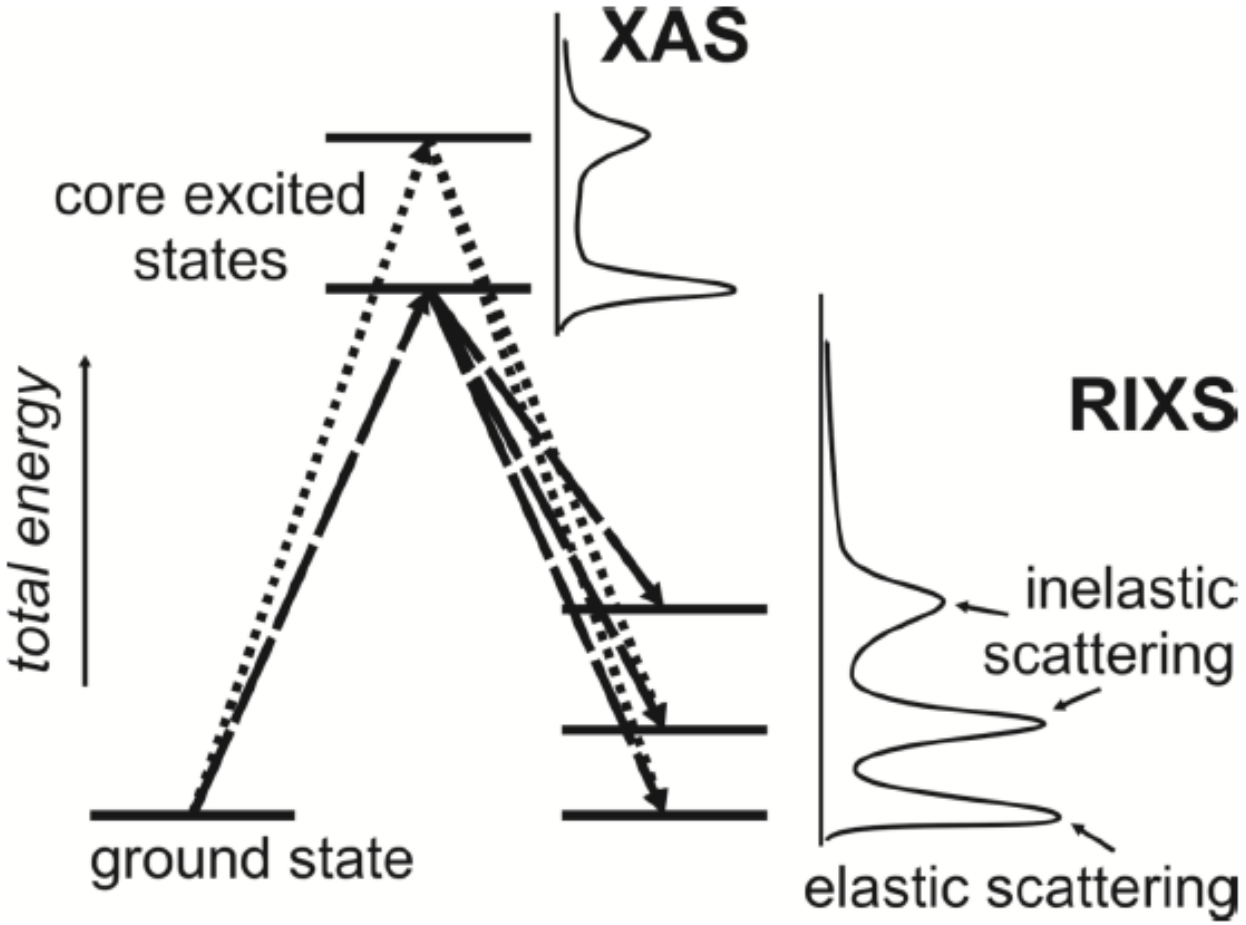
- X-ray absorption spectroscopy
- Multiplet calculations

- Resonant inelastic x-ray scattering

resonant inelastic x-ray scattering



resonant inelastic x-ray scattering



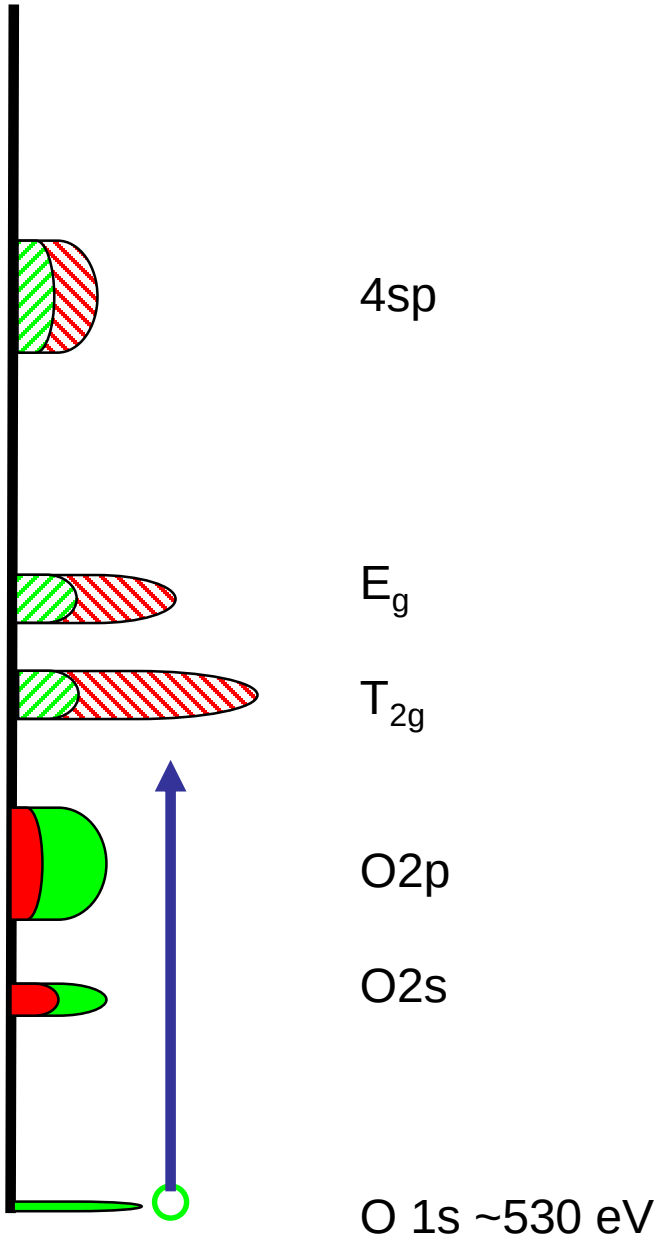
$$F(\Omega,\omega)=\sum_j\left|\sum_i\frac{<f|T_2|i><i|T_1|g>}{E_g+\hbar\Omega-E_i+\mathrm{i}\Gamma_i}\right|^2\times\frac{\Gamma_f/2\pi}{(E_g+\hbar\Omega-E_f-\hbar\omega)^2+\Gamma_f{}^2/4}$$

X-ray Absorption Spectroscopy

- Element specific
- Sensitive to low concentrations
- Applicable under extreme conditions

- SPACE: Combination with x-ray microscopy
- TIME: femtosecond XAS
- RESONANCE: RIXS, RPES, R diffraction

XAS: spectral shape (O 1s of TiO2)



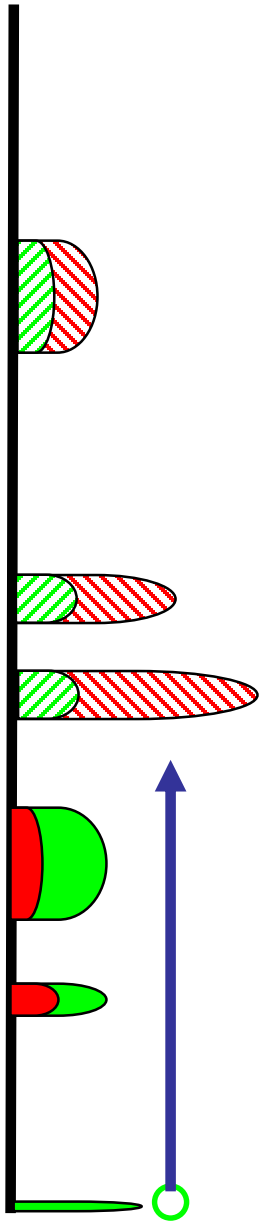
Electronic structure of a transition metal oxide

Main bonding:
O2p with metal 4sp
Gives valence band and conduction band,
Mixed in character

Additional bonding
O2p with metal 3d;
Gives mixed 3d bands split by crystal field in octahedral symmetry, T2g states have pi-bonding and Eg states have sigma-bonding.

oxygen 1s core state
is localized at an oxygen atom

XAS: spectral shape (O 1s of TiO2)



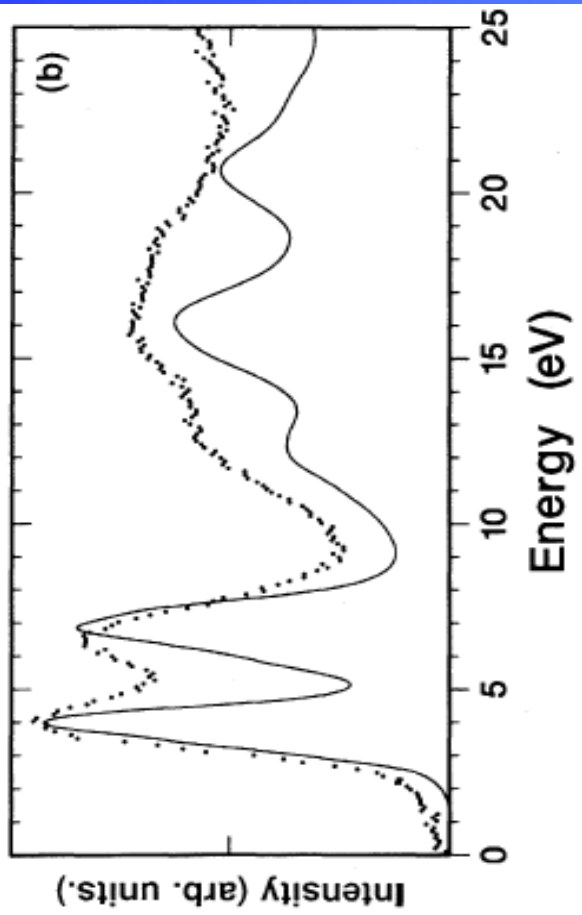
4sp

E_g

T_{2g}

O2p

O2s



transition from oxygen 1s state
to an empty state

oxygen 1s core state
is localized at an oxygen atom

local empty DOS

dipole selection rule:
p-projected DOS

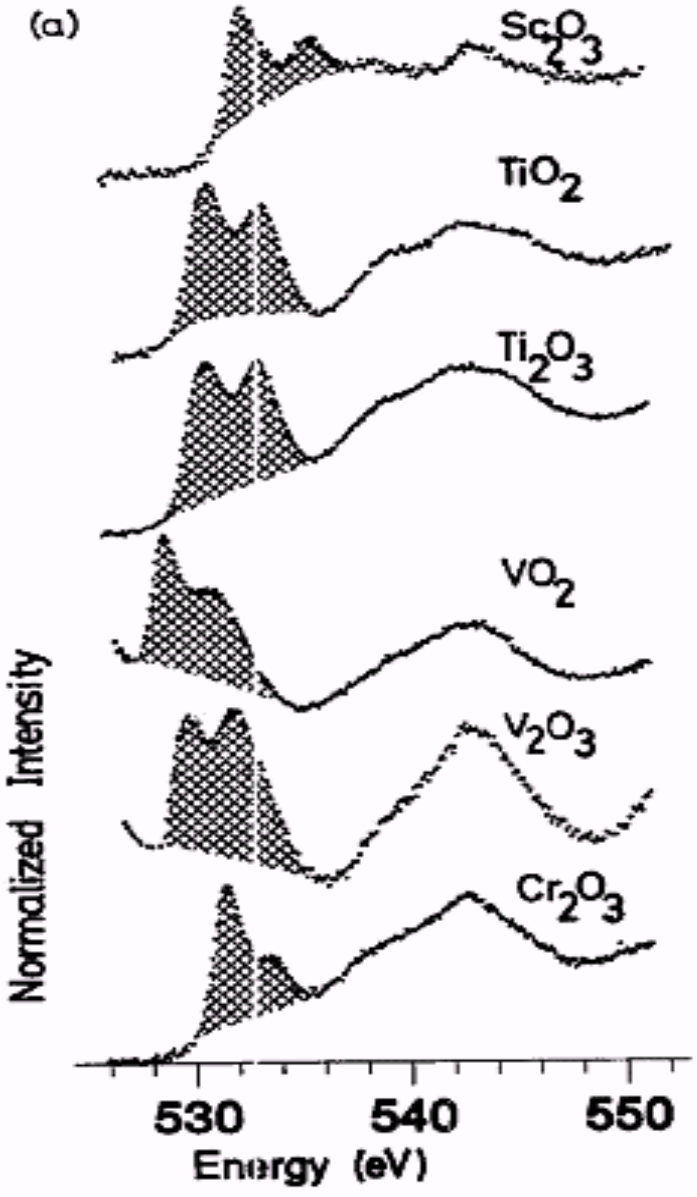
Fermi Golden Rule:

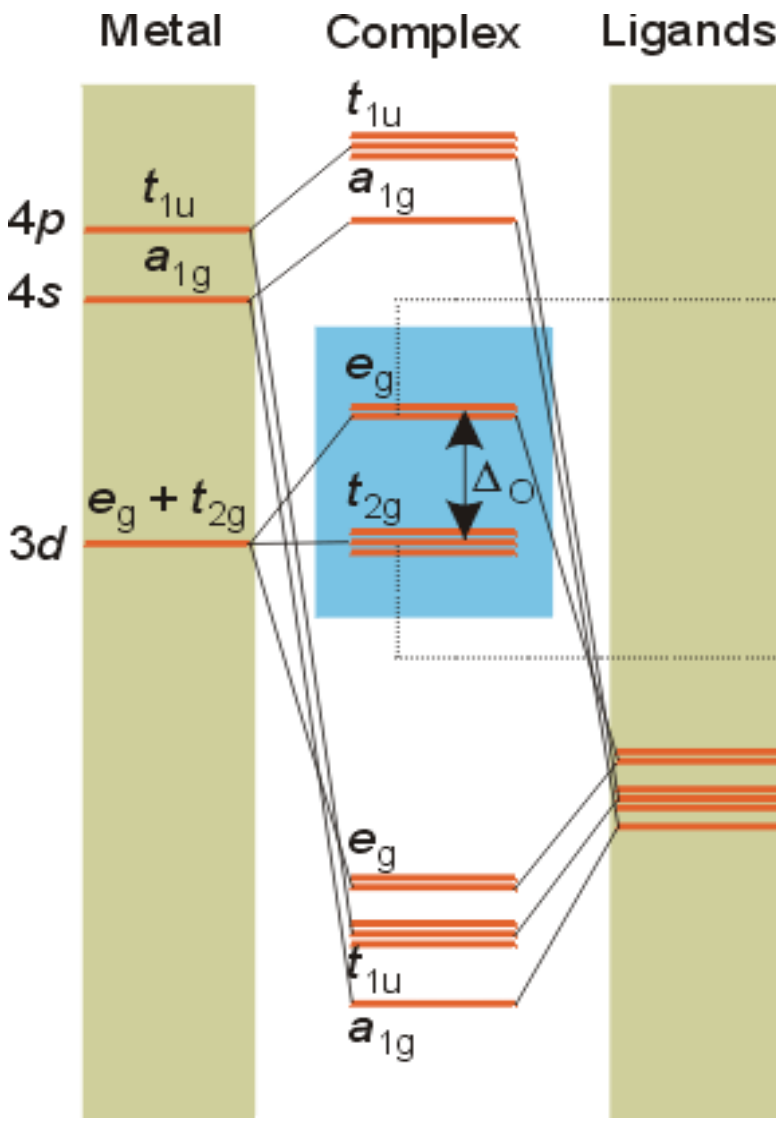
$$I_{XAS} = |\langle \Phi_f | \text{dipole} | \Phi_i \rangle|^2 \, \delta_{[\Delta E=0]}$$

O 1s ~530 eV

[Phys. Rev. B. 40, 5715 (1989); review in Chem. Rev. 120, 4056 (2020)]

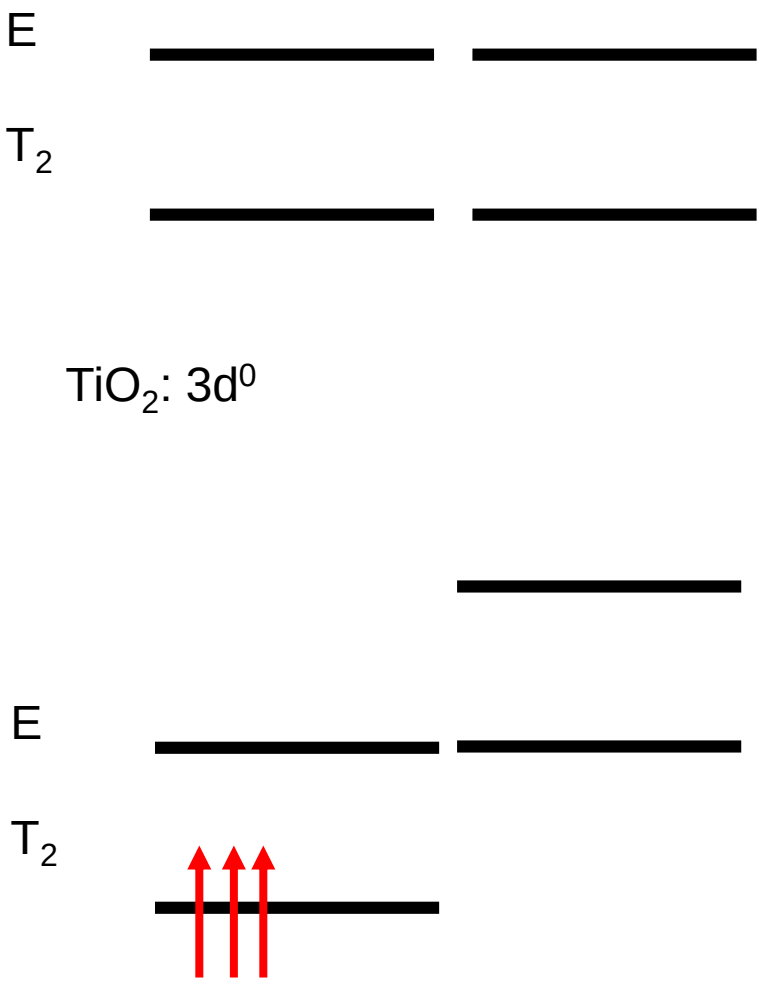
XAS: spectral shape (O 1s)

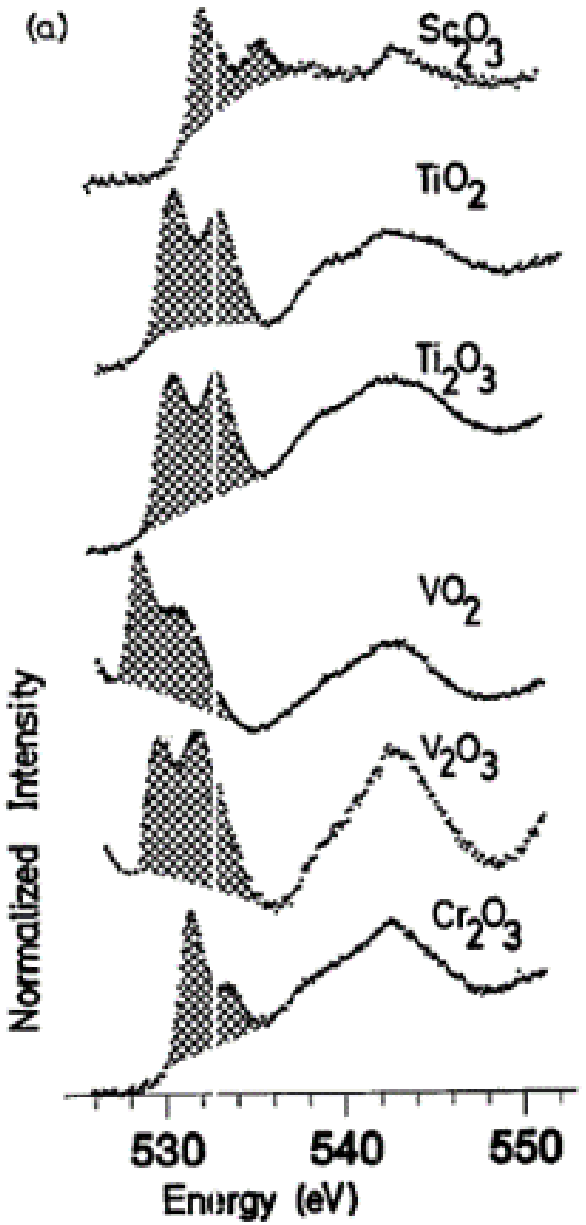




[Phys. Rev. B. 40, 5715 (1989); review in Chem. Rev. 120, 4056 (2020)]

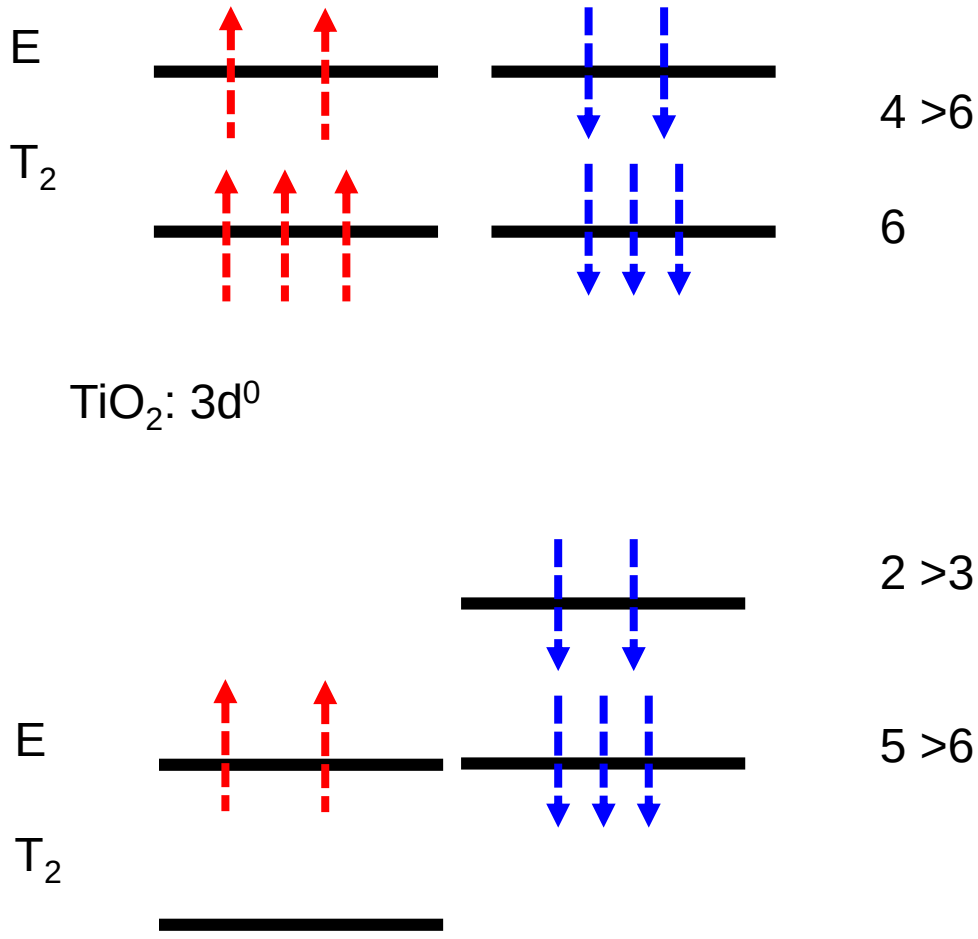
XAS: spectral shape

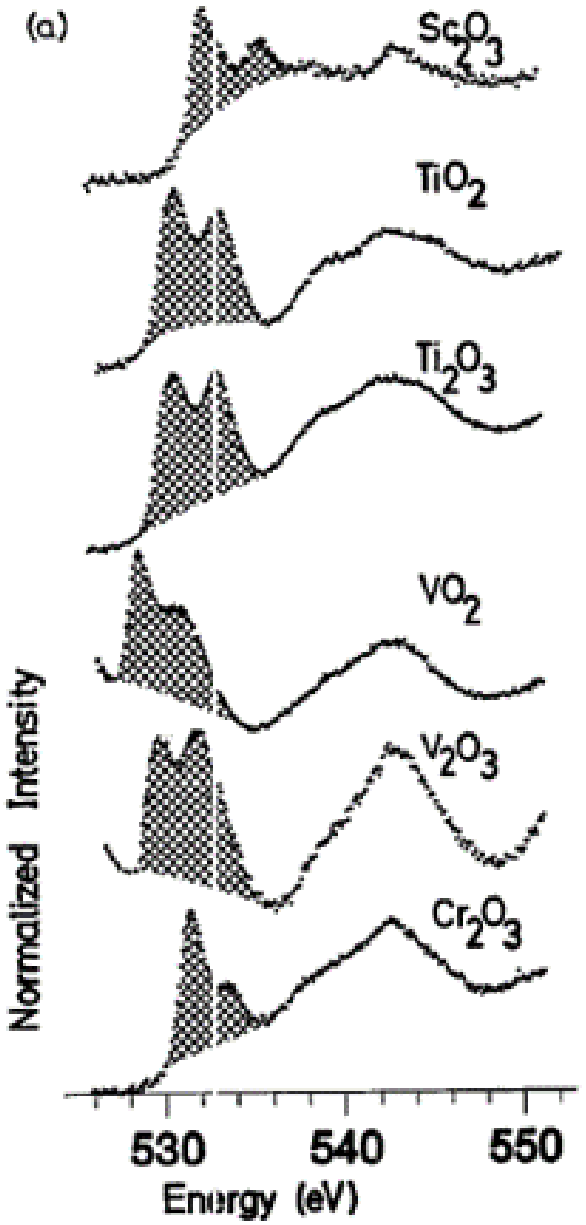




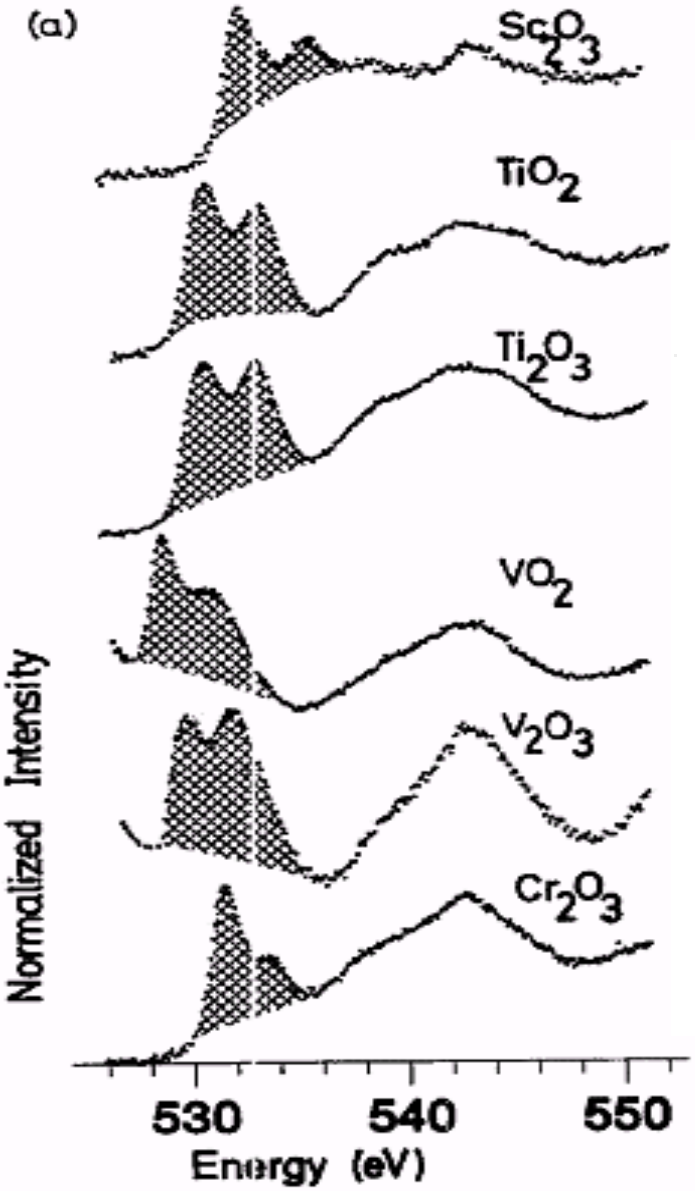
[Phys. Rev. B. 40, 5715 (1989); review in Chem. Rev. 120, 4056 (2020)]

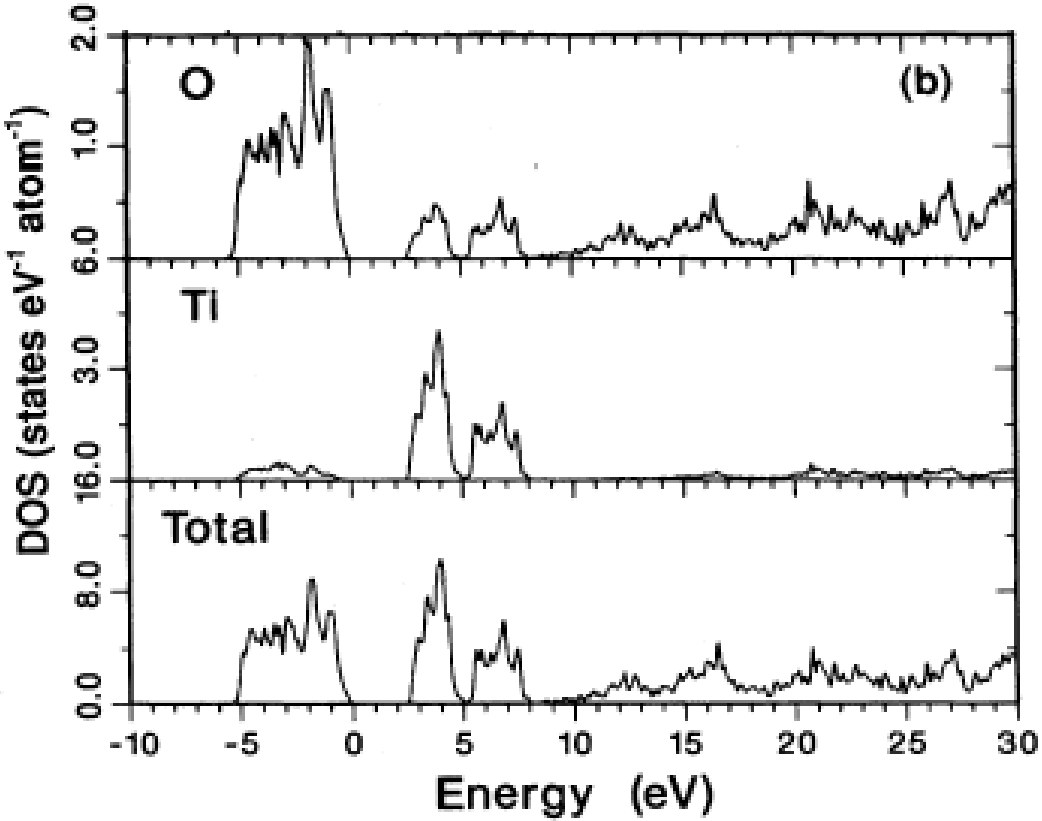
XAS: spectral shape





XAS: spectral shape (O 1s)

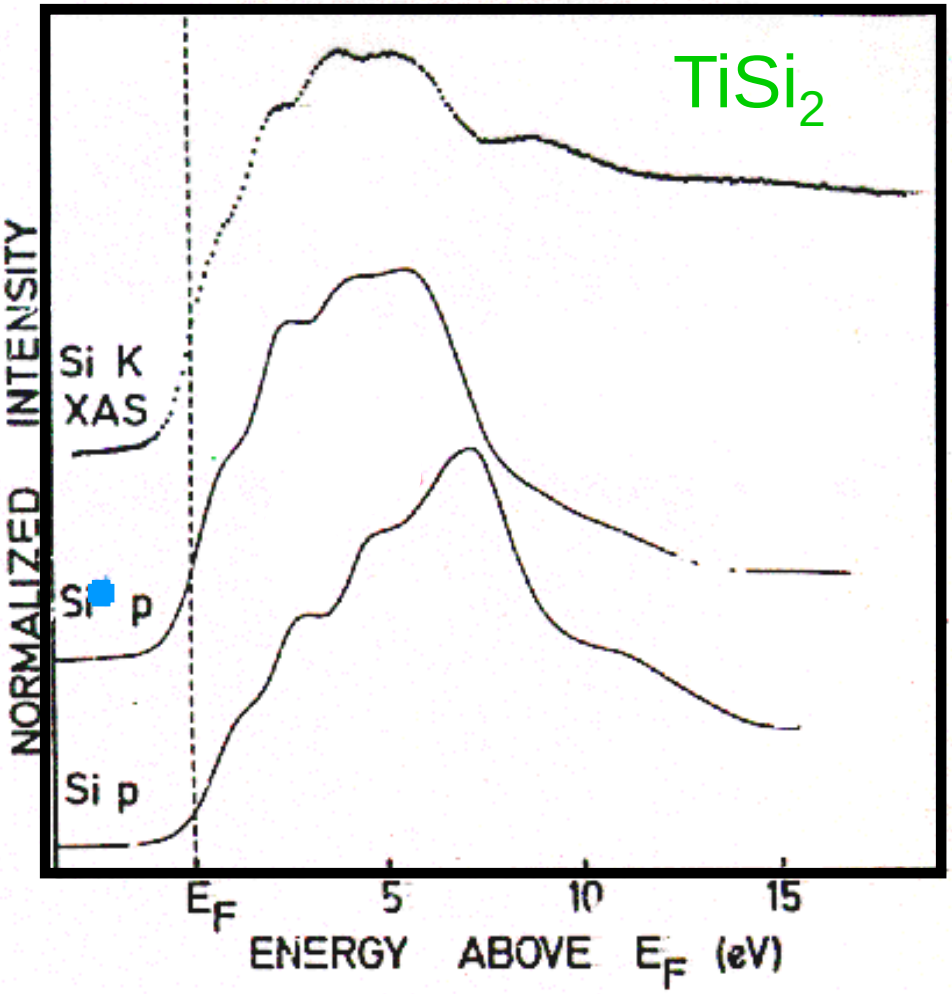




oxygen 1s > p DOS

[Phys. Rev. B. 40, 5715 (1989); 48, 2074 (1993)]

XAS: spectral shape

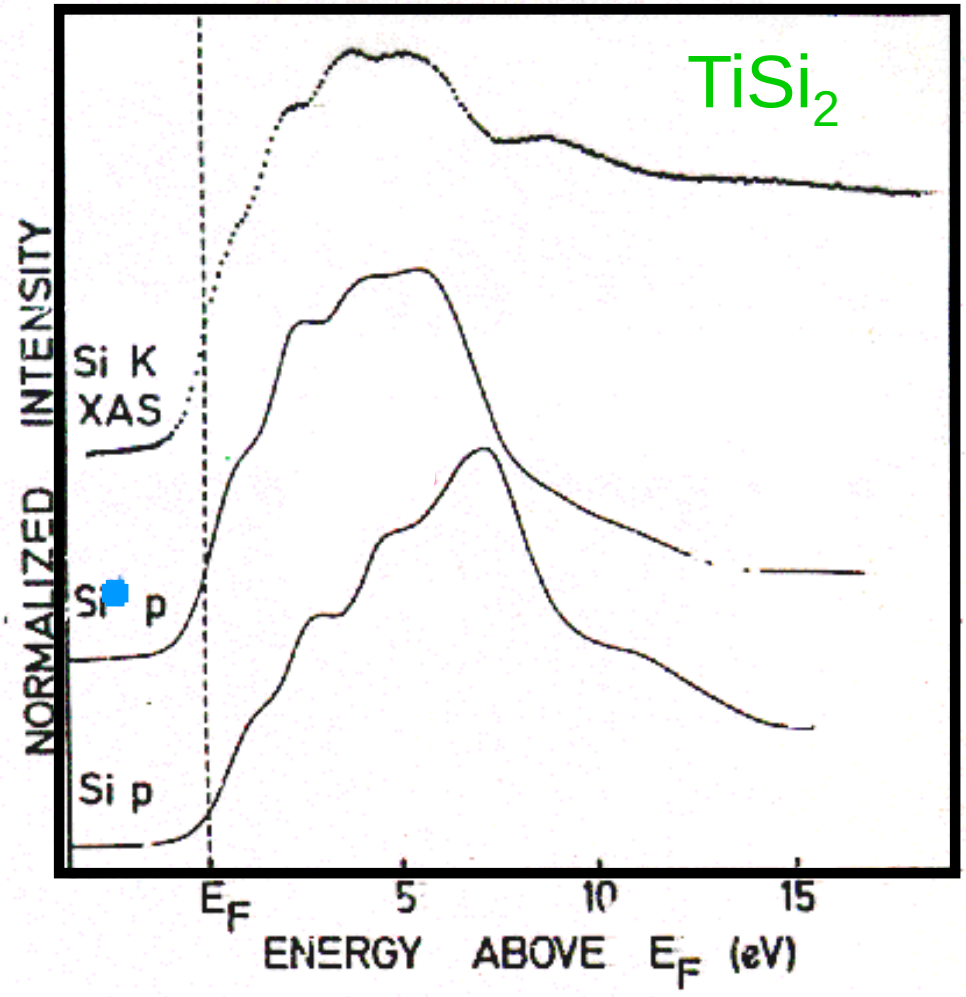


- **Final State Rule:** Spectral shape of XAS looks like final state DOS

(BSE, TDDFT calculations)

Phys. Rev. B. 41, 11899 (1991)

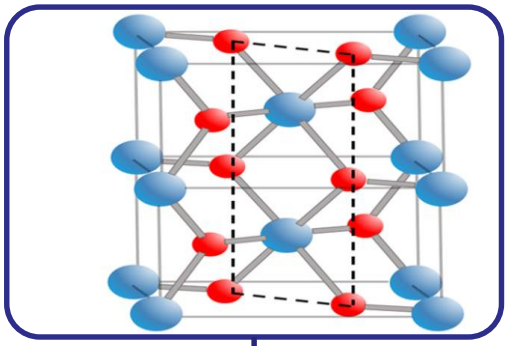
XAS: spectral shape



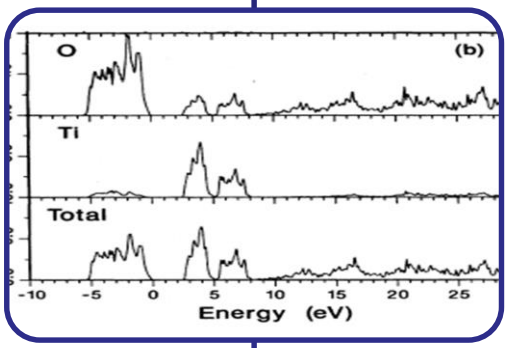
- **XAS codes:**
- Multiple scattering:
  FEFF, FDMNES, etc.
- Band structure:
  WIEN2K, VASP
  Quantumexpresso, etc.
- Real-space DFT:
  ADF,
  ORCA, etc.

Phys. Rev. B. 41, 11899 (1991)

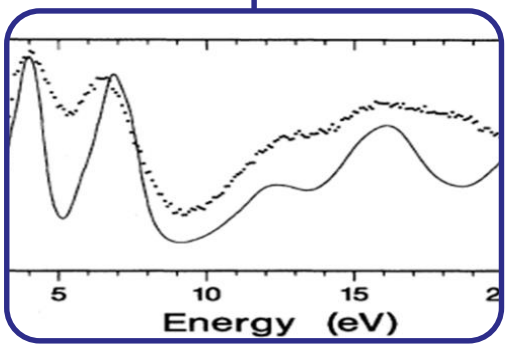
XAS: spectral shape (O 1s)



Crystal structure



Electronic structure calculation,
for example Density Functional Theory (DFT)
(in the presence of the core hole)

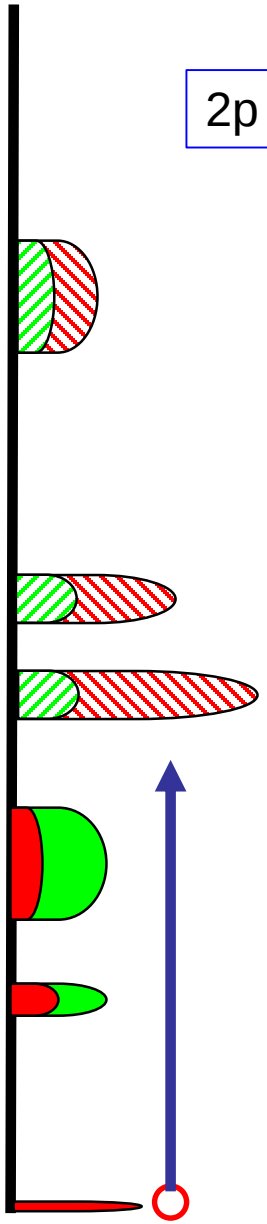


Calculation of the oxygen
p-projected local empty DOS

Compare with experiment

CODES: FEFF, Wien2K, VASP, QE, etc.

XAS: spectral shape (Ti 2p)



2p > 3d

4sp

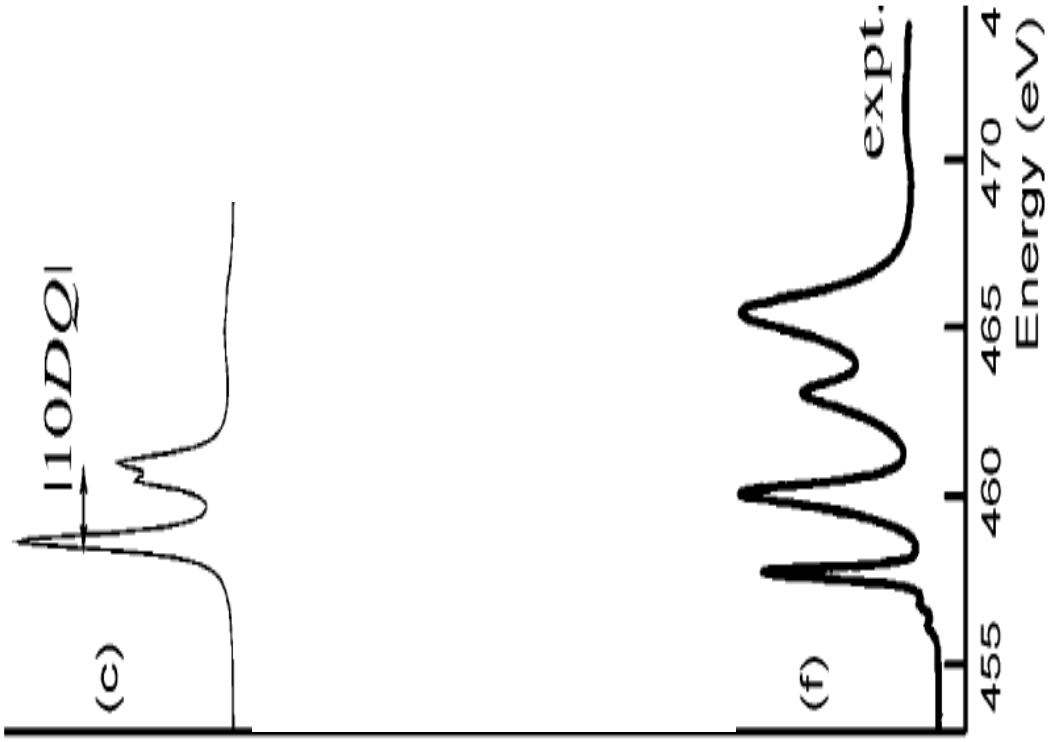
E_g

T_{2g}

O2p

O2s

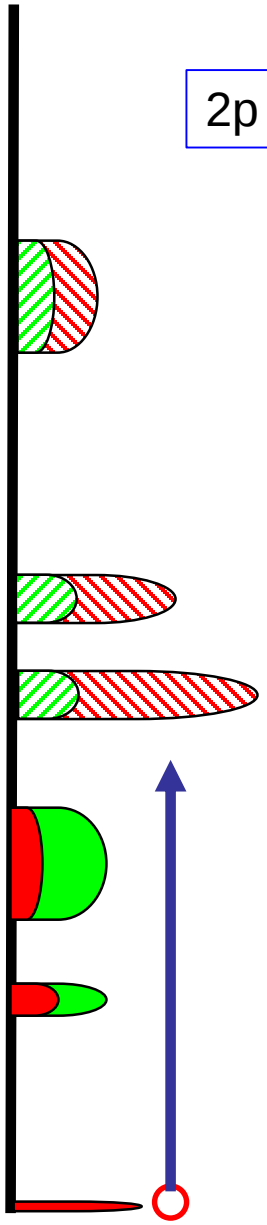
Ti 2p ~460 eV



Expect the ***d (and s-) projected Ti*** DOS

Why is experiment different?

XAS: spectral shape (Ti 2p)



2p > 3d

4sp

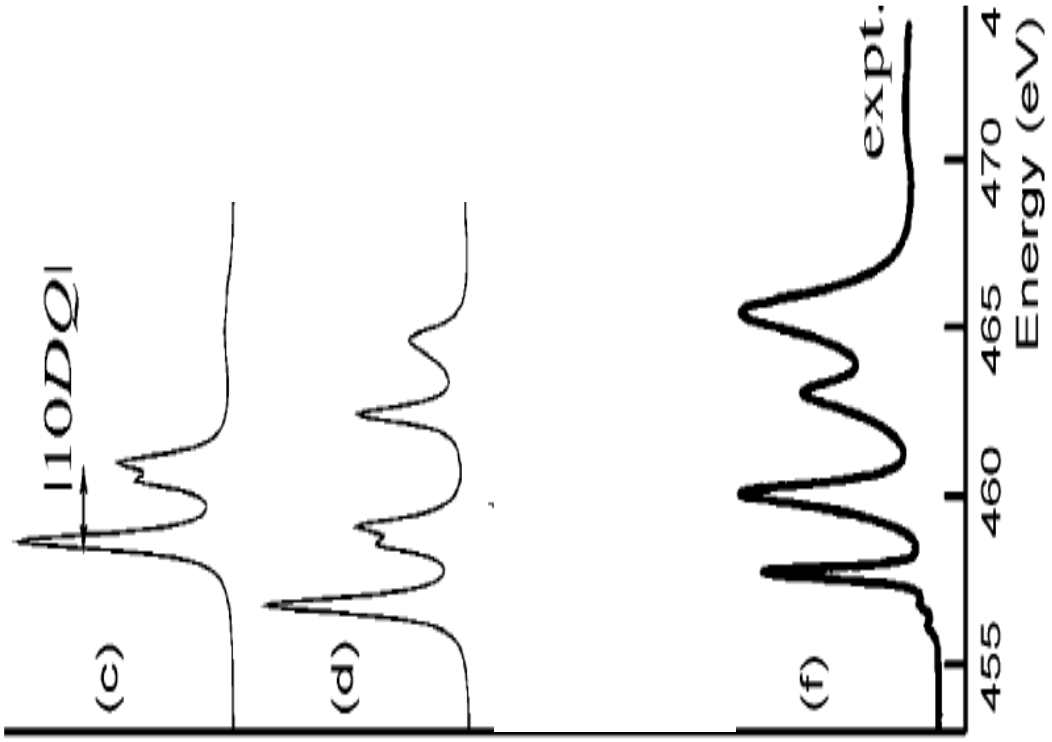
E_g

T_{2g}

O2p

O2s

Ti 2p ~460 eV

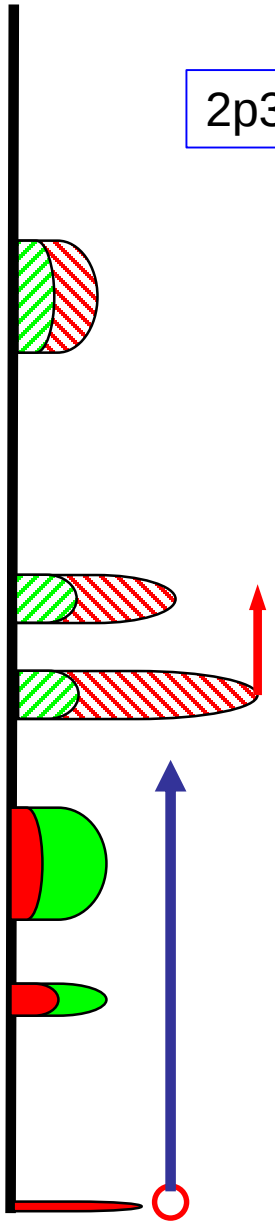


Expect the ***d (and s-) projected Ti*** DOS

2p spin-orbit coupling (~6 eV)

XAS: spectral shape (Ti 2p)

2p3d 2-electron integrals



4sp

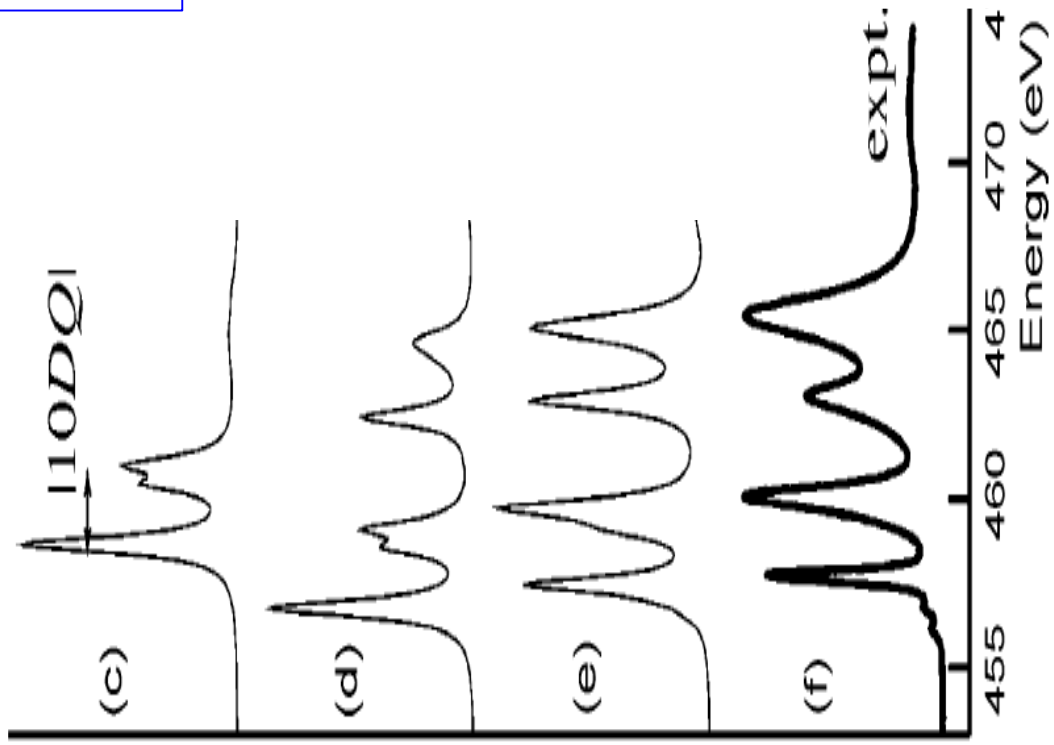
E_g

T_{2g}

O2p

O2s

Ti 2p ~460 eV



Expect ***local d-projected Ti*** DOS

Core spin-orbit splitting
Overlap of core 2p and valence 3d states
>> many electron excitations dominate

XAS: spectral shape (Ti 2p)

Fermi Golden Rule:

$I_{XAS} = |\langle \Phi_f | \text{dipole} | \Phi_i \rangle|^2 \ \delta_{[\Delta E=0]}$

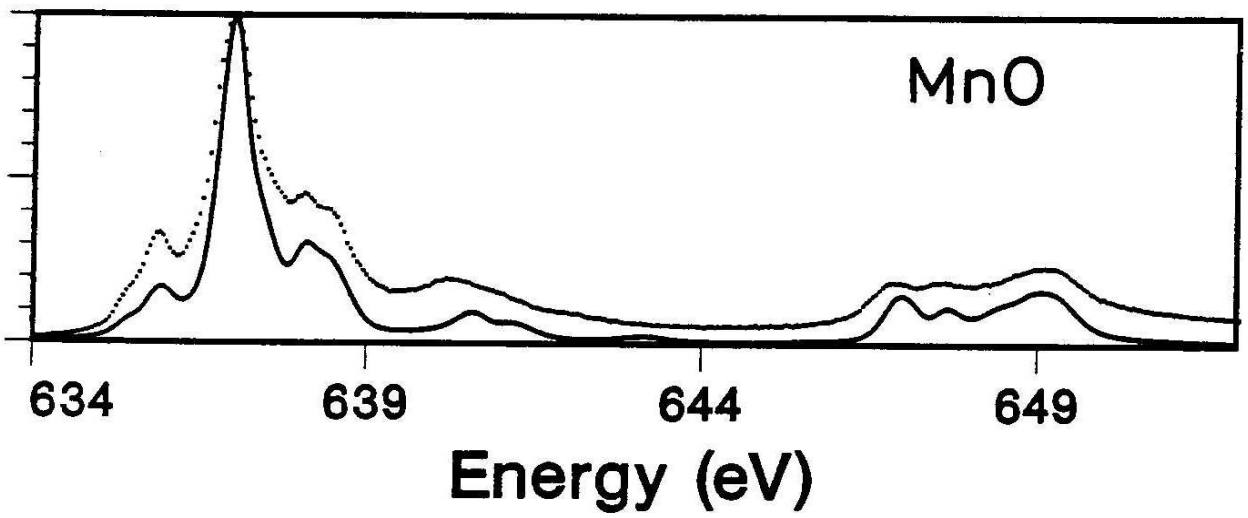
$I_{XAS} = |\langle \ 2p^5 \ 3d^1 \ | \text{dipole} | \ 3d^0 \rangle|^2 \ \delta_{[\Delta E=0]}$

1. Can NOT approximate 2p-3d interaction as extra potential
2. Large core hole spin-orbit coupling

Single electron (excitation) approximation breaks down :

~~$I_{XAS} = |\langle 3d | \text{dipole} | 2p \rangle|^2 \ \rho$~~

XAS: spectral shape (Mn 2p)



1. Can NOT neglect 3d-3d interactions
2. Can NOT approximate 2p-3d interaction as extra potential
3. Large core hole spin-orbit coupling

$$I_{XAS} = |< 2p^5\ 3d^6\ |dipole|\ 3d^5>|^2\ \delta_{[\Delta E=0]}$$

CODES: CRISPY/QUANTY, CTM4XAS

[Phys. Rev. B. 42, 5459 (1990); REVIEW: J. Elec. Spec 249, 147061 (2021)]

XAS: spectral shape (O 1s)

Fermi Golden Rule:

$$I_{XAS} = |\langle \Phi_f | \text{dipole} | \Phi_i \rangle|^2 \ \delta_{[\Delta E=0]}$$

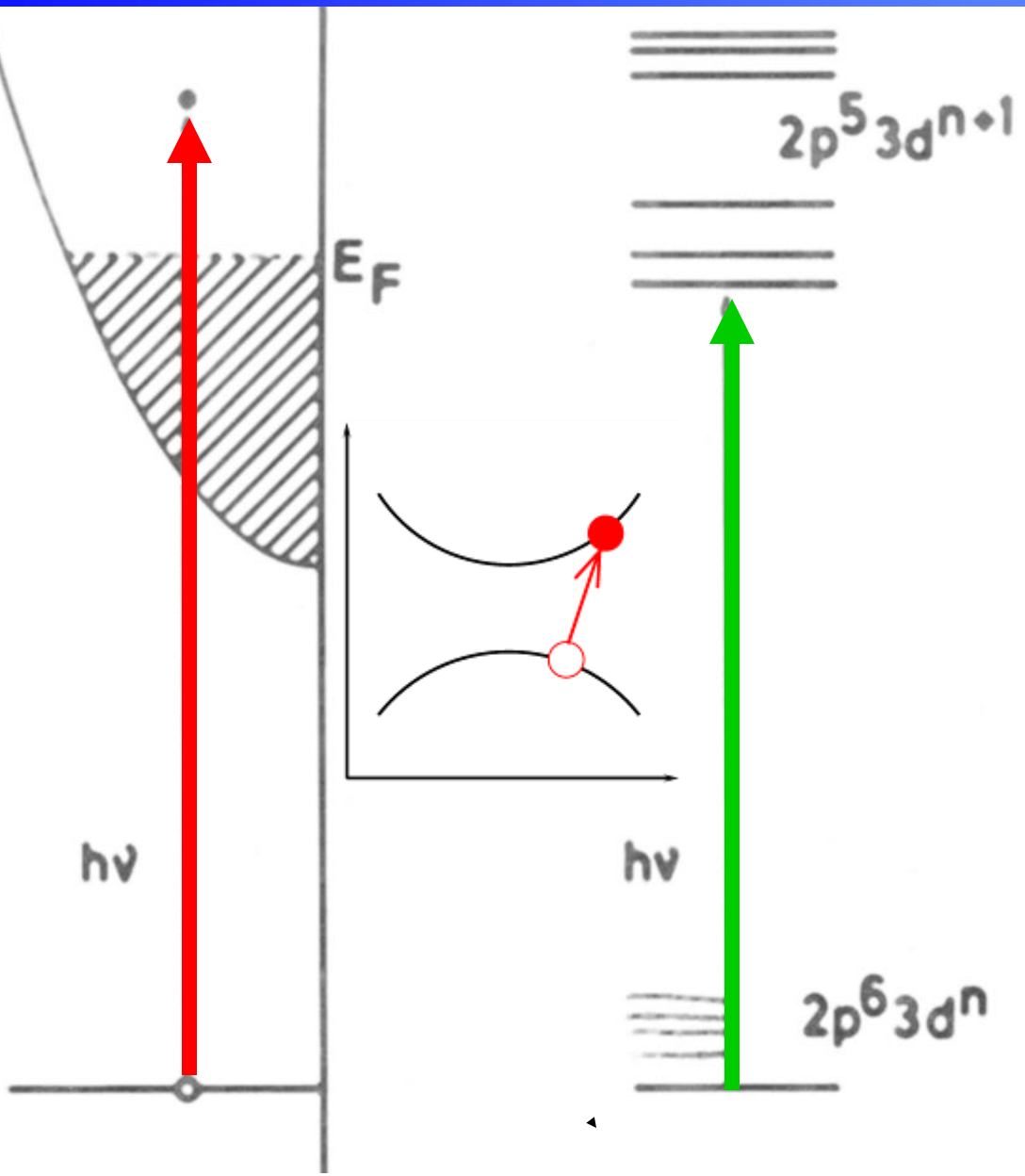
$$I_{XAS} = |\langle 1s^1 2p^5 | \text{dipole} | 2p^4 \rangle|^2 \ \delta_{[\Delta E=0]}$$

1. Can neglect local 2p-2p interaction
2. Can approximate 1s-2p interaction as extra potential
3. No core hole spin-orbit coupling

Single electron (excitation) approximation :

$$I_{XAS} = |\langle 2p | \text{dipole} | 1s \rangle|^2 \ \rho$$

Interpretation of XAS



1-particle:

1s edges

(DFT + core hole +U)

2-particle:

+ all edges of closed shell systems

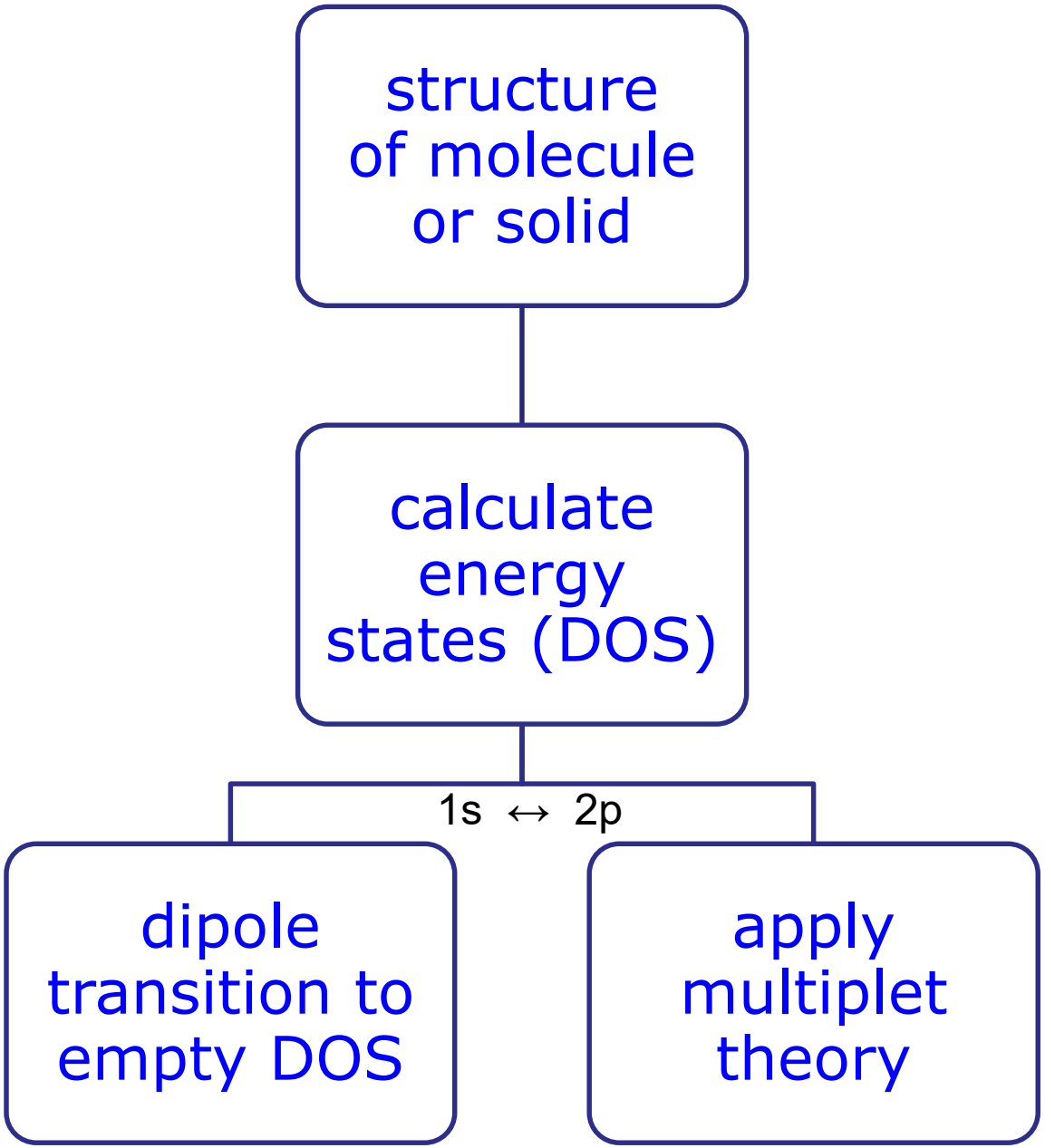
(TDDFT, BSE)

many-particle:

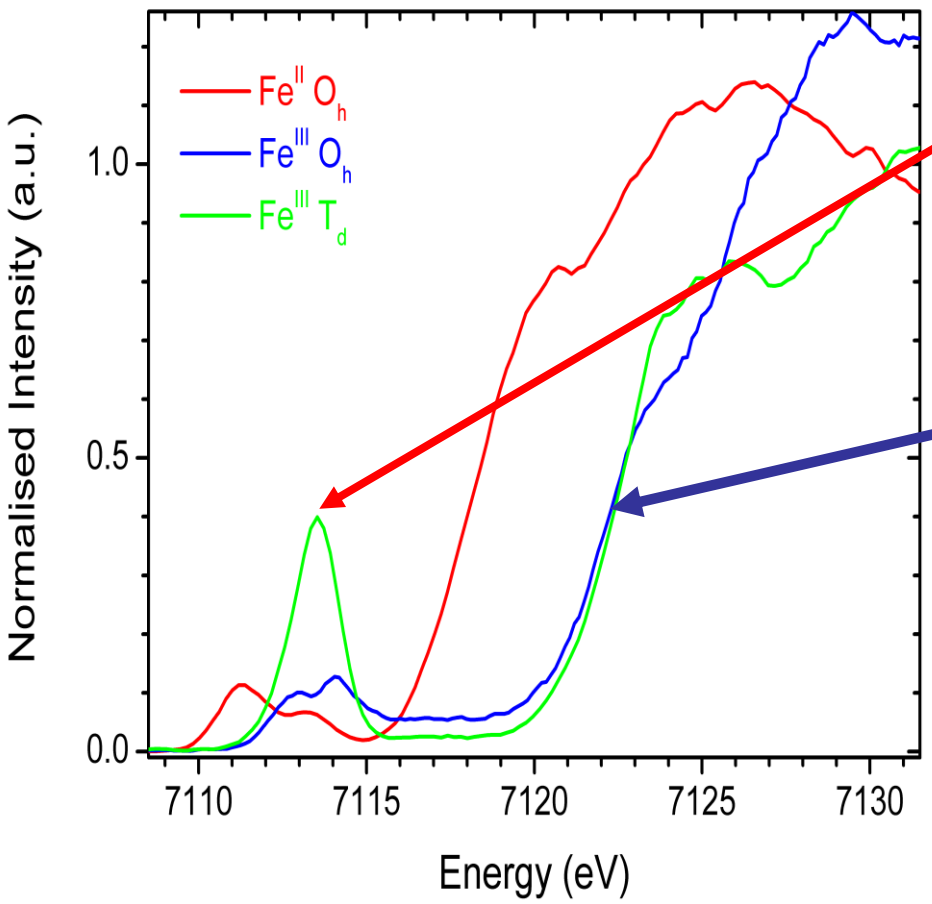
open shell systems

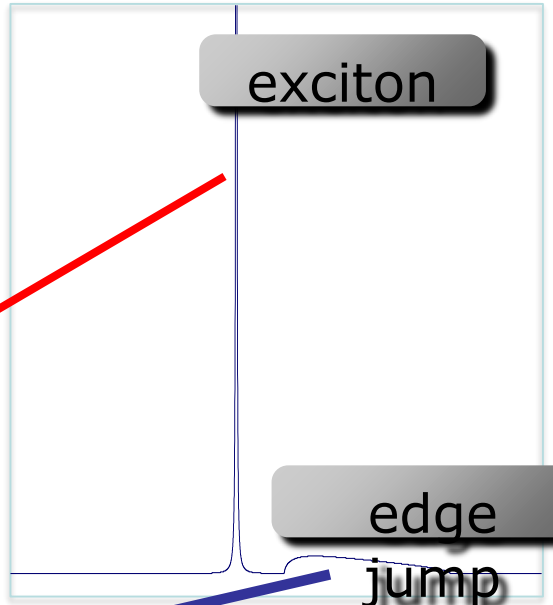
(CTM4XAS)

XAS spectral shape



Metal K edges: dipole & quadrupole

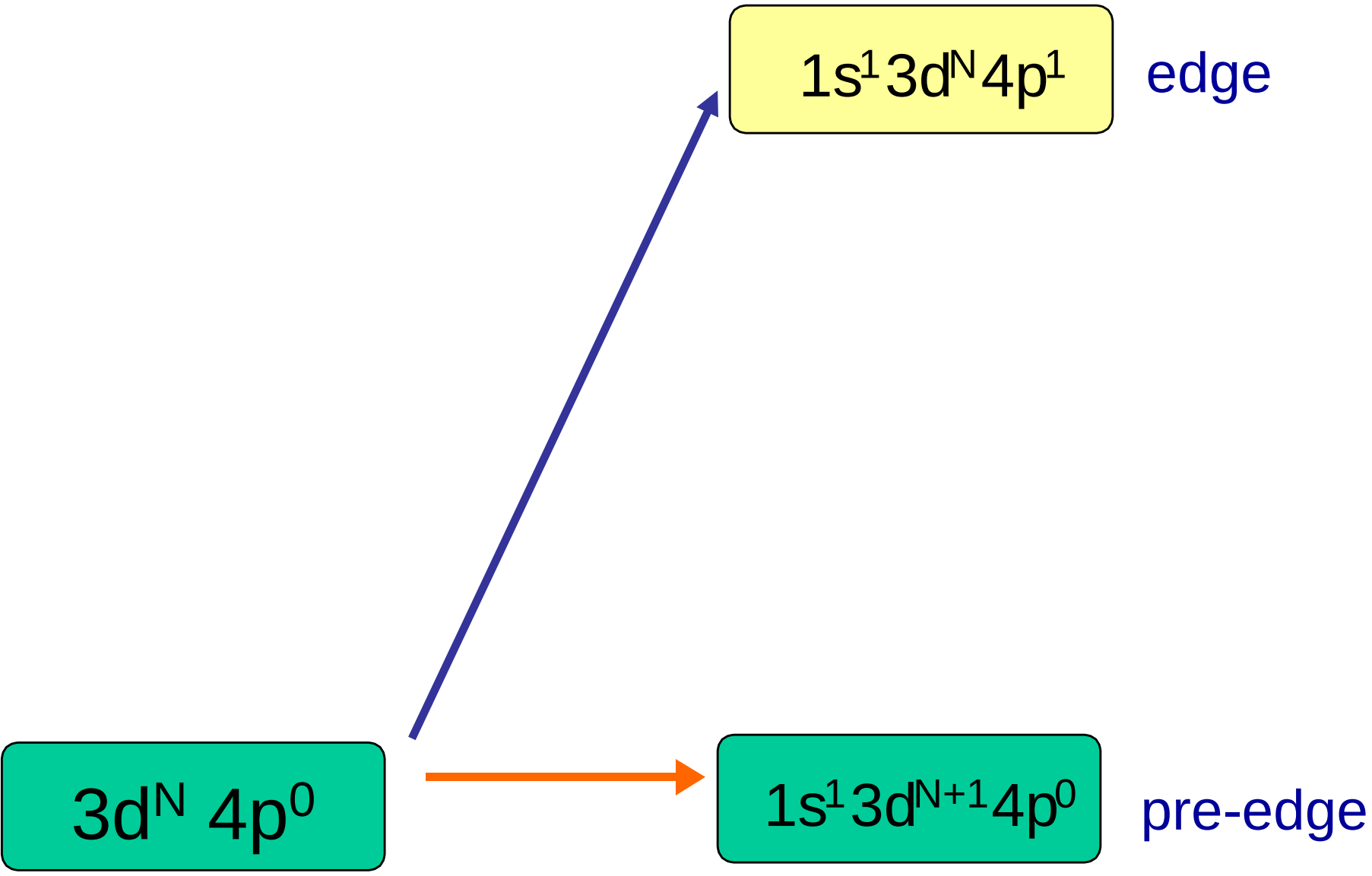




3d systems
1s > p dipole
1s > 3d quadrupole

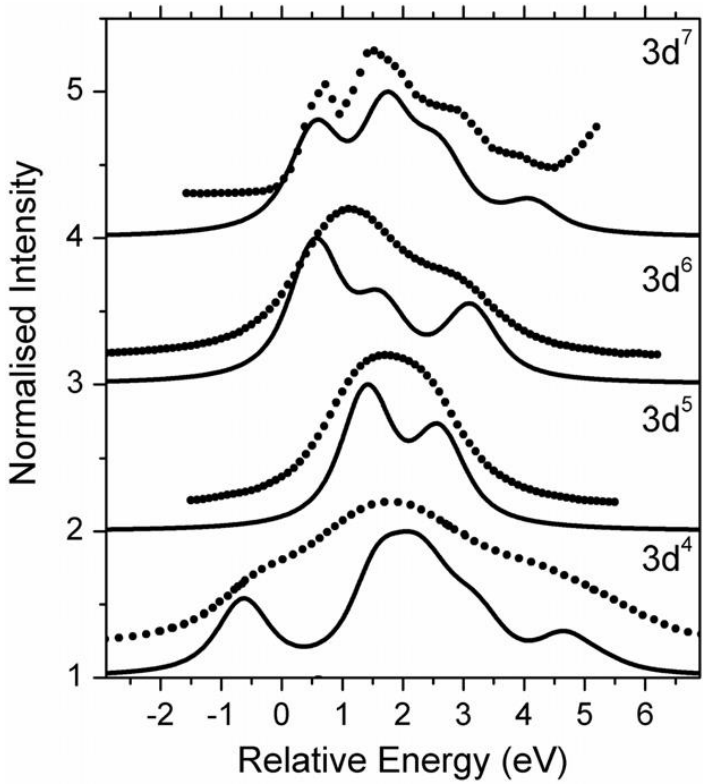
[J. Phys. Chem. B. 109, 20751 (2005)]

pre-edge (interpretation)



pre-edge (interpretation)

$1s^1 3d^N 4p^1$ edge

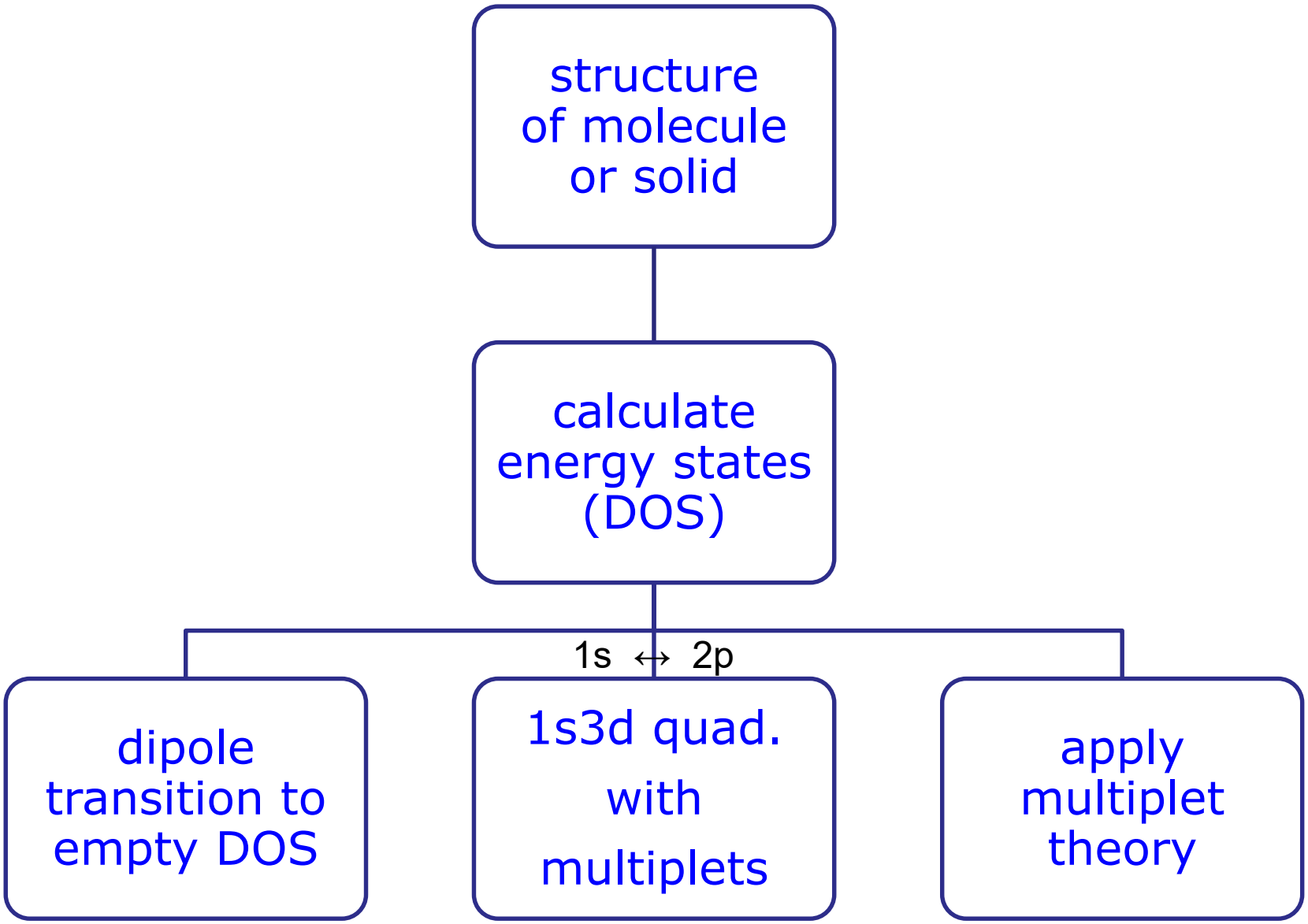


$3d^N\ 4p^0$

$1s^1 3d^{N+1} 4p^0$ pre-edge

[J. Phys. Cond. Matt. 21, 104207 (2009)]

XAS spectral shape



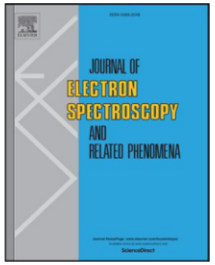
XAS multiplet codes

Journal of Electron Spectroscopy and Related Phenomena 249 (2021) 147061

Contents lists available at ScienceDirect

Journal of Electron Spectroscopy and Related Phenomena

journal homepage: www.elsevier.com/locate/elspec

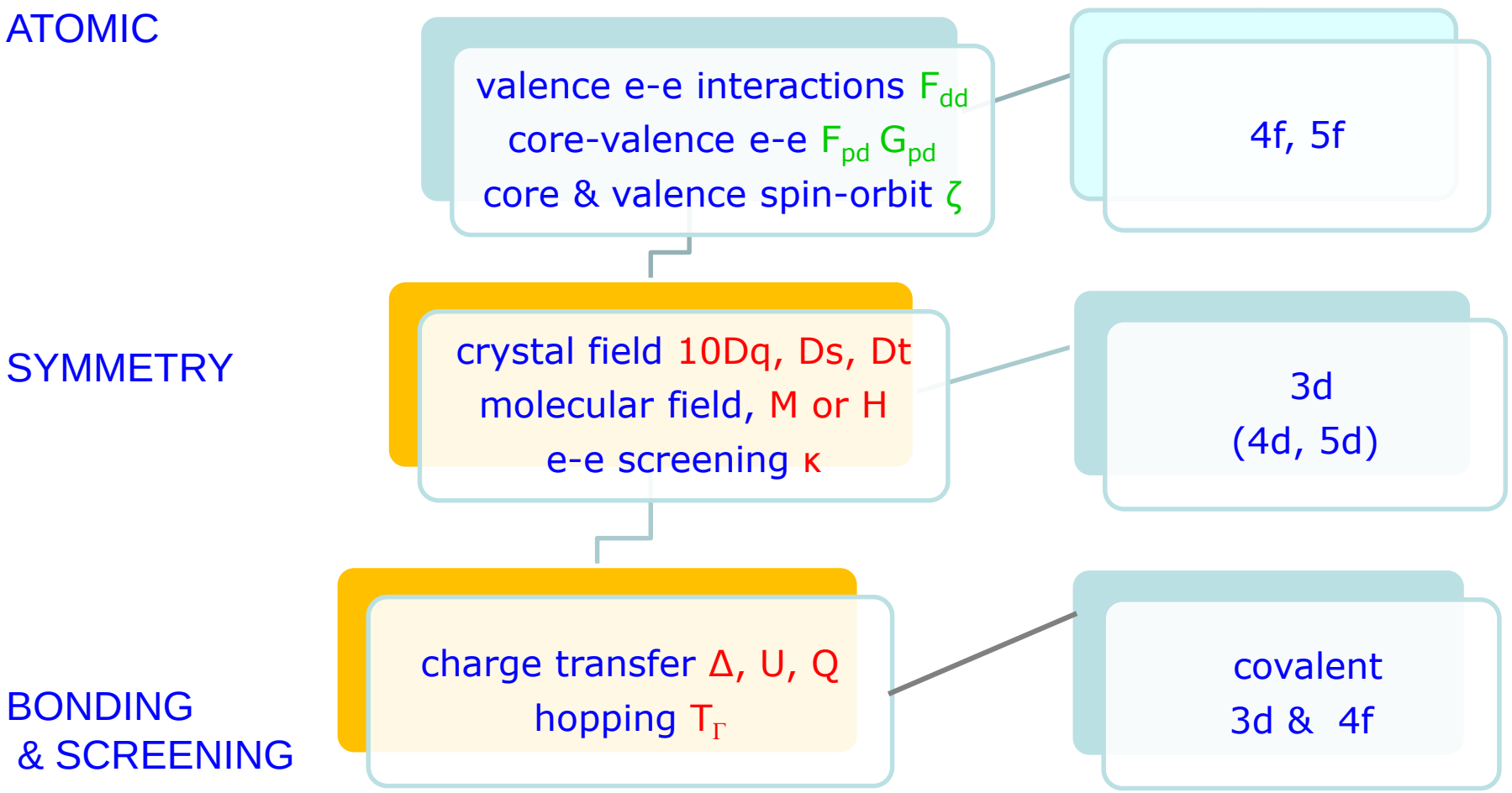


2p x-ray absorption spectroscopy of 3d transition metal systems

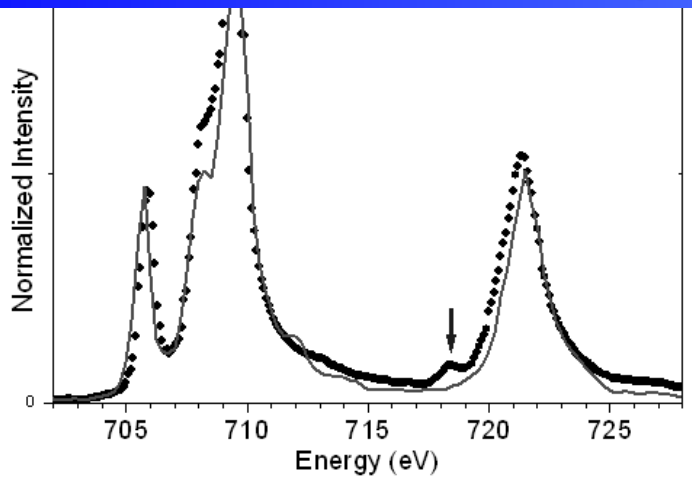
Frank M.F. de Groot [a,*], Hebatalla Elnaggar [a], Federica Frati [a], Ru-pan Wang [a], Mario U. Delgado-Jaime [b], Michel van Veenendaal [c,d], Javier Fernandez-Rodriguez [e], Maurits W. Haverkort [f], Robert J. Green [g,h], Gerrit van der Laan [i], Yaroslav Kvashnin [j], Atsushi Hariki [k], Hidekazu Ikeno [l], Harry Ramanantoanina [m], Claude Daul [n], Bernard Delley [o], Michael Odelius [p], Marcus Lundberg [q], Oliver Kuhn [r], Sergey I. Bokarev [r], Eric Shirley [s], John Vinson [s], Keith Gilmore [t], Mauro Stener [u], Giovanna Fronzoni [u], Piero Decleva [u], Peter Kruger [v], Marius Retegan [w], Yves Joly [x], Christian Vorwerk [y], Claudia Draxl [y], John Rehr [z], Arata Tanaka [A]

CODES: CTM, QUANTY, multiX, etc.

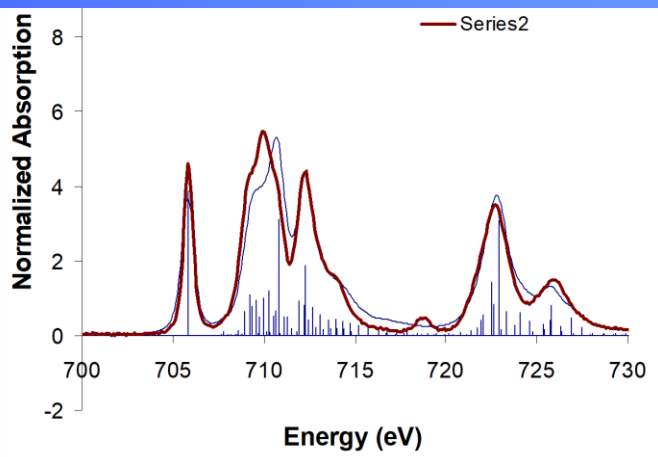
Multiplet calculations



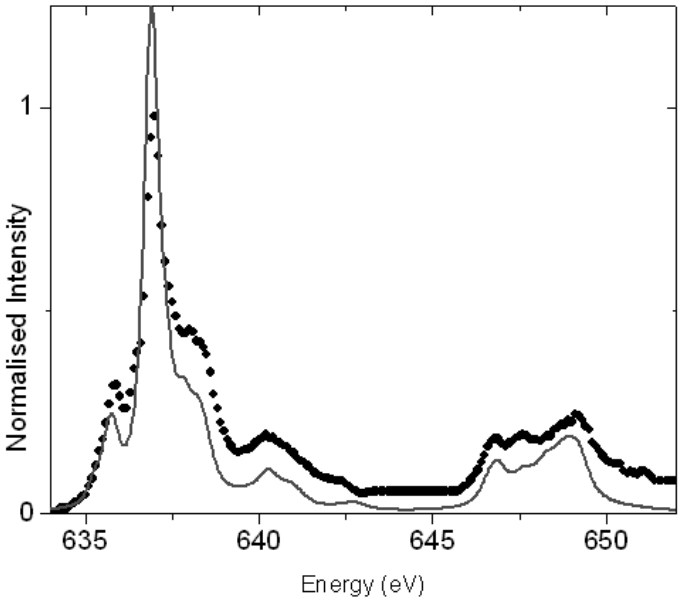
Multiplet calculations



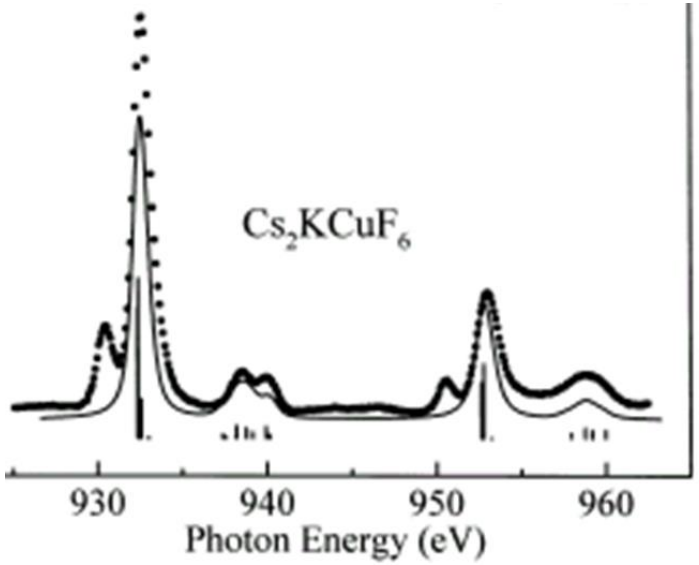
Fe(III)-tacn (low-spin Oh)



Fe(III)-CN (MLCT & LMCT)



MnO (high-spin Oh)



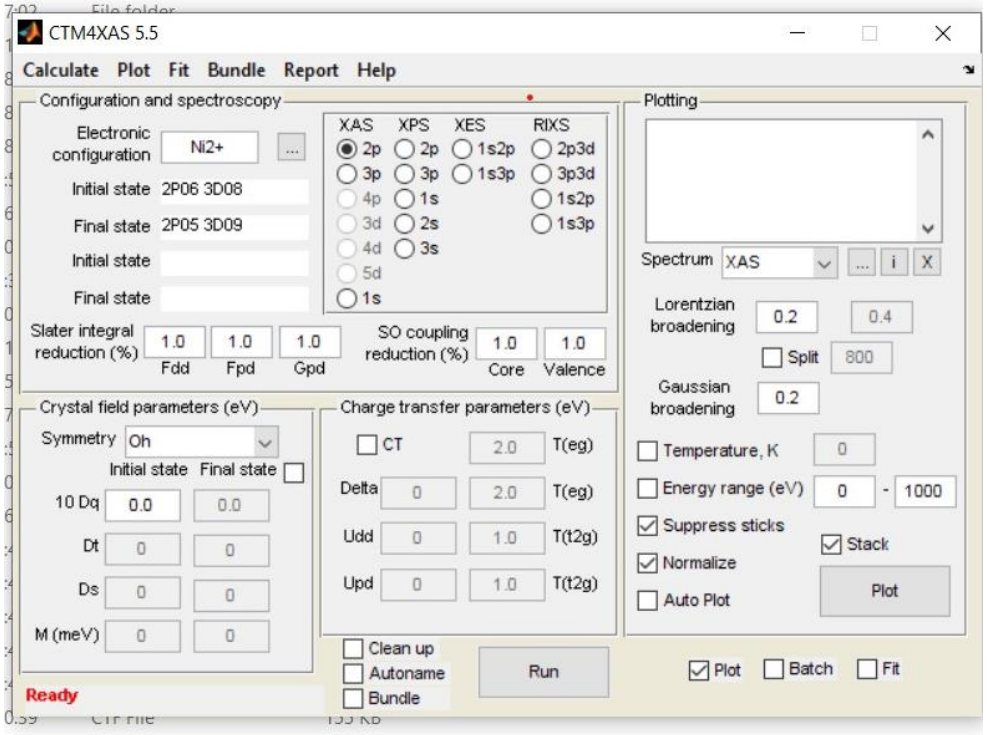
Cu(III) (strong LMCT)

Multiplet calculations: CTM4XAS

- Calculations for all core level spectroscopies of open shell systems (when DFT and TD-DFT break down)
- Interfaces: XAS & XMCD; XPS; XES & RIXS

- Also: Auger, resonant photoemission, coincidence (not in interface)

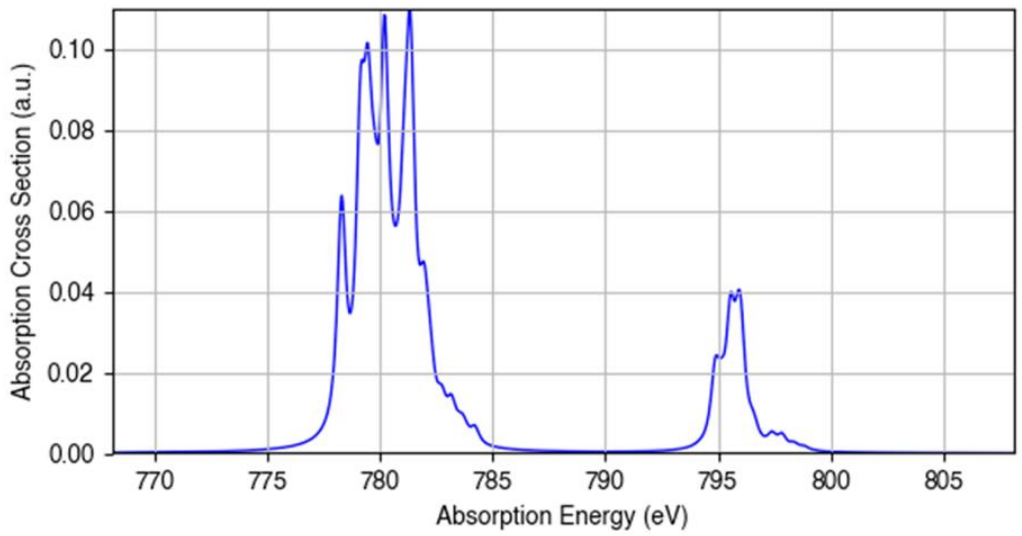
- Monday or Tuesday break: can teach how to get started with calculations CTM4XAS and/or QUANTY



f.m.f.degroot@uu.nl

Multiplet calculations: quanty

Crispy - Co2+_L-edge.lua



Analysis of the initial Hamiltonian:

i	<E>	<S^2>	<L^2>	<J^2>	<Sz>	<Lz>	<Jz>	<N_2p>	<N_3d>
1	-3.0980	3.7459	11.7904	23.0136	-0.1208	-0.0831	-0.2039	6.0000	7.0000
2	-3.0980	3.7459	11.7904	23.0136	0.1208	0.0831	0.2039	6.0000	7.0000

Spectrum calculation for each of the selected states:

i	dZ
1	1.00E+00
2	1.00E+00

Quanty

General Setup

Element and Experiment

Co | 2+ | Oh

XAS | L2,3 (2p)

Experimental Conditions

Temperature (K): 10.0

Magnetic Field (T): 0.0

Absorbtion Energy

Range (eV): 768.1 — 808.1

Number of Points: 1000

Broadening FWHM (eV)

Lorentzian: 0.43

Gaussian: 0.1

Wave and Polarization Vectors

$\mathbf{k}_{in}$ [x, y, z]: [0, -1, 0]

$\boldsymbol{\varepsilon}_{in}$ [x, y, z]: [0, 0, 1]

Spectra

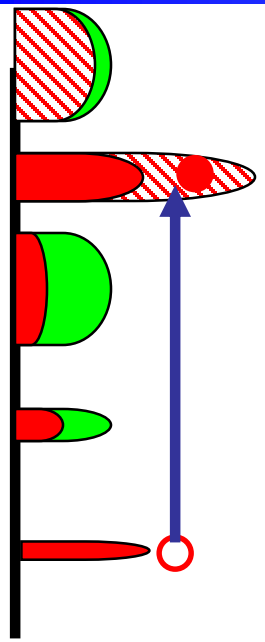
☑ Isotropic ☐ XMCD ☐ X(M)LD

Hamiltonian Setup

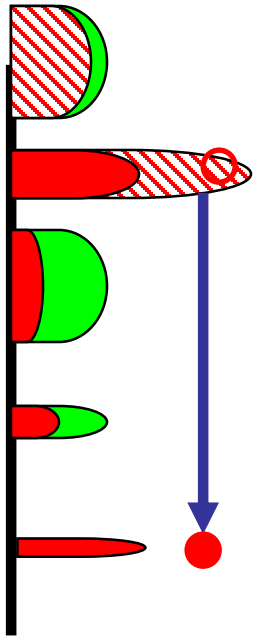
Results

Save Input As... | Run

Decay of the core hole



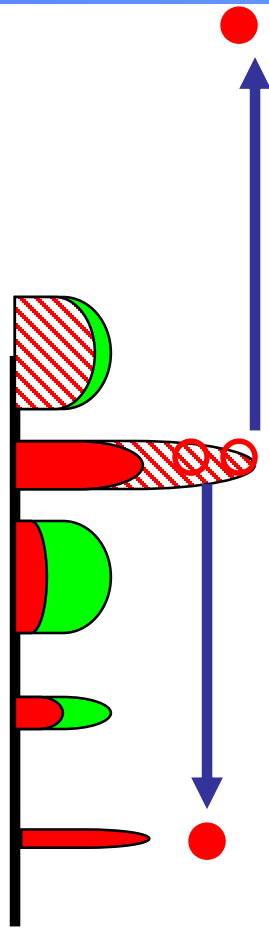
XAS



x-ray emission
1%

(2 meV)

500 nm



Auger
99%

200 meV

5 nm

XAS: detection techniques

Transmission

(homogeneous, saturation > **thin samples**)

below ~50 nm

Electron Yield

> **surface** sensitive (5 nm)

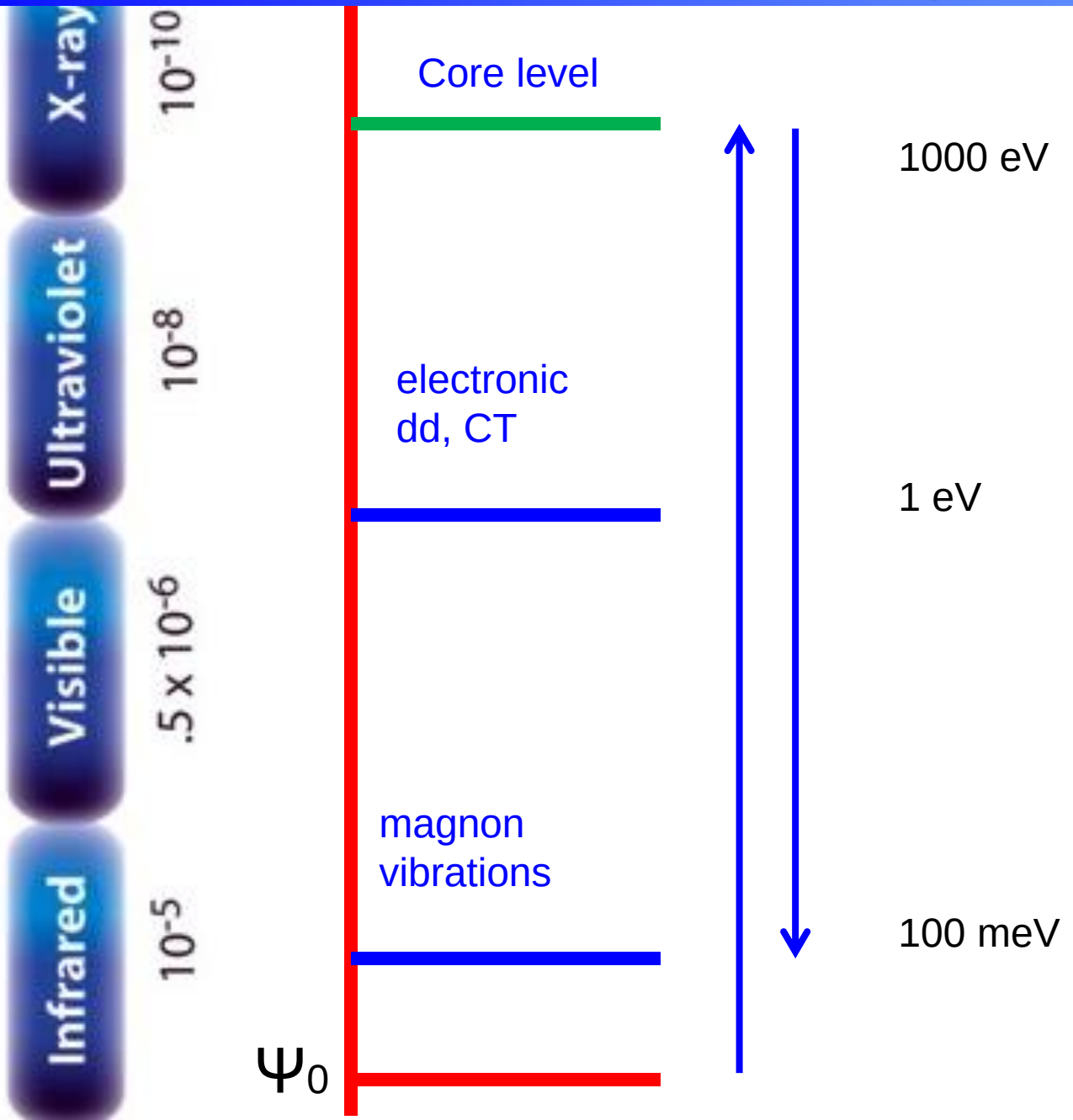
Fluorescence Yield

saturation = energy dep. probing depth
self-absorption = re-absorption emitted x-rays

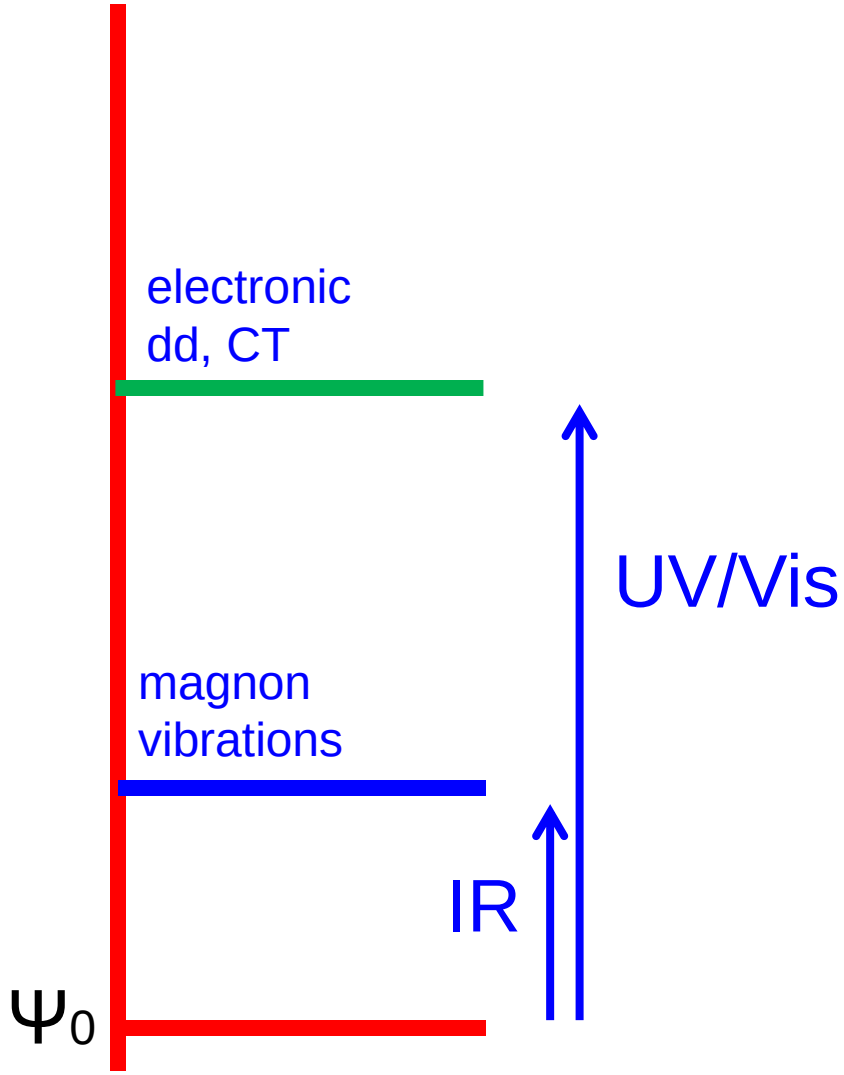
> **dilute samples** below ~5%

[L edges are intrinsically distorted]

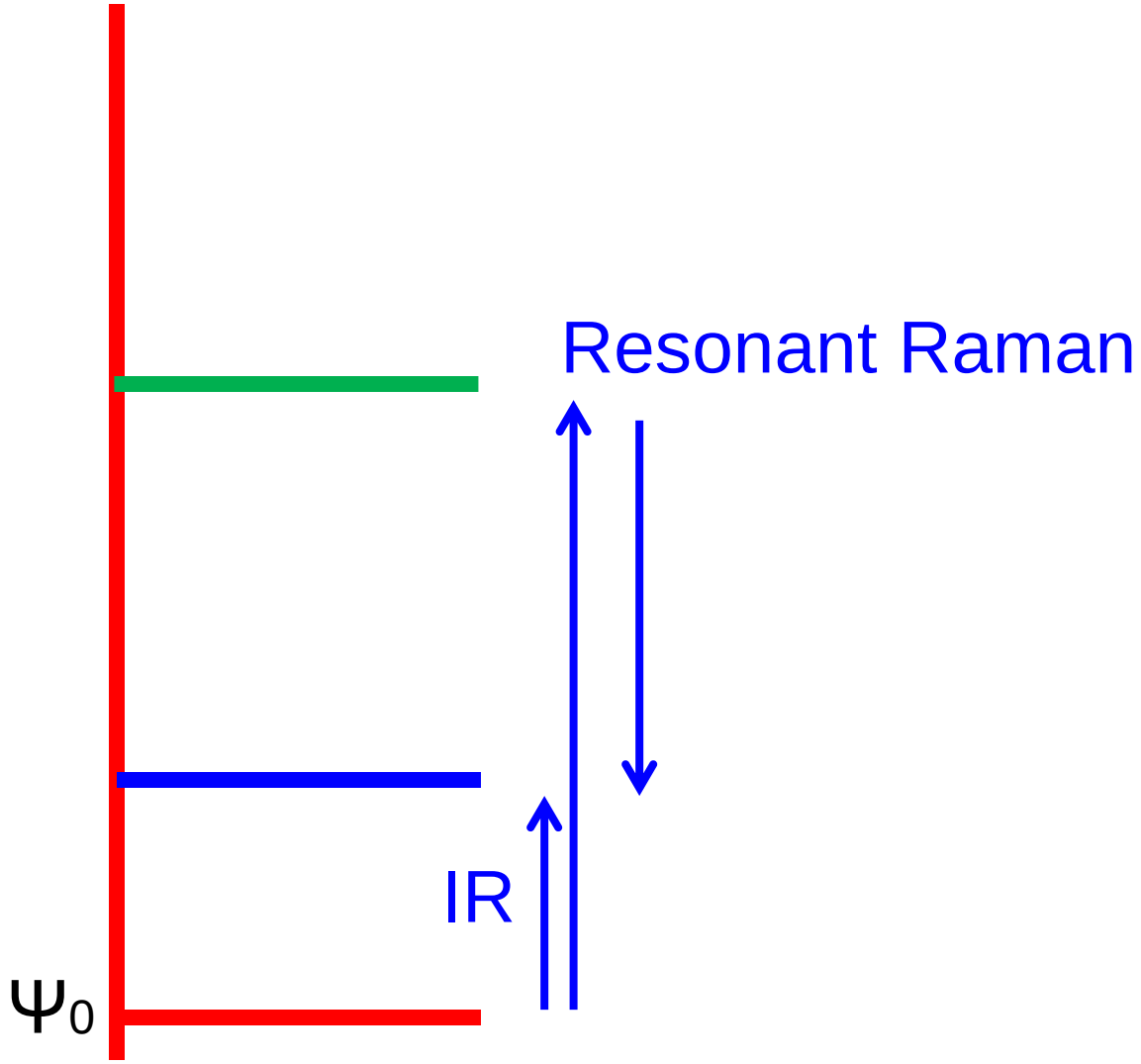
resonant inelastic x-ray scattering



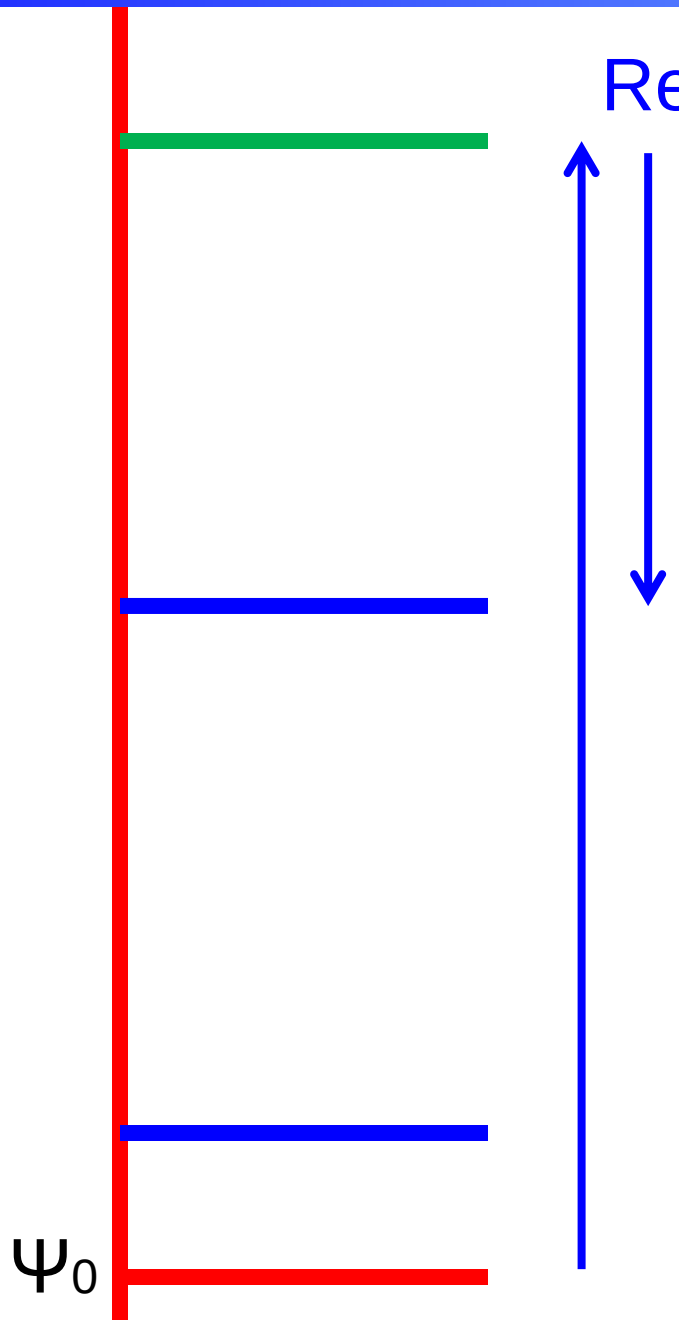
resonant inelastic x-ray scattering



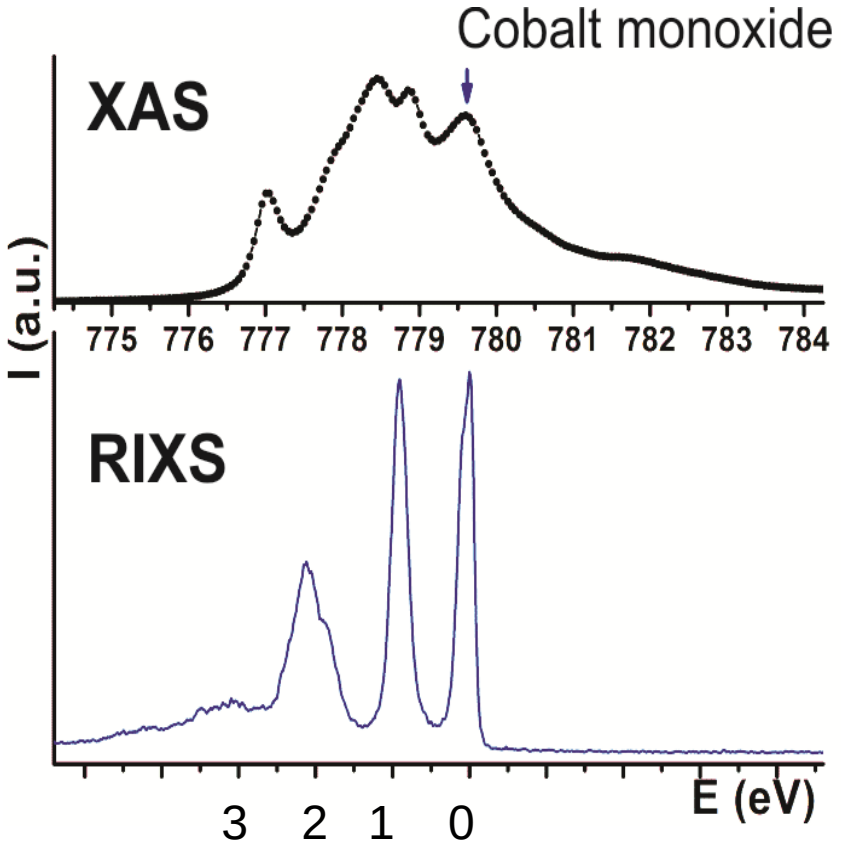
resonant inelastic x-ray scattering



resonant inelastic x-ray scattering



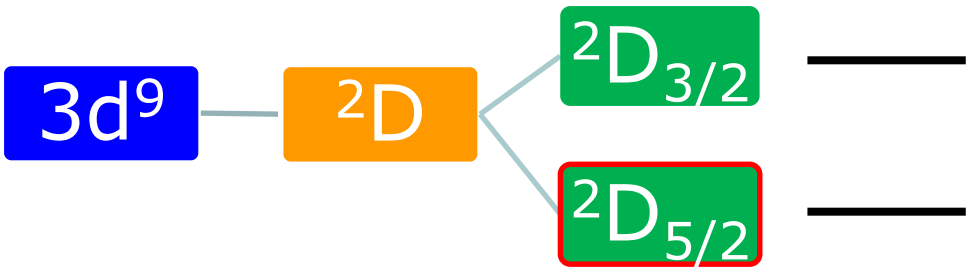
Resonant X-ray Raman



Cu2+ 2p3d RIXS (from $3d^9$ to $2p^5 3d^{10}$ to $3d^9$)

ATOMIC

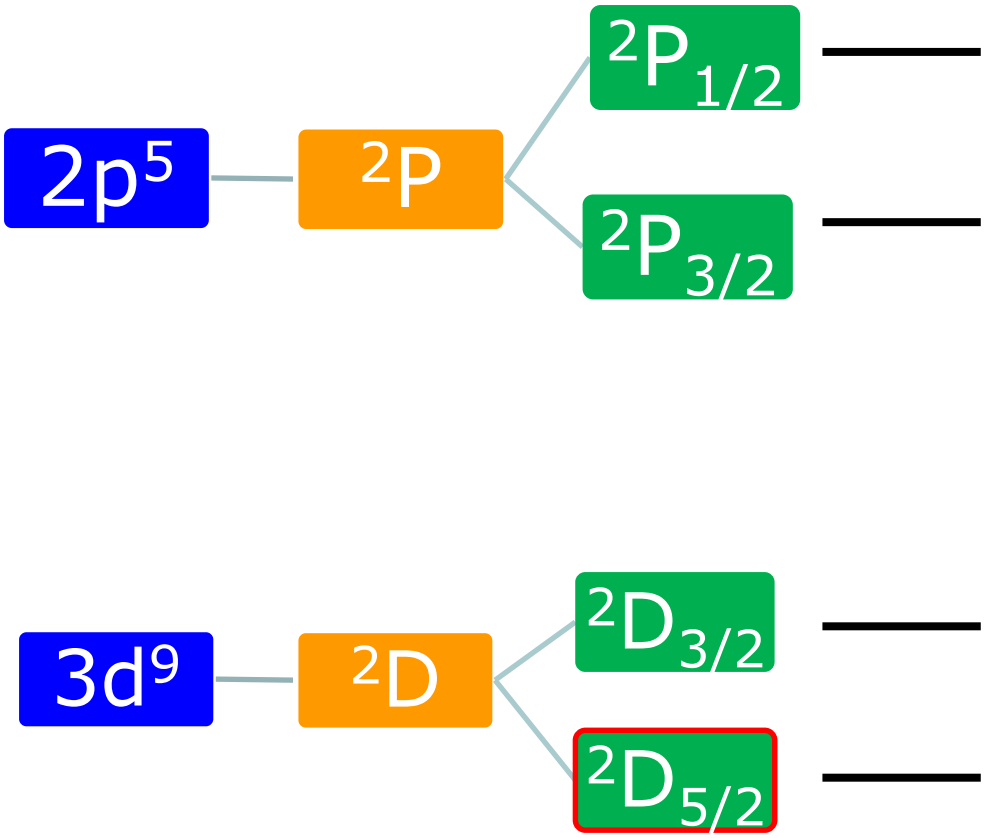
Dipole selection rule:
ΔJ=-1, 0 or +1
J=J'≠0



Cu2+ 2p3d RIXS (from $3d^9$ to $2p^5 3d^{10}$ to $3d^9$)

ATOMIC

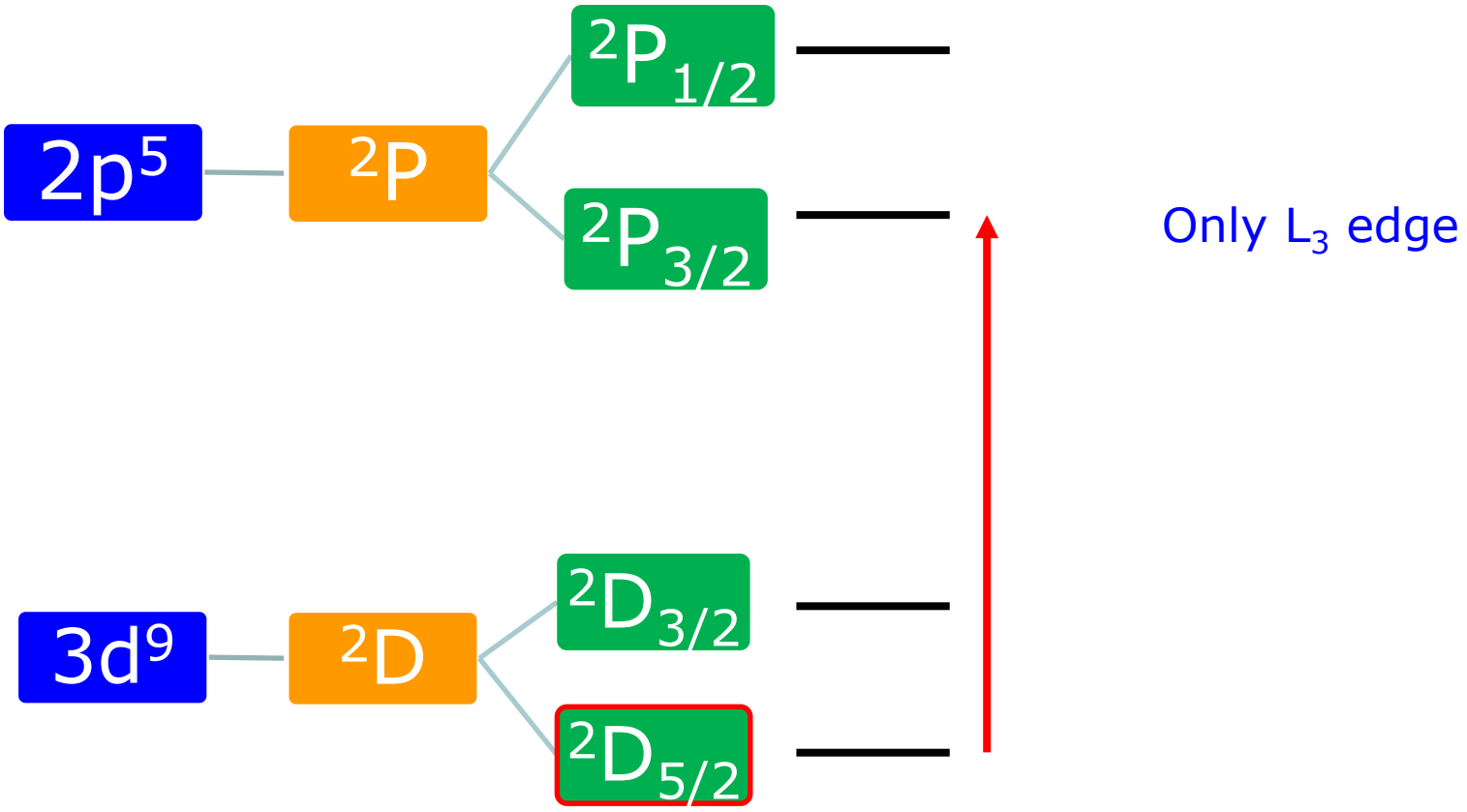
Dipole selection rule:
ΔJ=-1, 0 or +1
J=J'≠0



Cu2+ 2p XAS (from $3d^9$ to $2p^5 3d^{10}$)

ATOMIC

Dipole selection rule:
$\Delta J = -1, 0 \text{ or } +1$
$J = J' \neq 0$

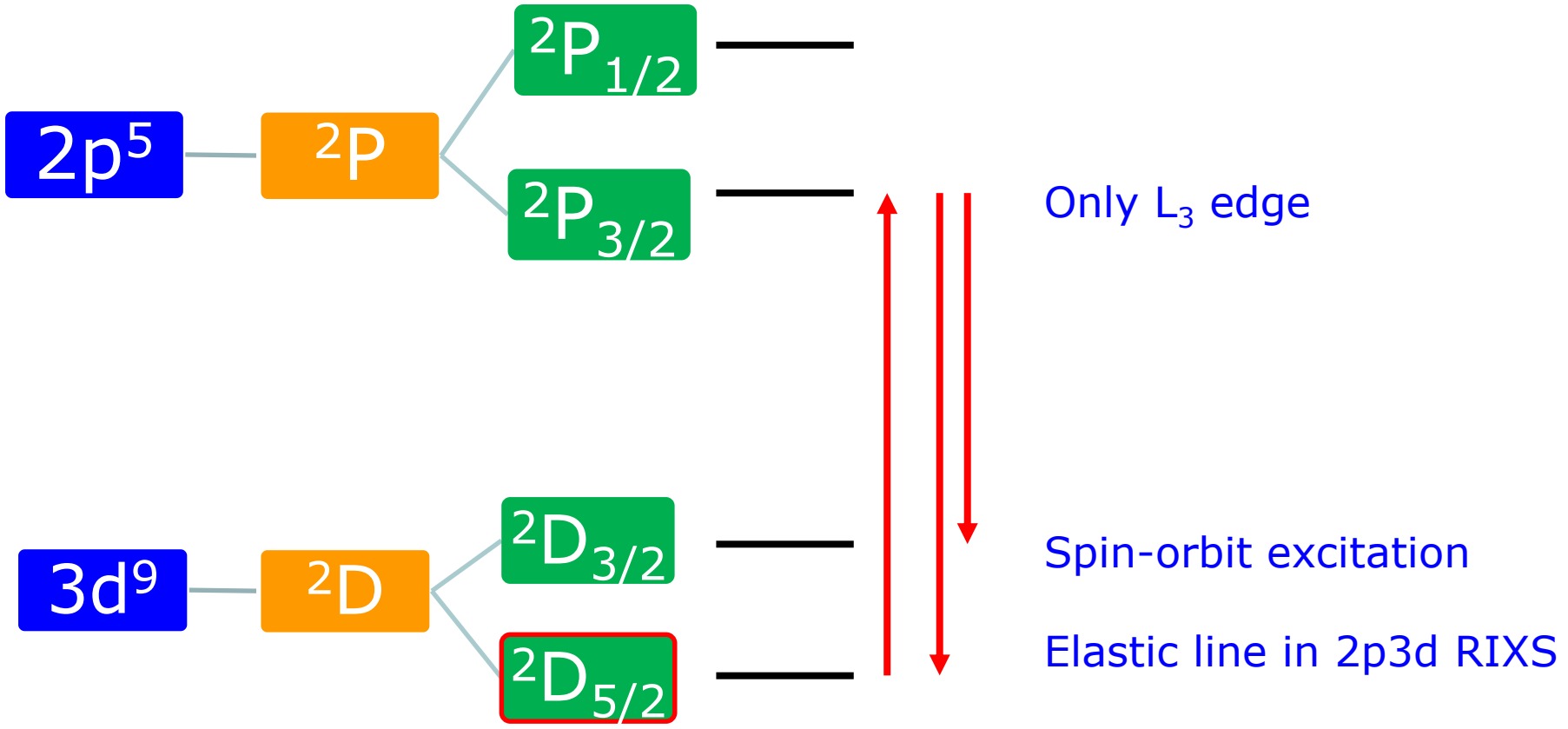


Only L_3 edge

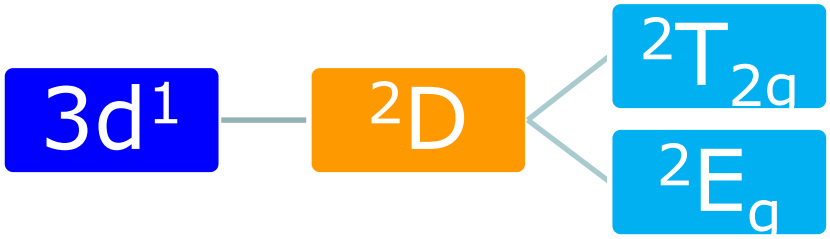
Cu2+ 2p3d RIXS (from $3d^9$ to $2p^5 3d^{10}$ to $3d^9$)

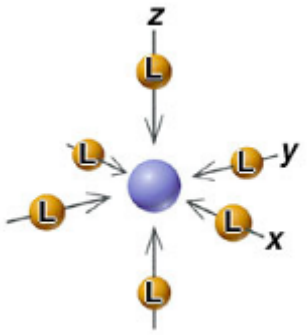
ATOMIC

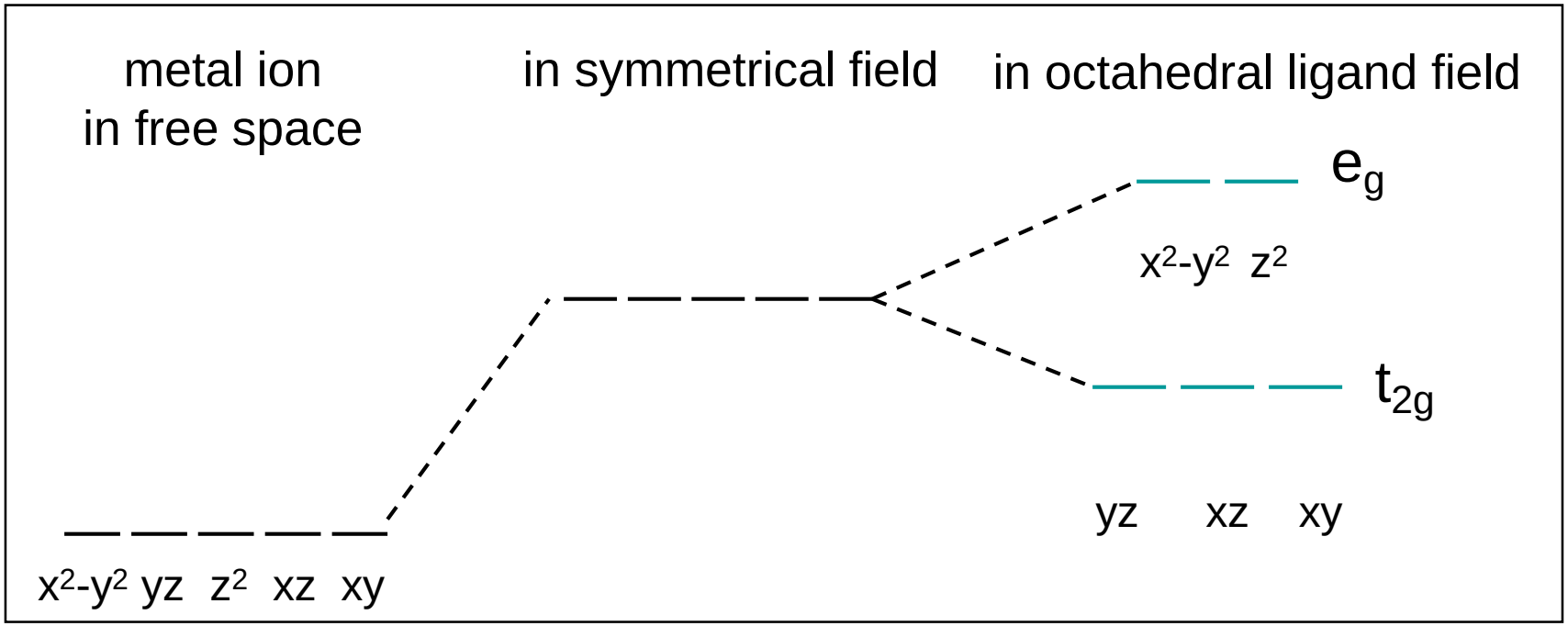
Dipole selection rule:
ΔJ=-1, 0 or +1
J=J'≠0



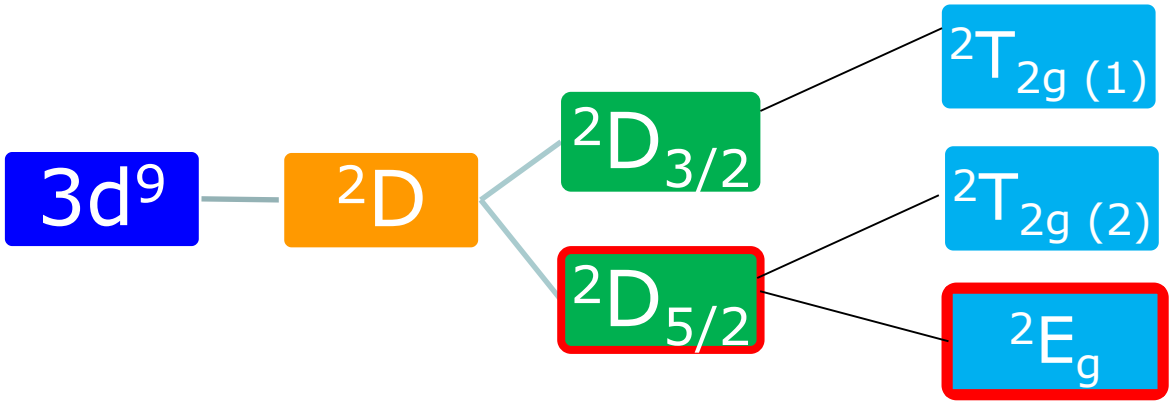
CRYSTAL FIELD EFFECT

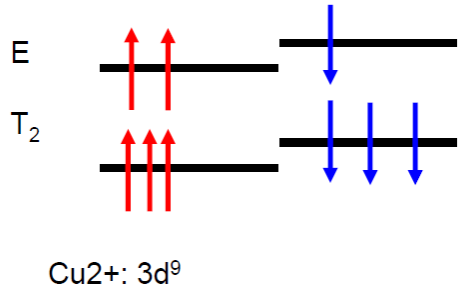


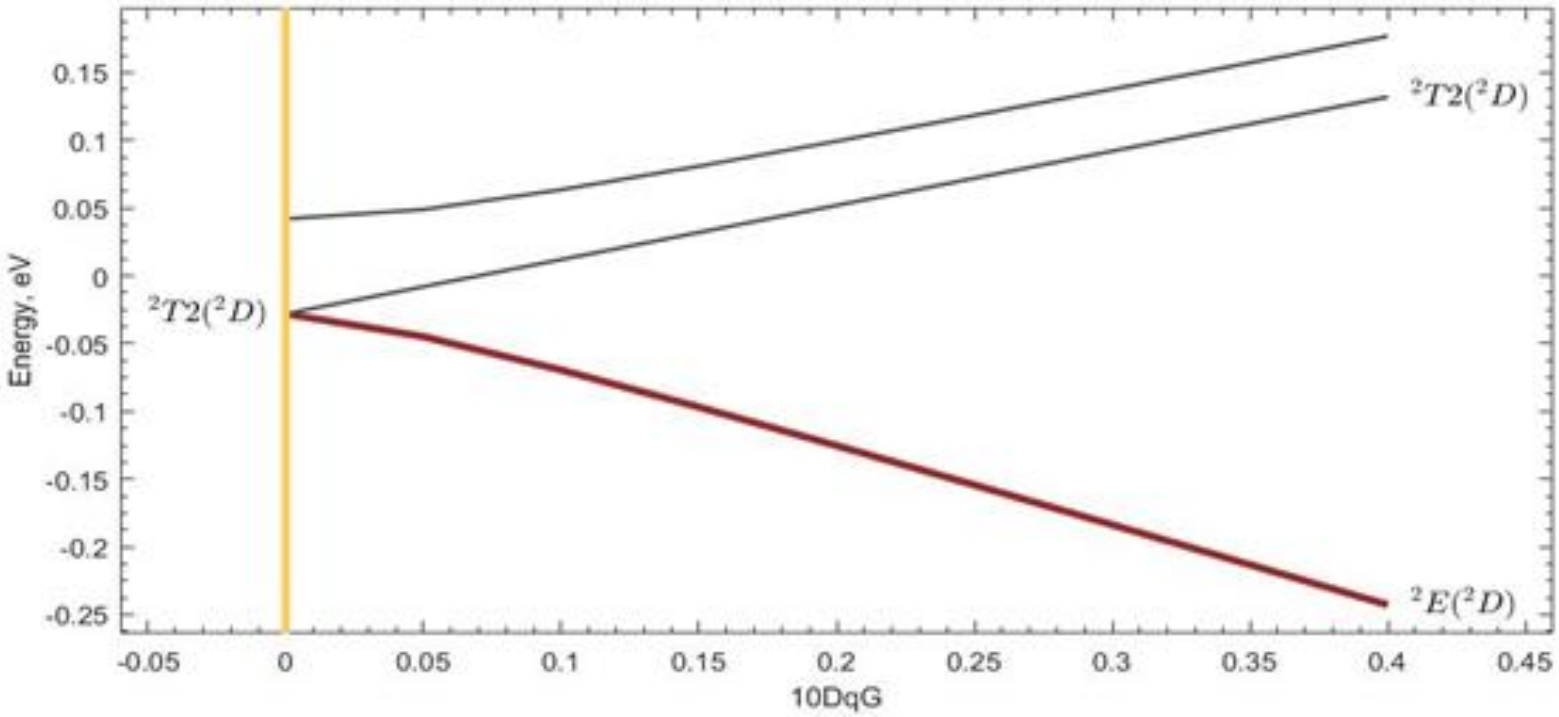




CRYSTAL FIELD EFFECT



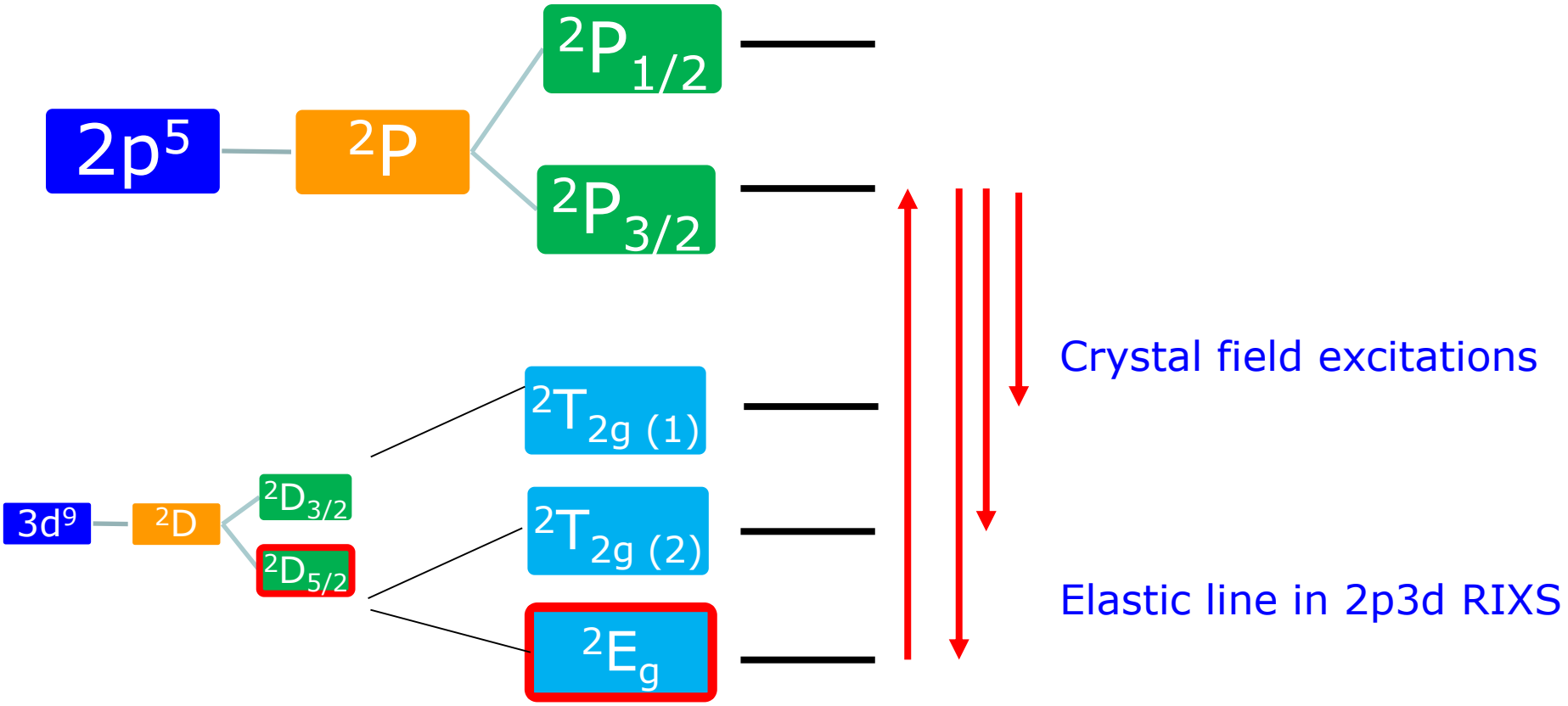




Cu2+ 2p3d RIXS (from $3d^9$ to $2p^5 3d^{10}$ to $3d^9$)

OCTAHEDRAL

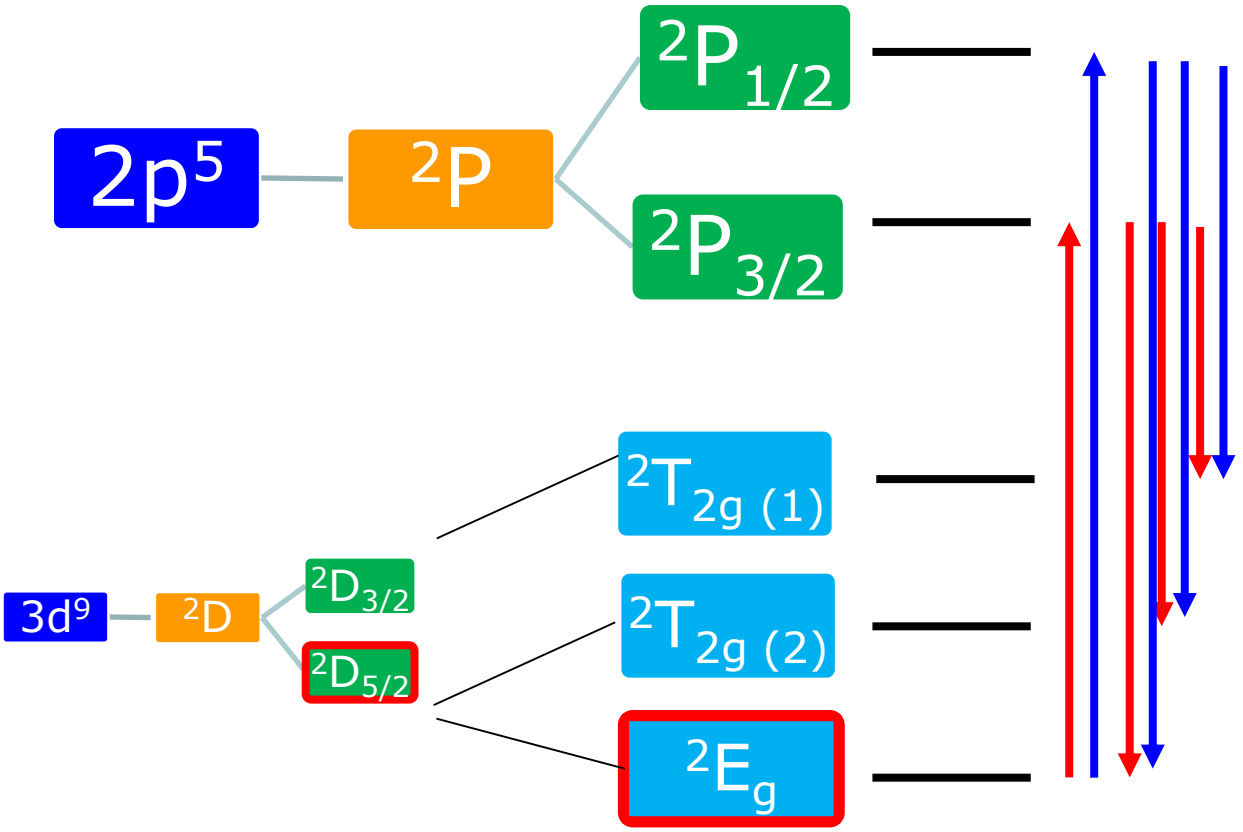
Dipole selection rule:
ΔJ=-1, 0 or +1
J=J'≠0



Cu2+ 2p3d RIXS (from $3d^9$ to $2p^5 3d^{10}$ to $3d^9$)

OCTAHEDRAL

Dipole selection rule:
$\Delta J = -1, 0 \text{ or } +1$
$J = J' \neq 0$



Crystal field mixes J states

Both L_3 and L_2 edges

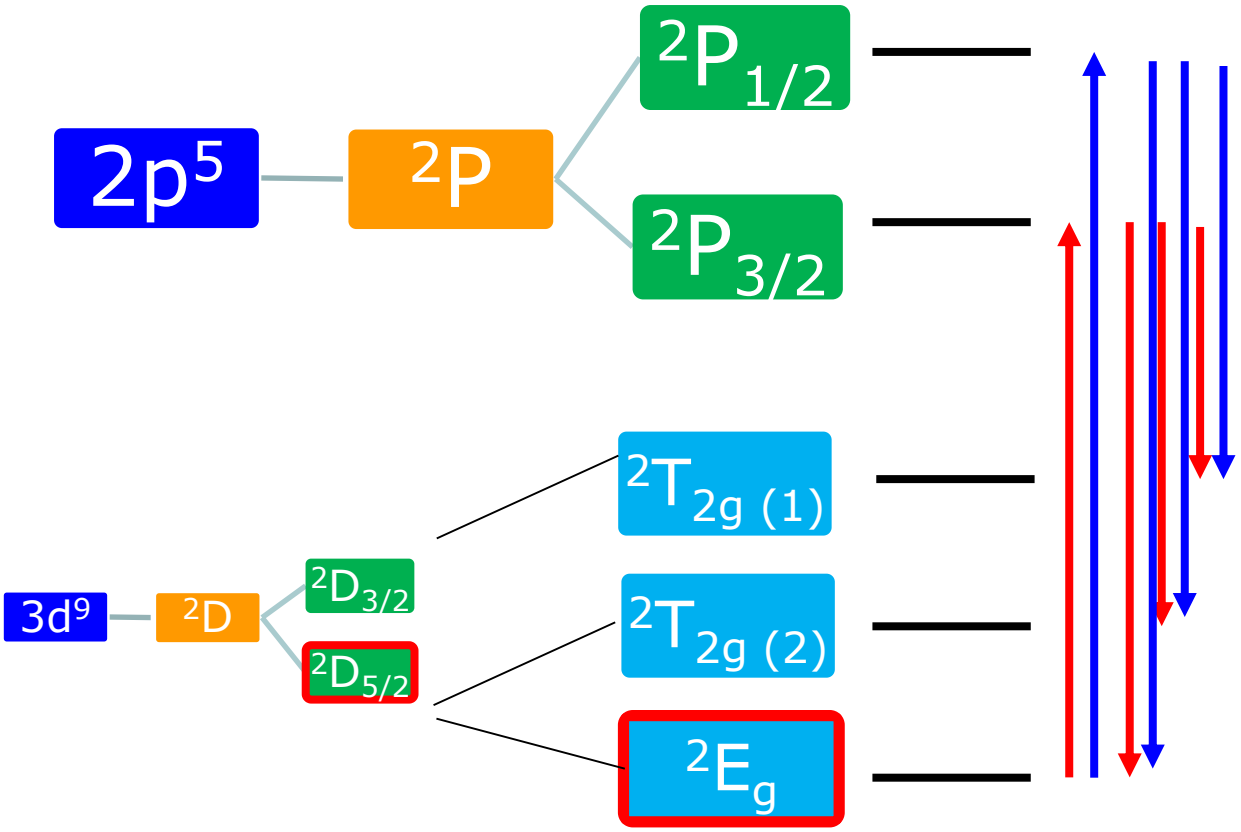
Crystal field excitations

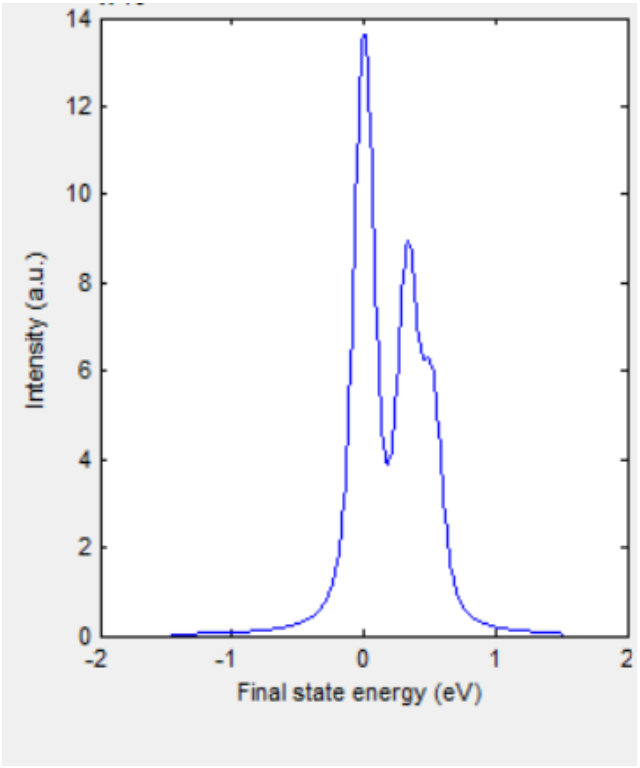
Elastic line in 2p3d RIXS

Cu2+ 2p3d RIXS (from $3d^9$ to $2p^5 3d^{10}$ to $3d^9$)

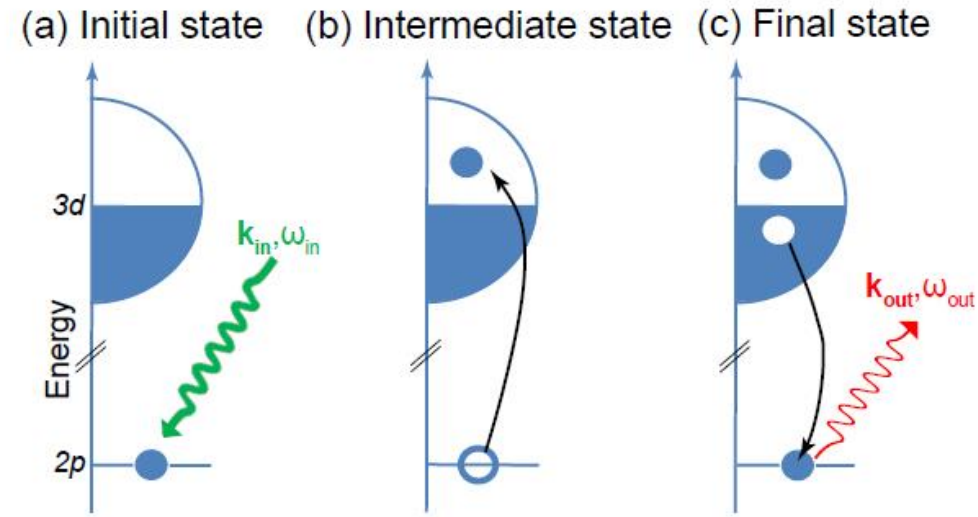
OCTAHEDRAL

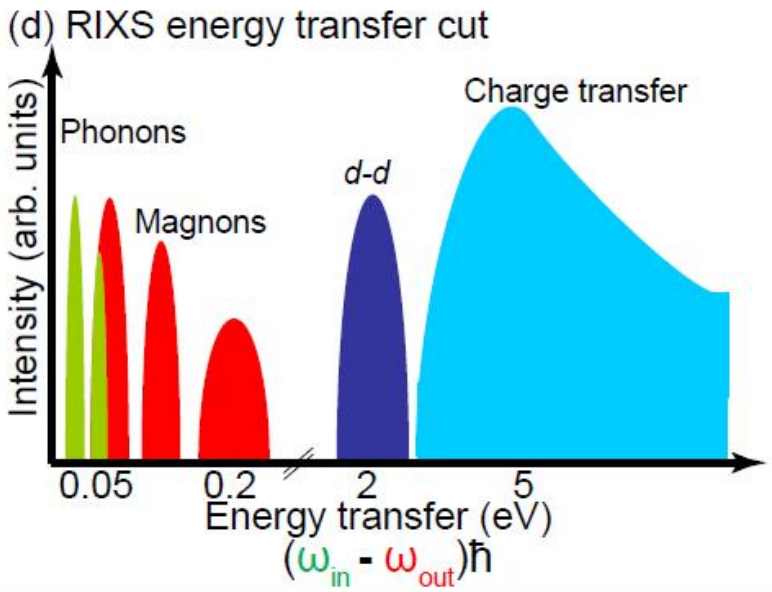
Dipole selection rule:
ΔJ=-1, 0 or +1
J=J'≠0

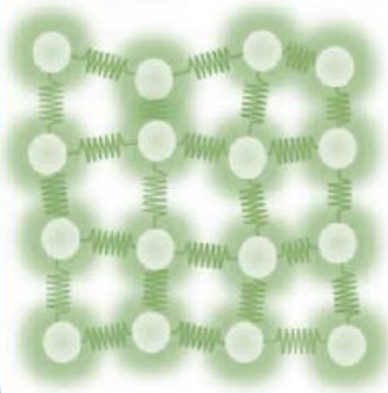


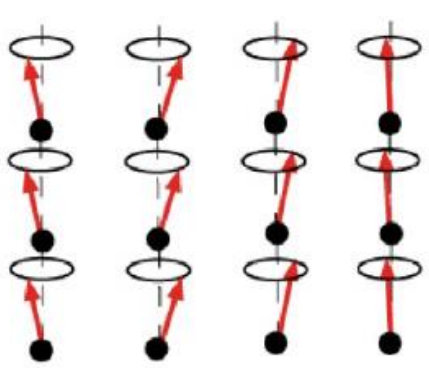


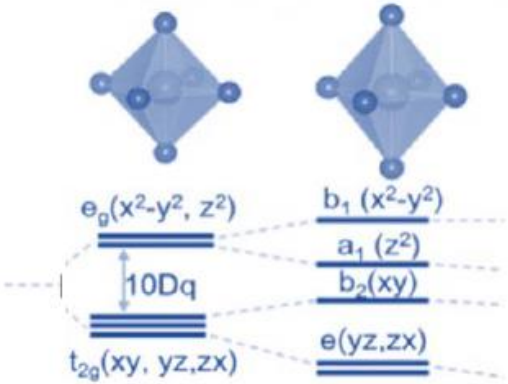
2p3d RIXS of transition metal ions

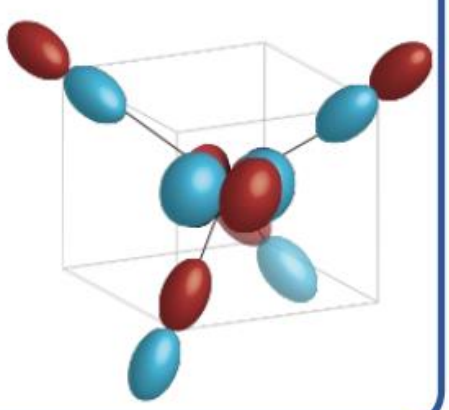












2p3d RIXS of transition metal ions

10^{-10}

10^{-8}

$.5 \times 10^{-6}$

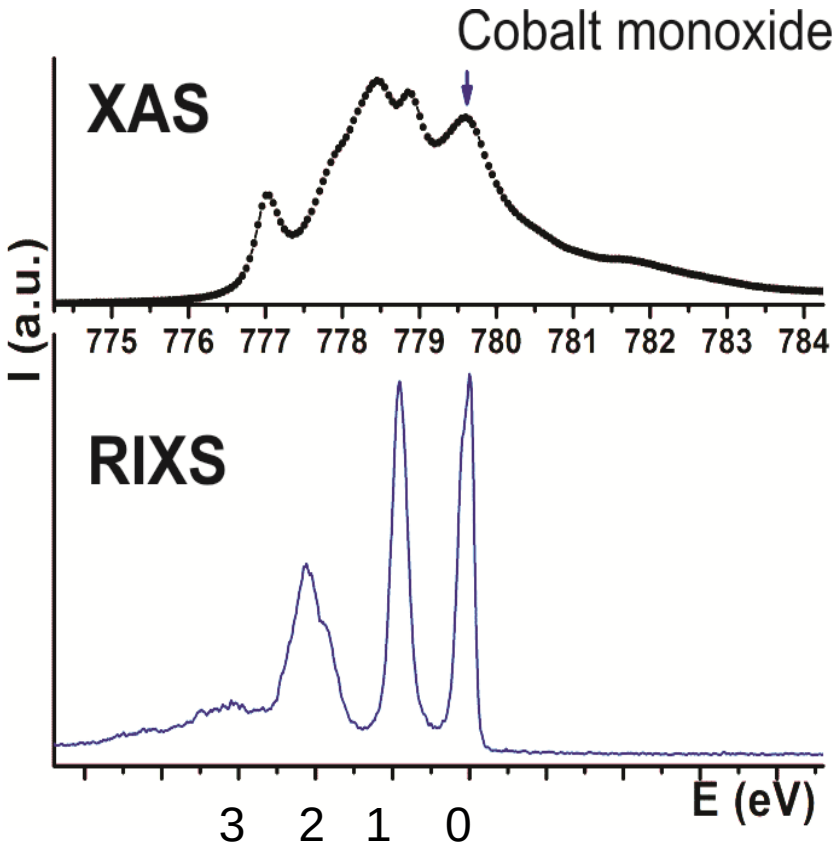
10^{-5}

core

electronic
dd, CT

magnon
vibrations

Ψ_0



2p3d RIXS

polarization, angles
(in, sample, out)

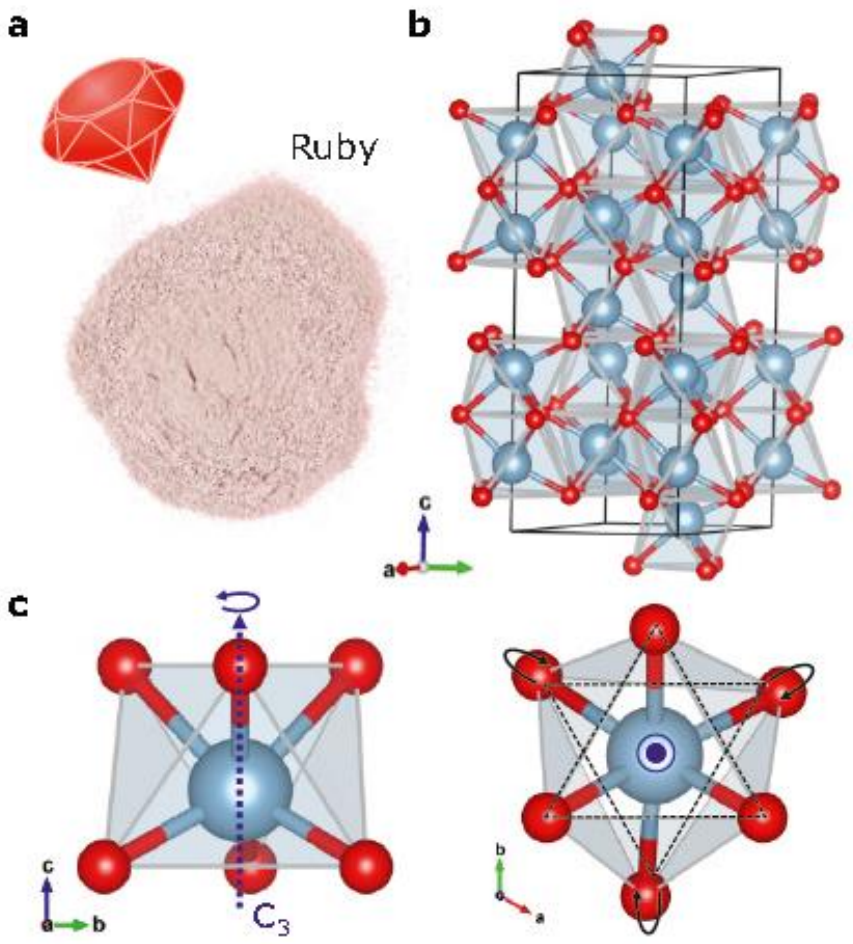
eV
electron-electron
crystal field
charge transfer

meV
spin-orbit, magnetic
distortions
vibrations

RIXS1998:
500 meV

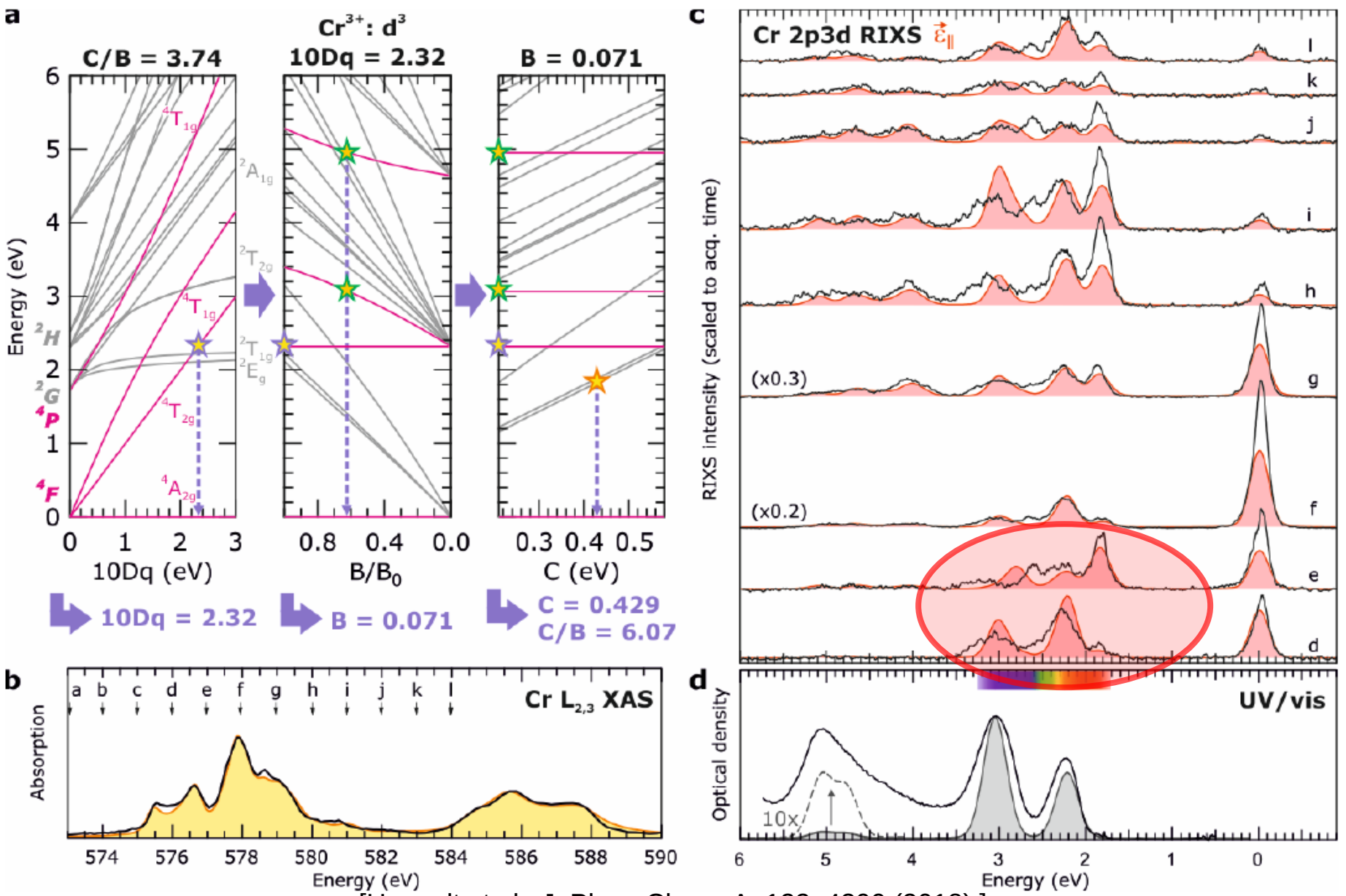
RIXS 2022:
20 meV

2p3d RIXS of isolated chromium ions (ruby)



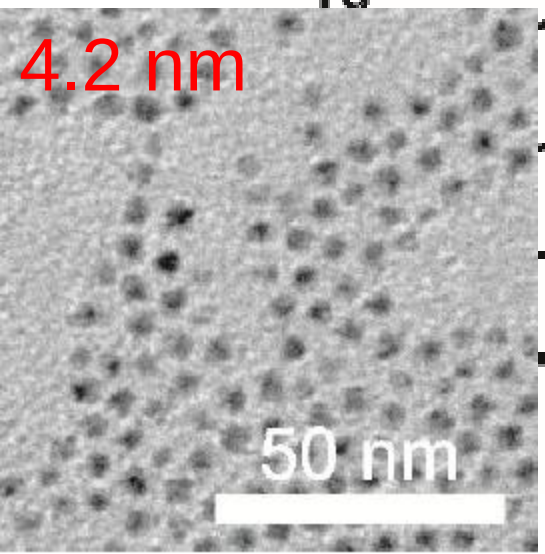
[Hunault et al., J. Phys. Chem. A. 122, 4399 (2018)]

Multiplet challenge: 2p3d RIXS on Cr^{3+}



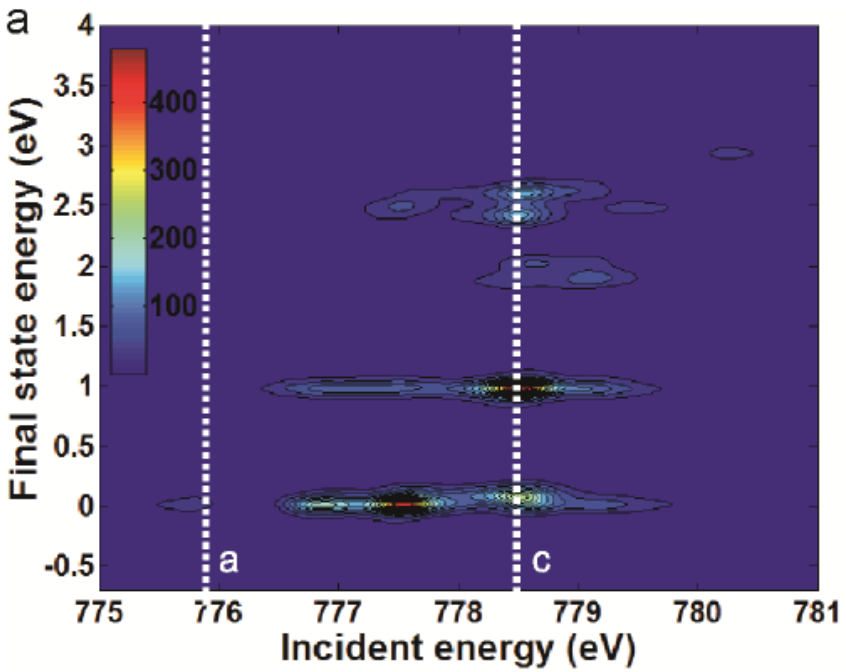
[Hunault et al., J. Phys. Chem. A. 122, 4399 (2018)]

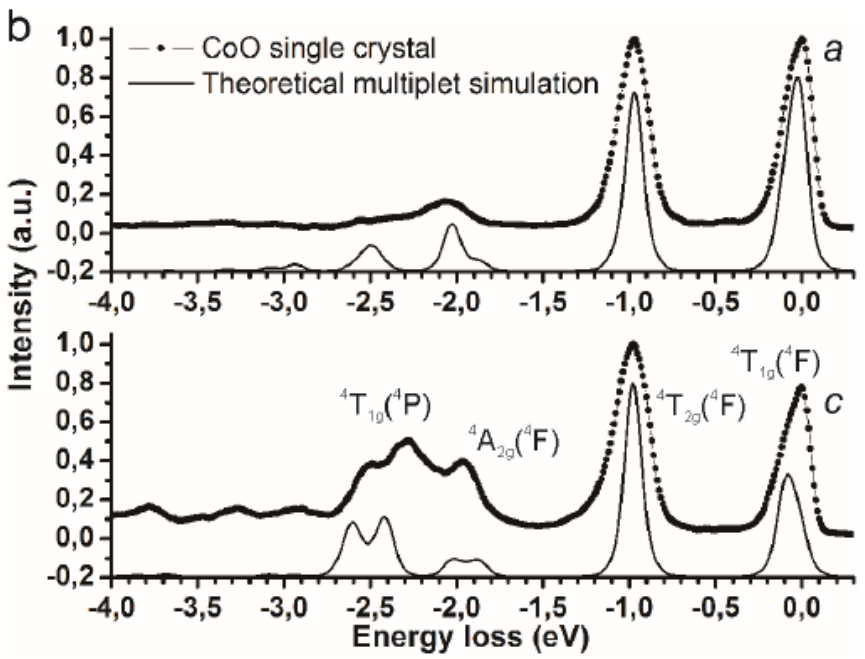
2p3d RIXS of CoO

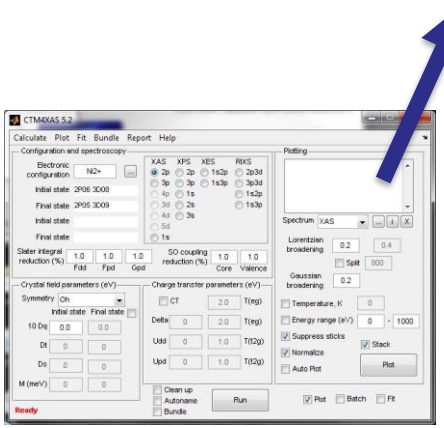


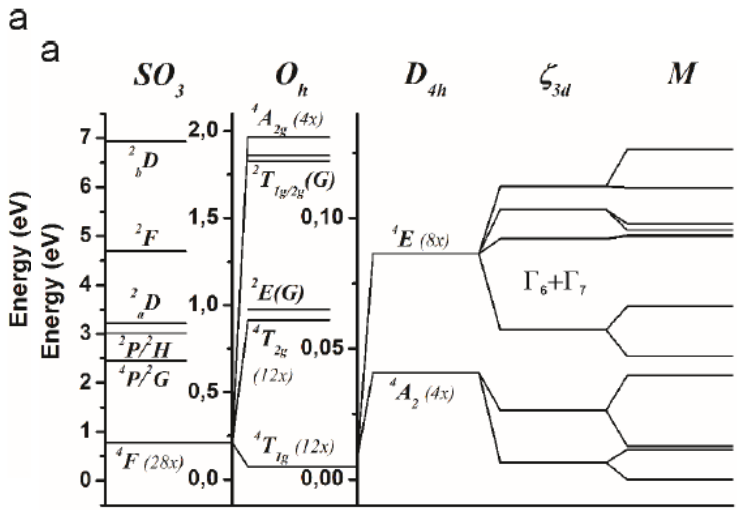
[van Schooneveld, J. Phys. Chem. C. 116, 15218 (2012)]

2p3d RIXS of CoO



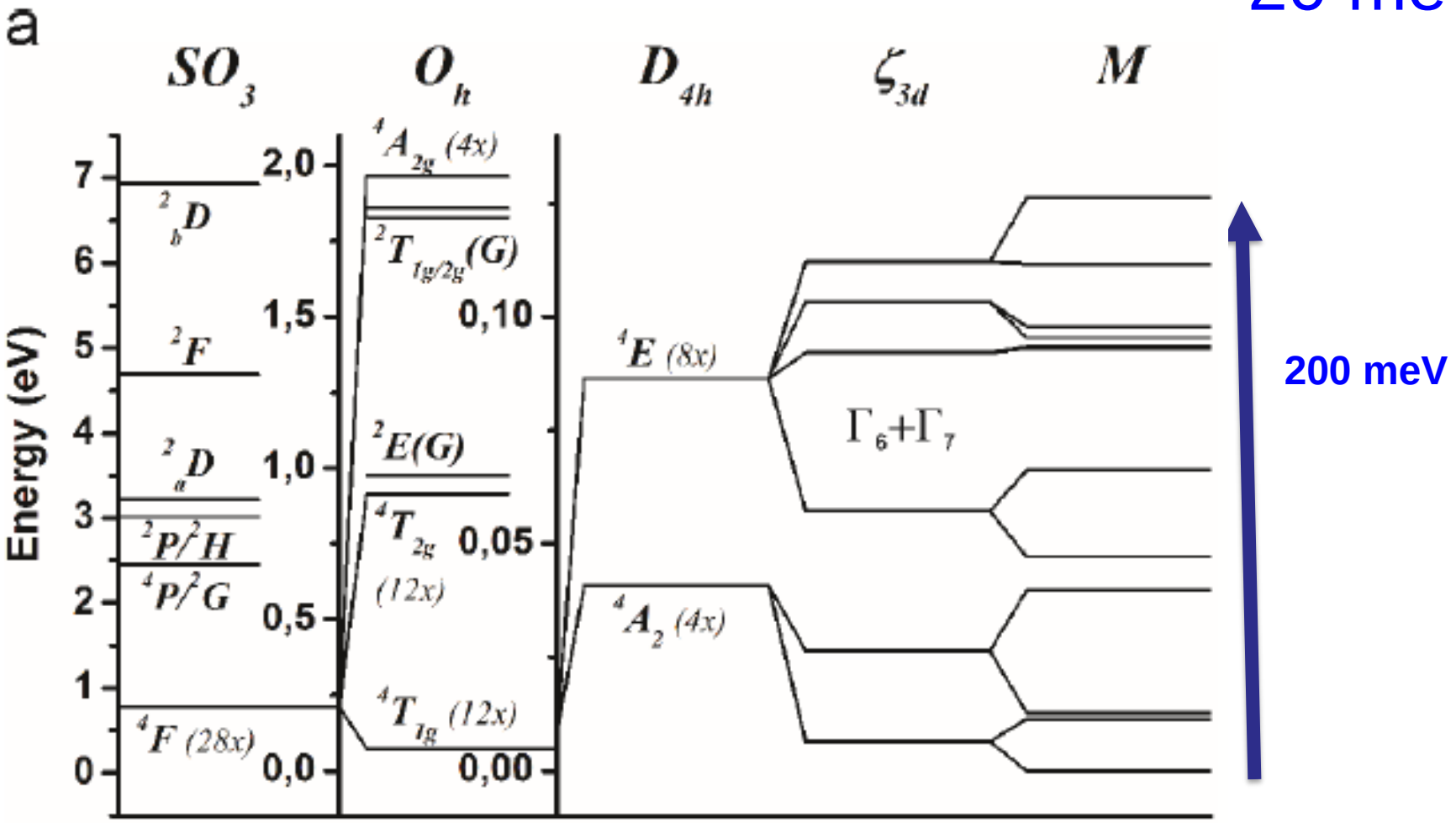






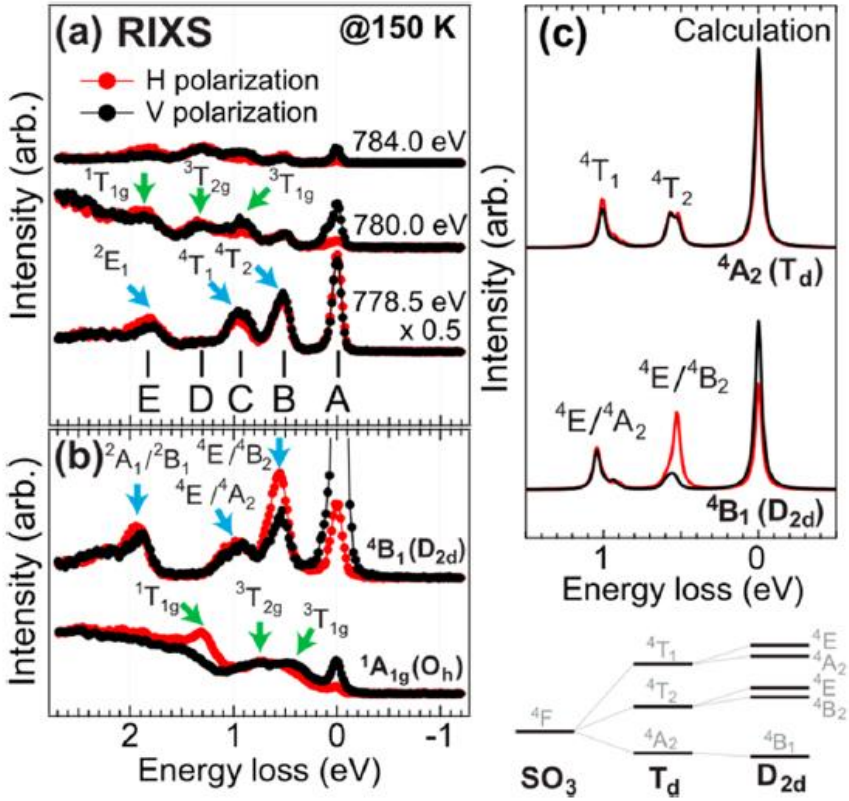
2p3d RIXS of CoO

RIXS2016:
20 meV



(+ phonons, charge transfer, dispersion)

2p3d RIXS of Co3O4 (separate valences)



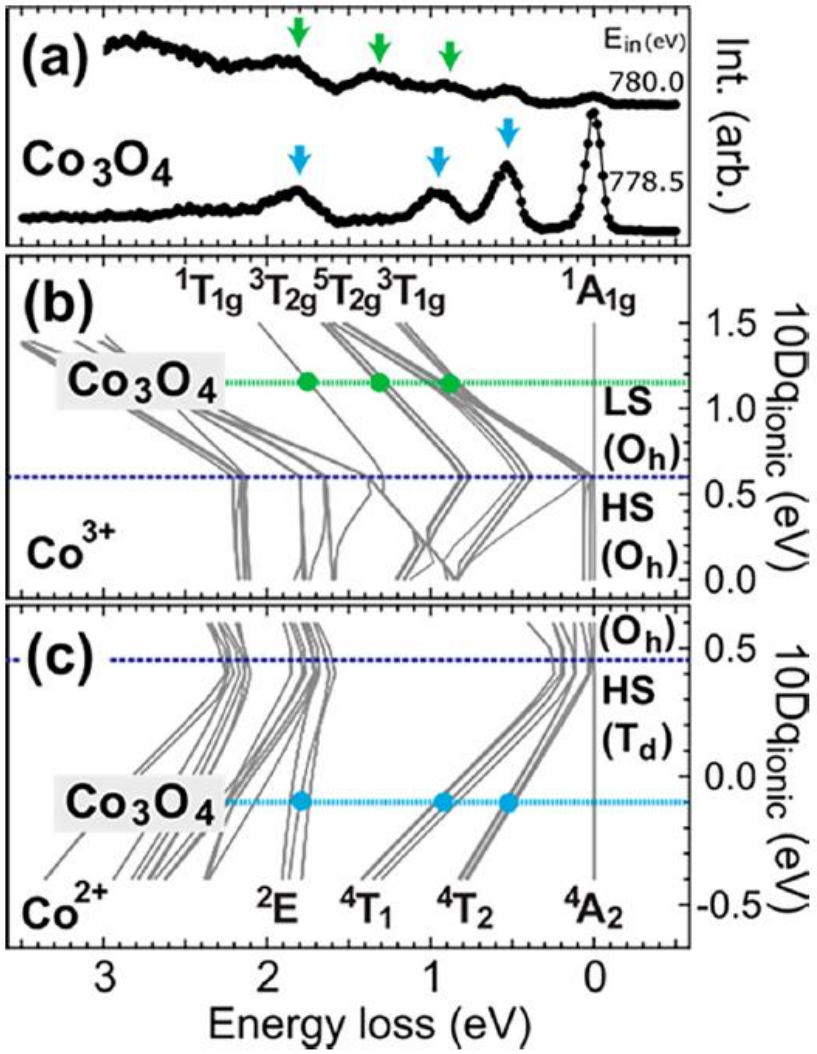
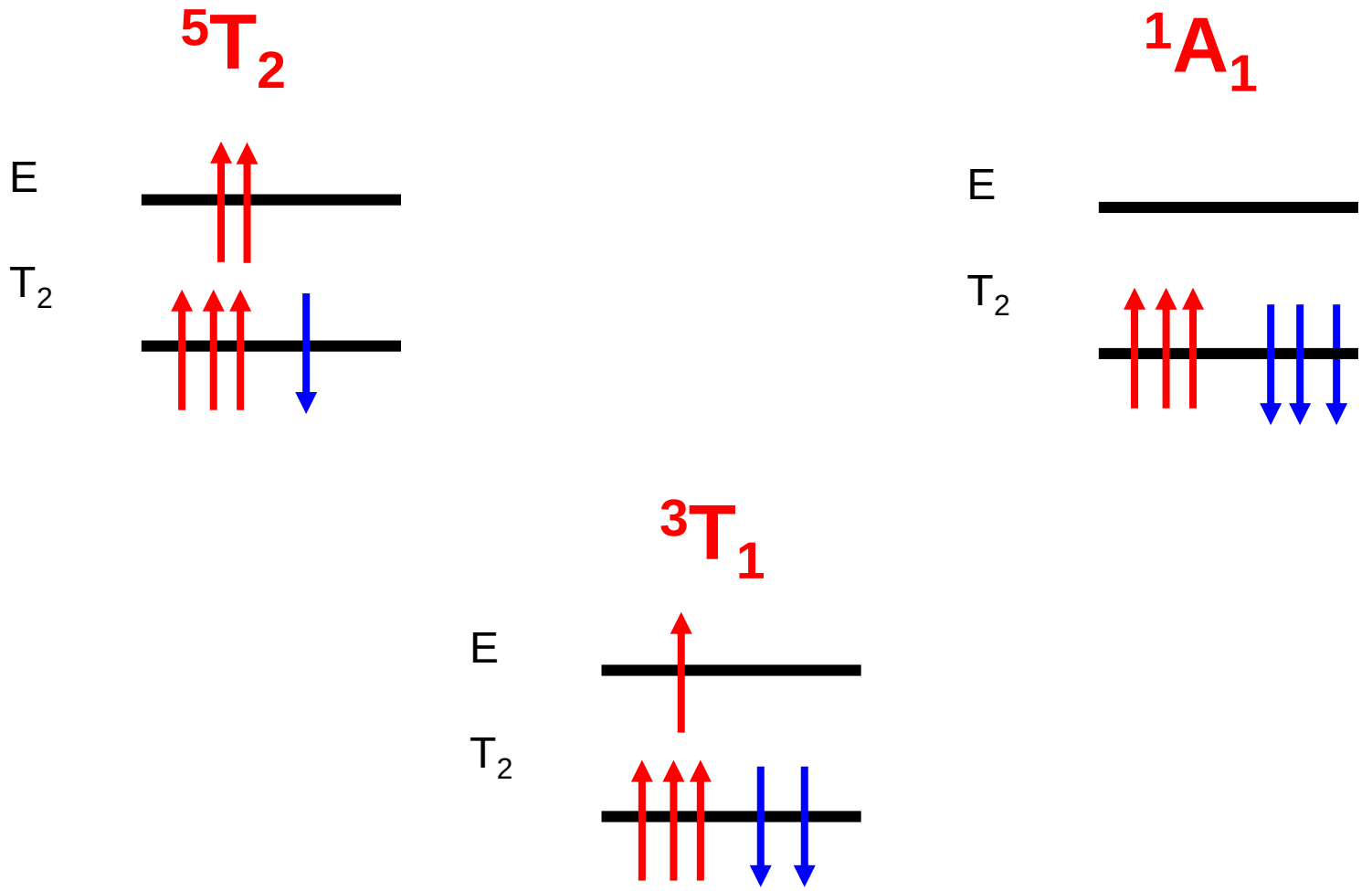


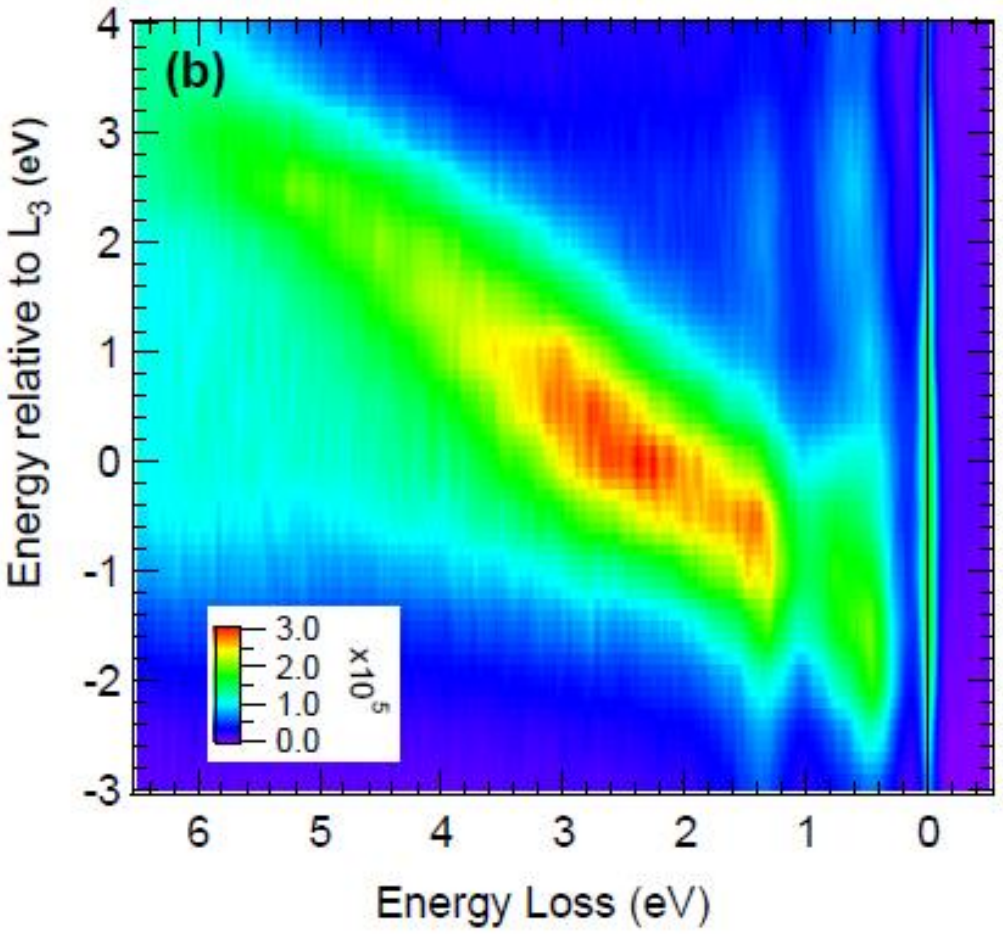
Figure 2. Comparison of H- and V-polarization RIXS spectra of (a) the Co_3O_4 and (b) the $^4B_1(D_{2d})$ and $^1A_{1g}(O_h)$ ground states from refs 44 and 45. The blue (green) arrows indicate the characteristic features of the $Co^{2+}(Co^{3+})$ site. (c) The calculated 2p3d RIXS polarization comparison of distorted and nondistorted tetrahedral Co^{2+} using parameters in ref 44 without considering the ligand-to-model charge transfer.

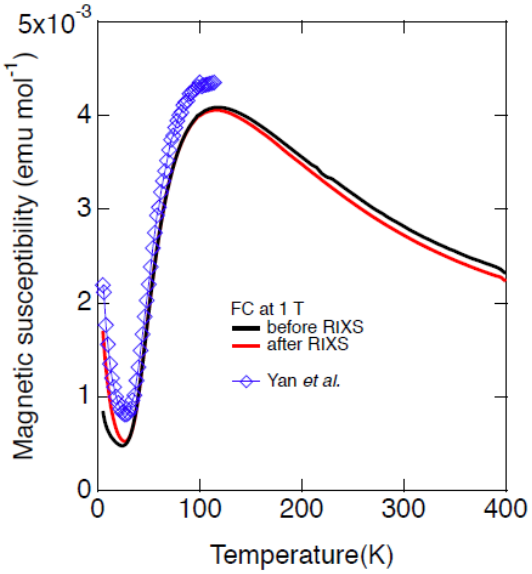
Spin state of $LaCoO_3$

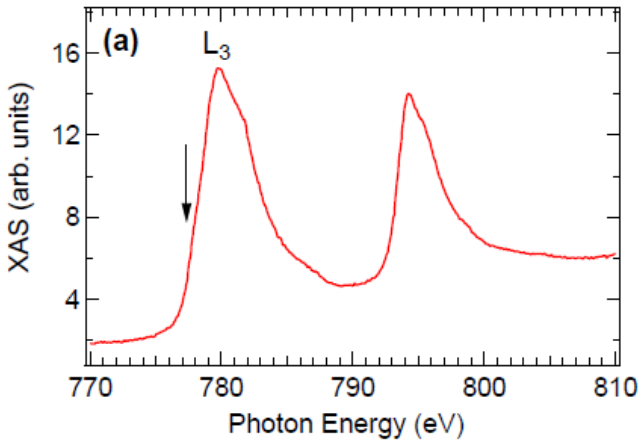


NOTE: Term symbols and orbital occupations are only indications: they are mixed by electron-electron, spin-orbit, etc.

Spin state of $LaCoO_3$



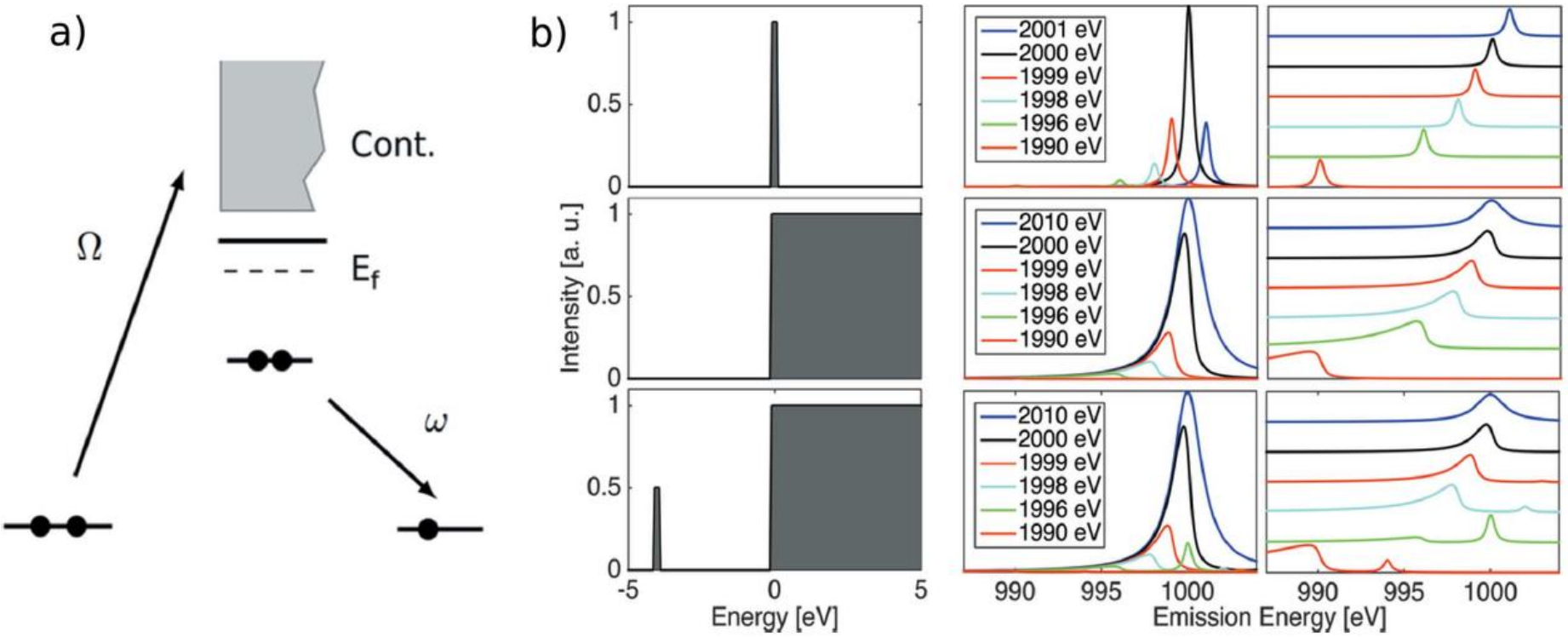




dd-excitations + fluorescence

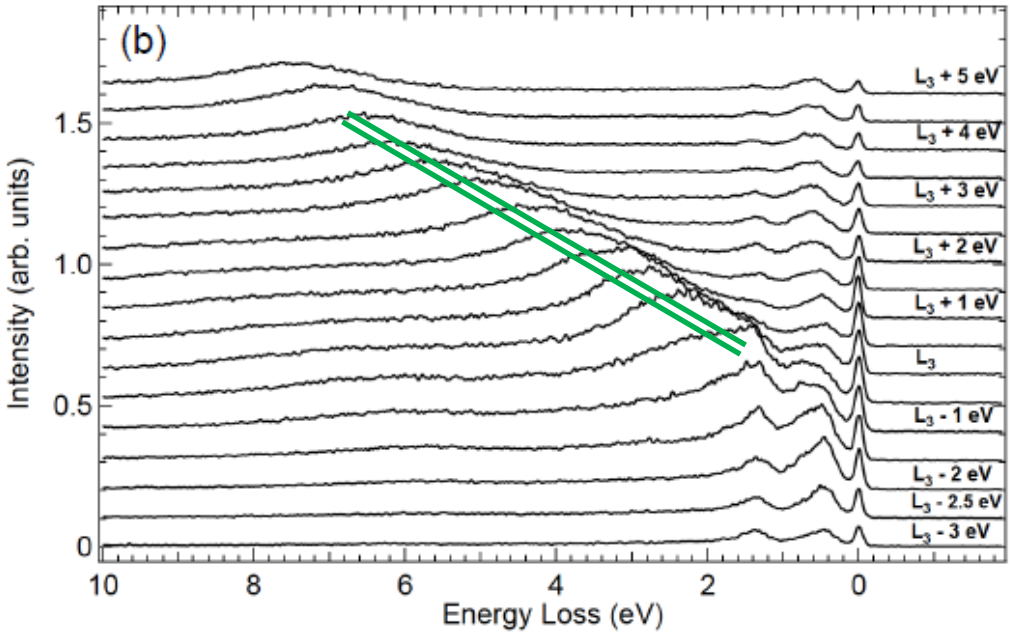
[Tomiyasu et al. PRL 8, 119, 196402 (2017)]

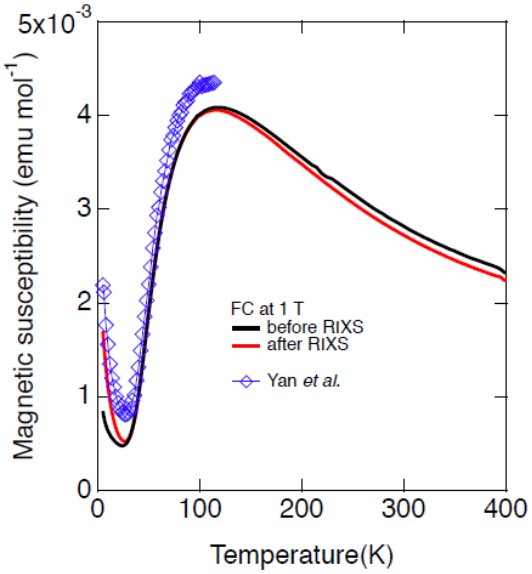
Excitons and continuum excitations

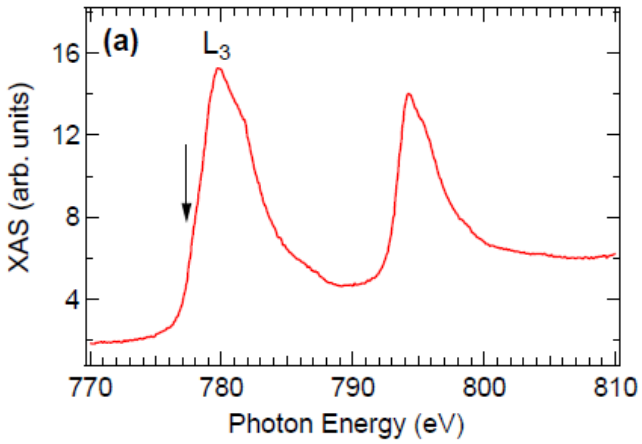


dd-excitations + fluorescence

Spin state of $LaCoO_3$



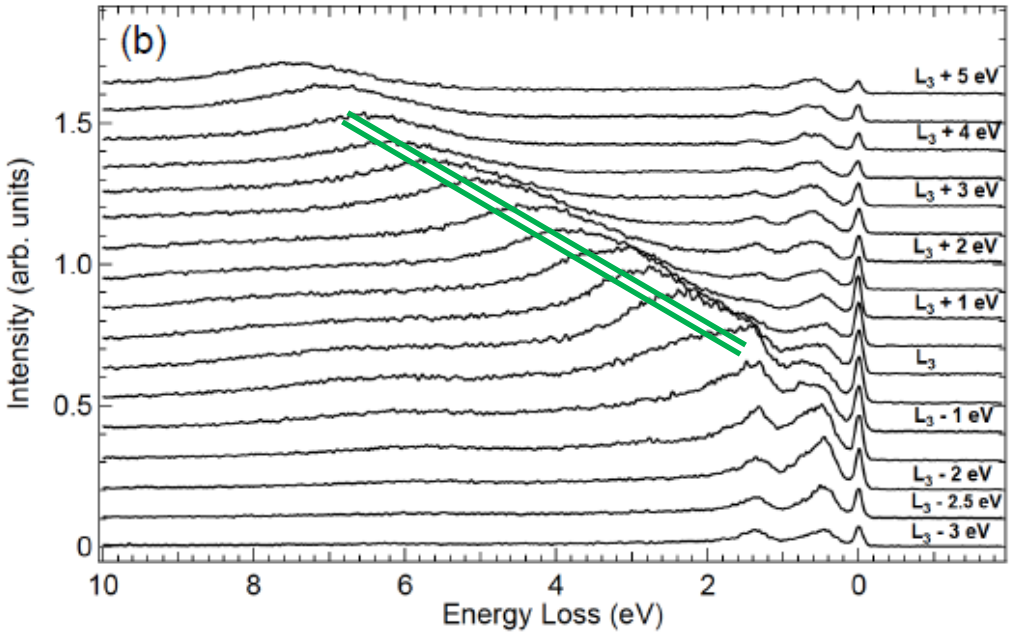




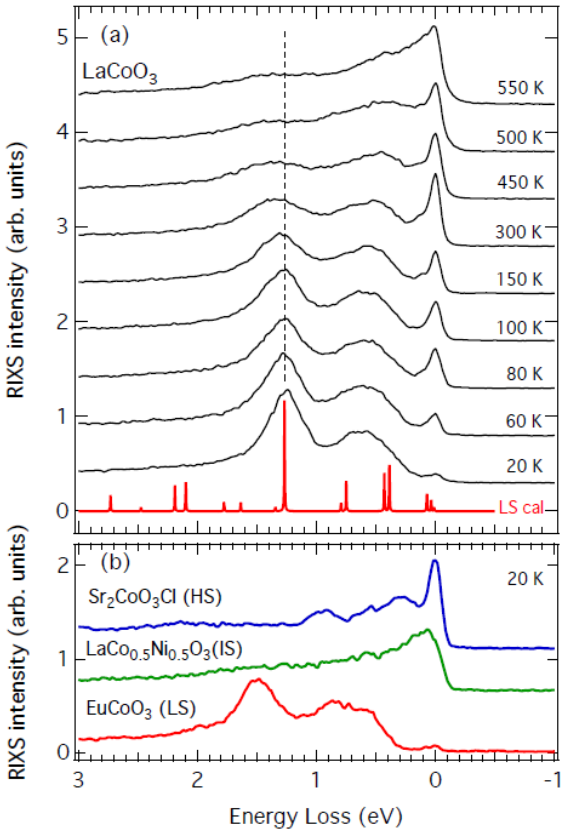
dd-excitations + fluorescence

[Tomiyasu et al. PRL 8, 119, 196402 (2017)]

Spin state of $LaCoO_3$

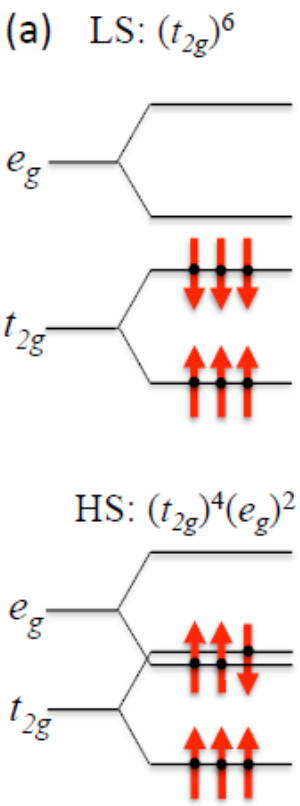


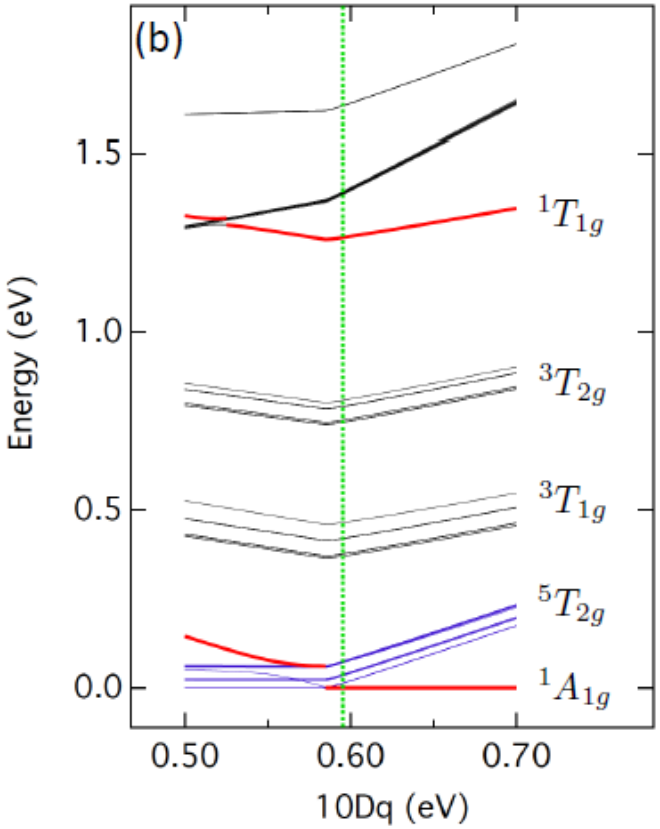
dd-excitations + fluorescence

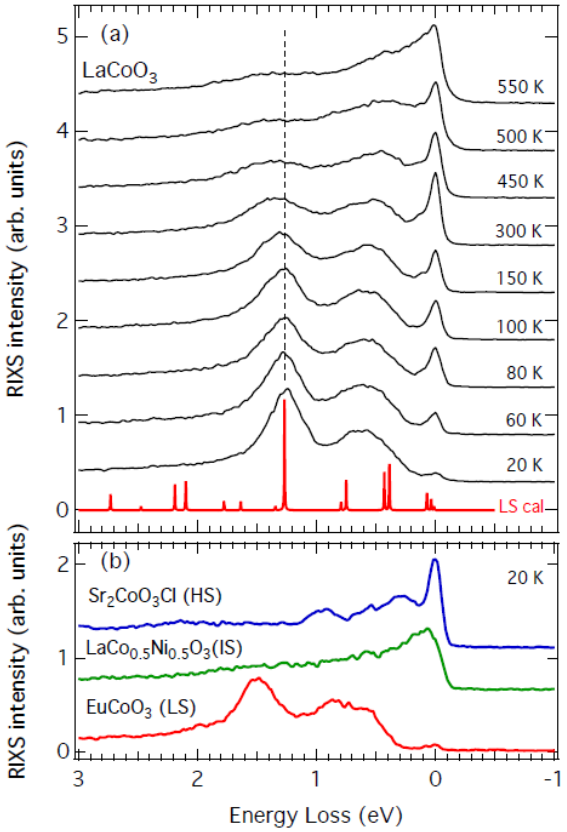


[Tomiyasu et al. PRL 8, 119, 196402 (2017)]

Spin state of $LaCoO_3$

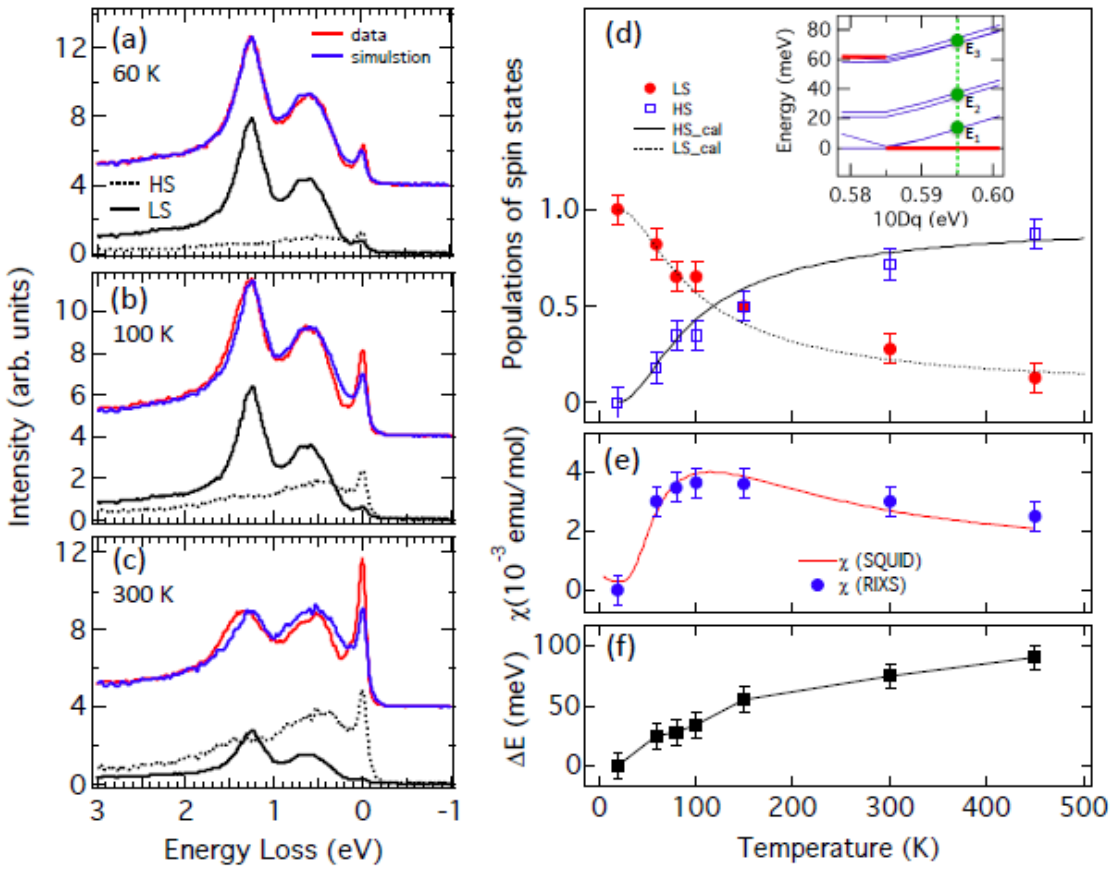






[Tomiyasu et al. PRL 8, 119, 196402 (2017)]

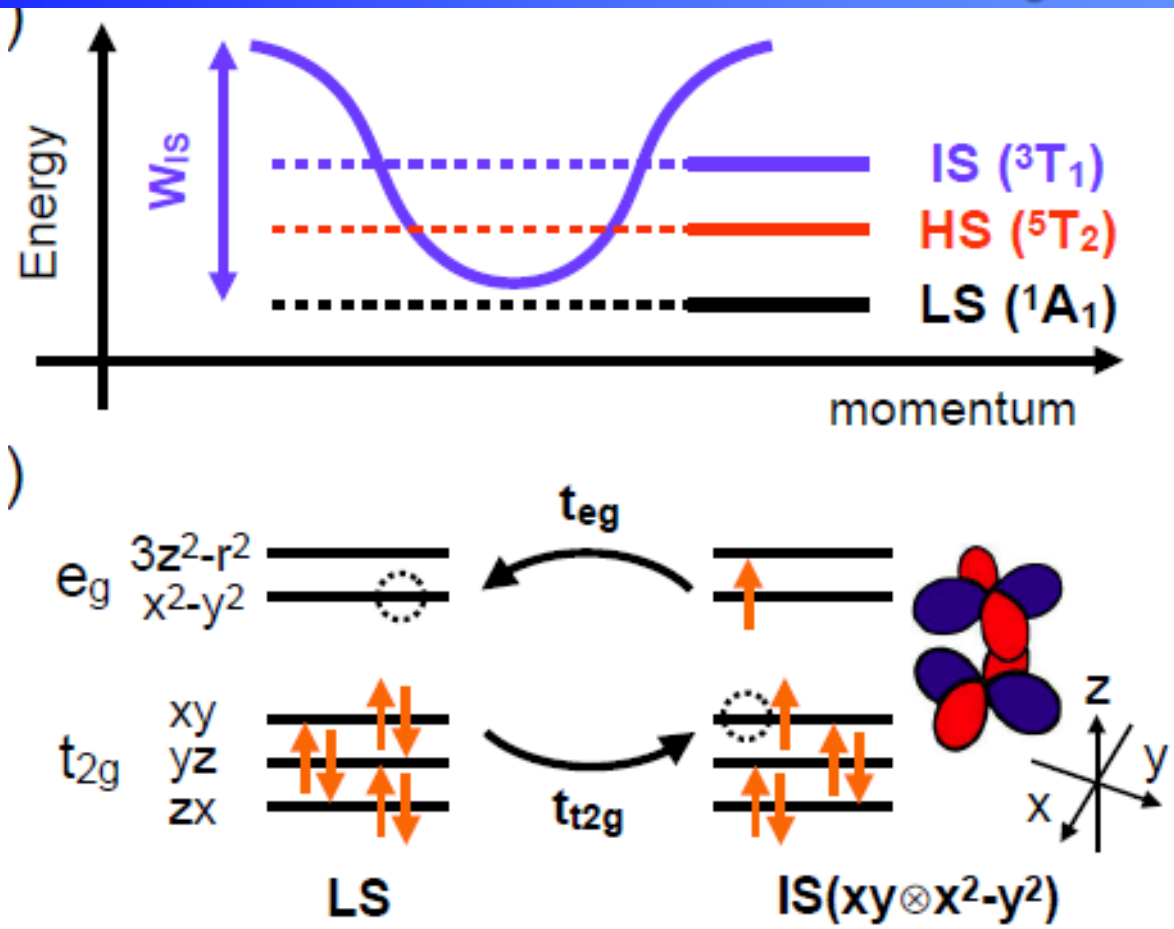
Spin state of $LaCoO_3$



Spin transition is from low-spin to high-spin

[Tomiyasu et al. PRL 8, 119, 196402 (2017)]

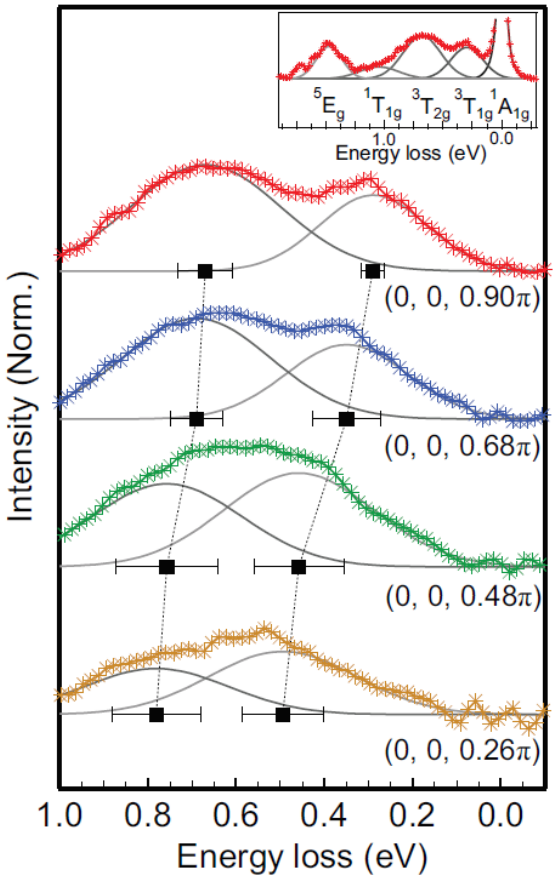
Spin state of $LaCoO_3$



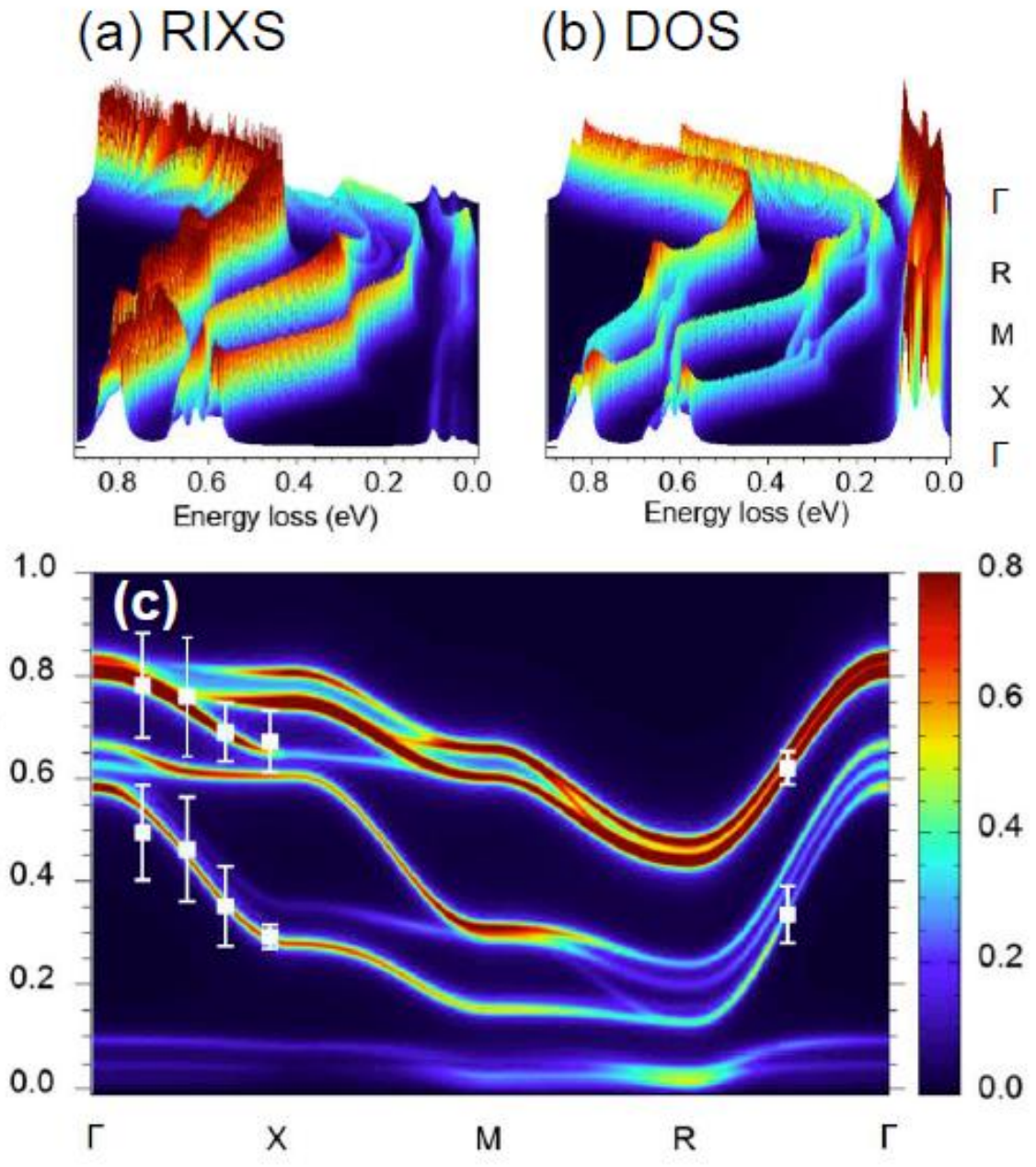
Order of states at zero Kelvin: LS < HS < IS
Strong coupling between LS and IS (not with HS)
Large dispersion of IS: **Excitonic Insulator**

[Sotnikov & KUnes, Sci. Rep 6, 30510 (2016); Wang et al. submitted]

Spin state of $LaCoO_3$

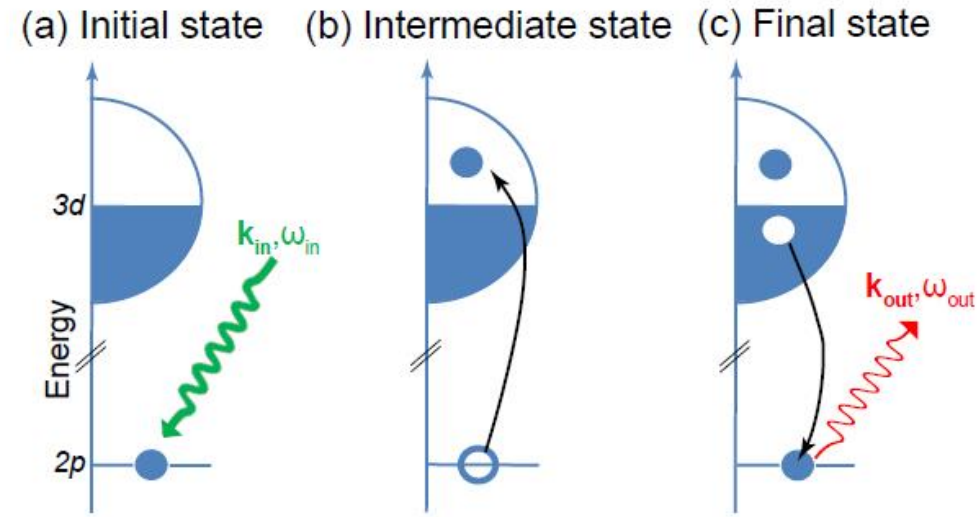


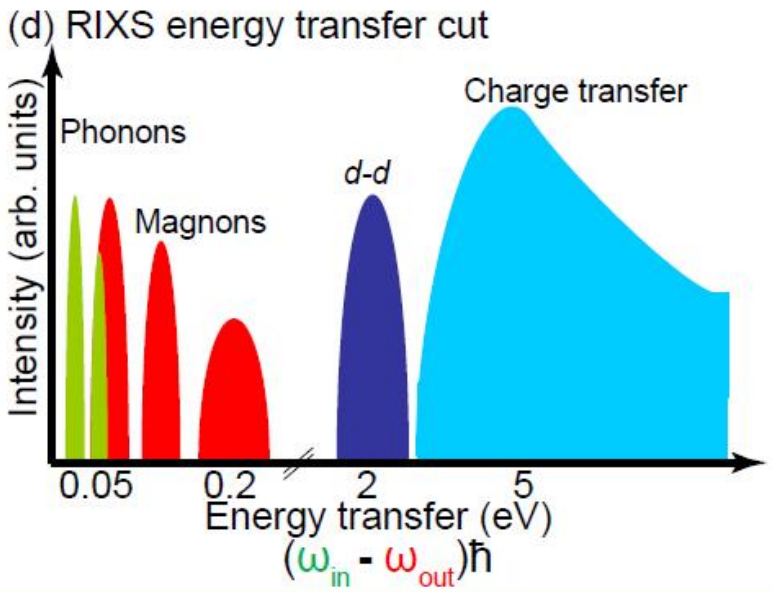
q-dep. RIXS

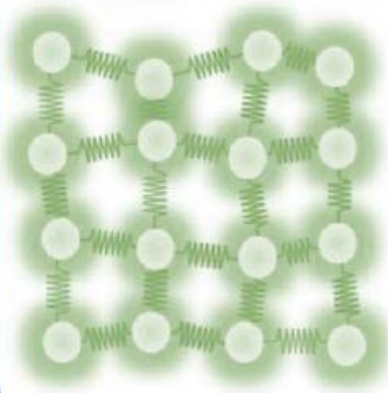


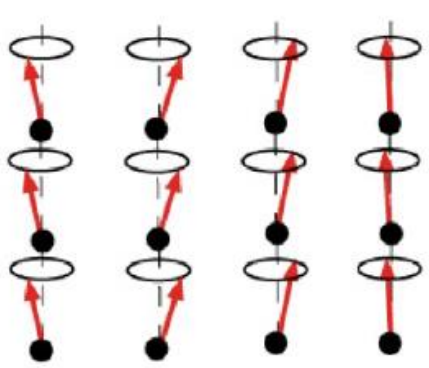
[Wang et al. 2018]

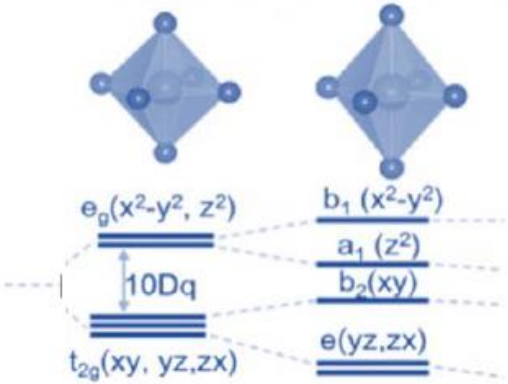
2p3d RIXS of transition metal ions

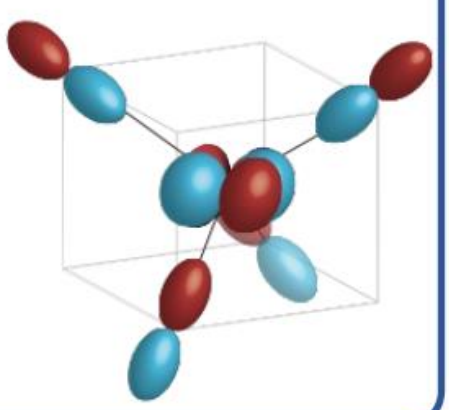








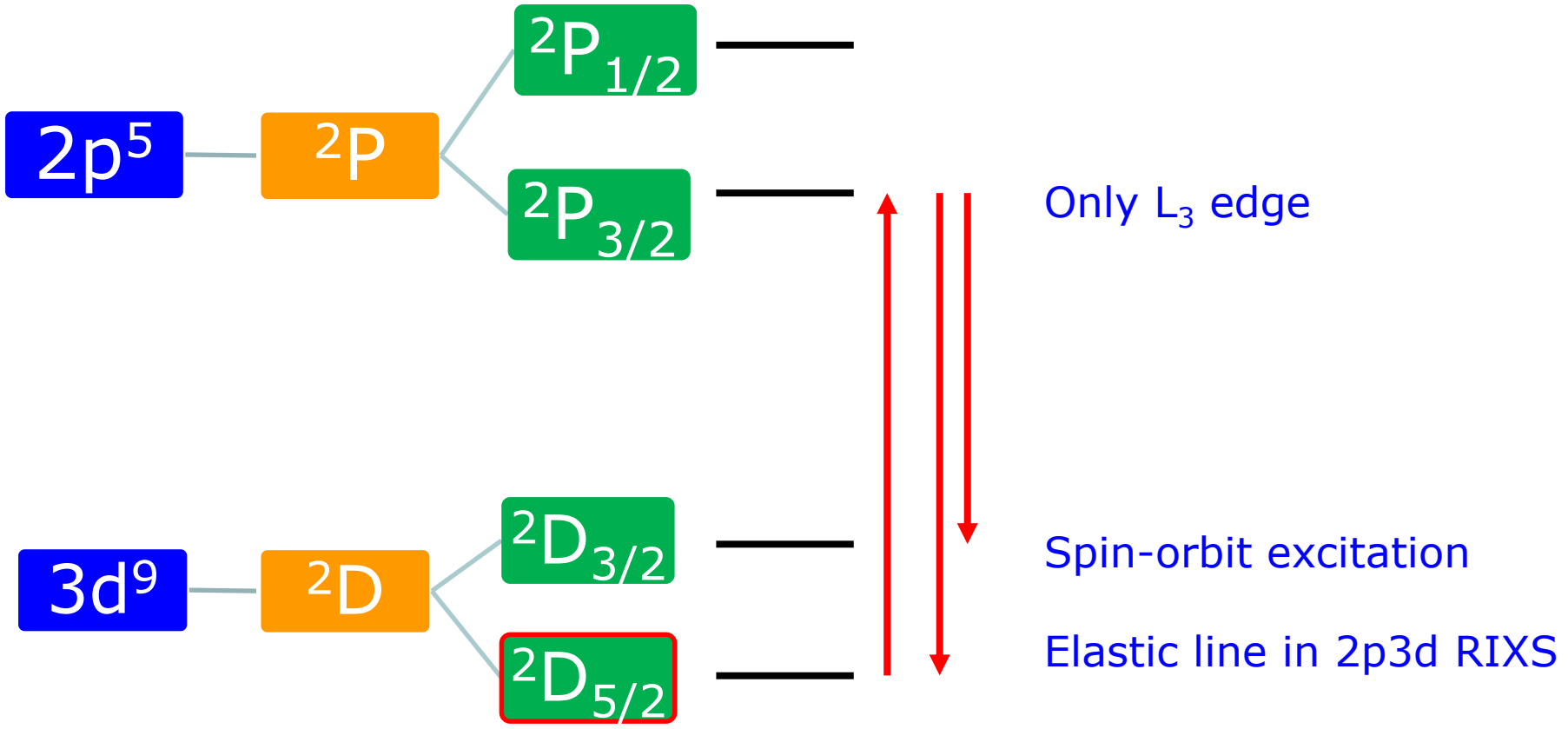




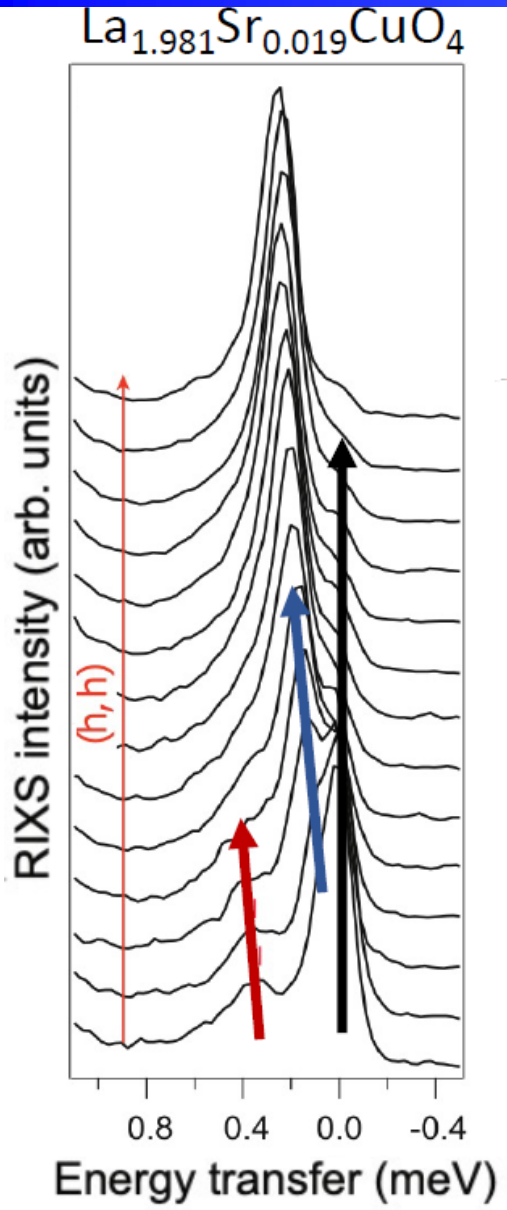
Cu2+ 2p3d RIXS (from $3d^9$ to $2p^5 3d^{10}$ to $3d^9$)

ATOMIC

Dipole selection rule:
ΔJ=-1, 0 or +1
J=J'≠0



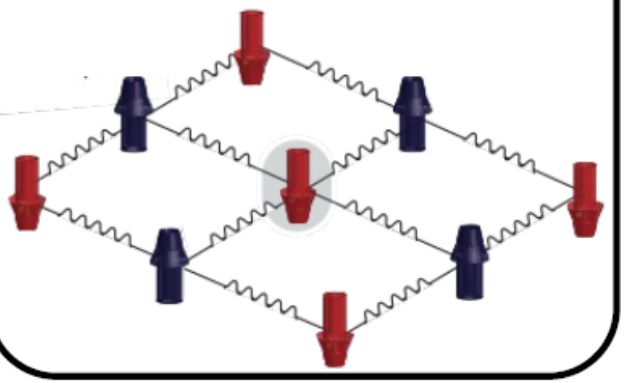
Magnon 2p3d RIXS in cuprates



Elastic

E = 0 eV

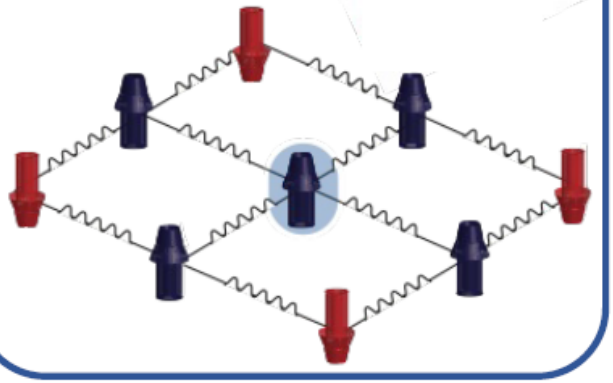
$\Delta M_S = 0$



Magnon

E = 0.2 eV

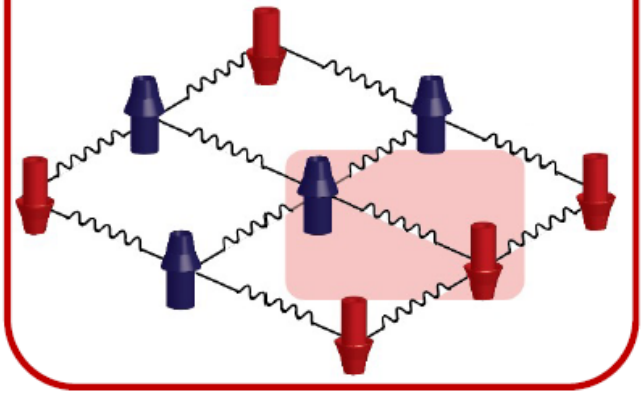
$\Delta M_S = 1$



Bimagnon

E = 0.4 eV

$\Delta M_S = 0$



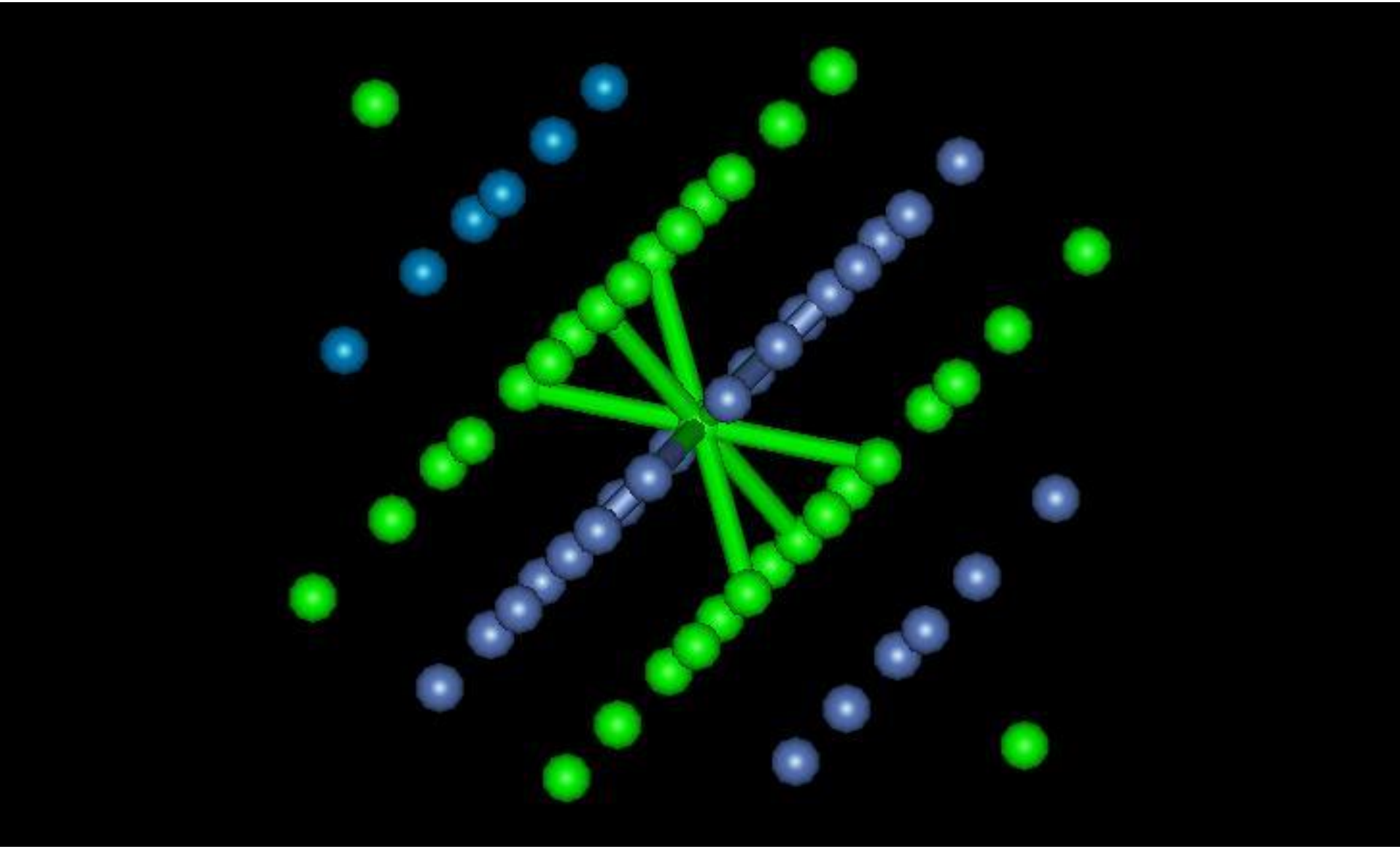
What we Know

- ❑ Single site, single magnon
- ❑ Two sites, single magnon

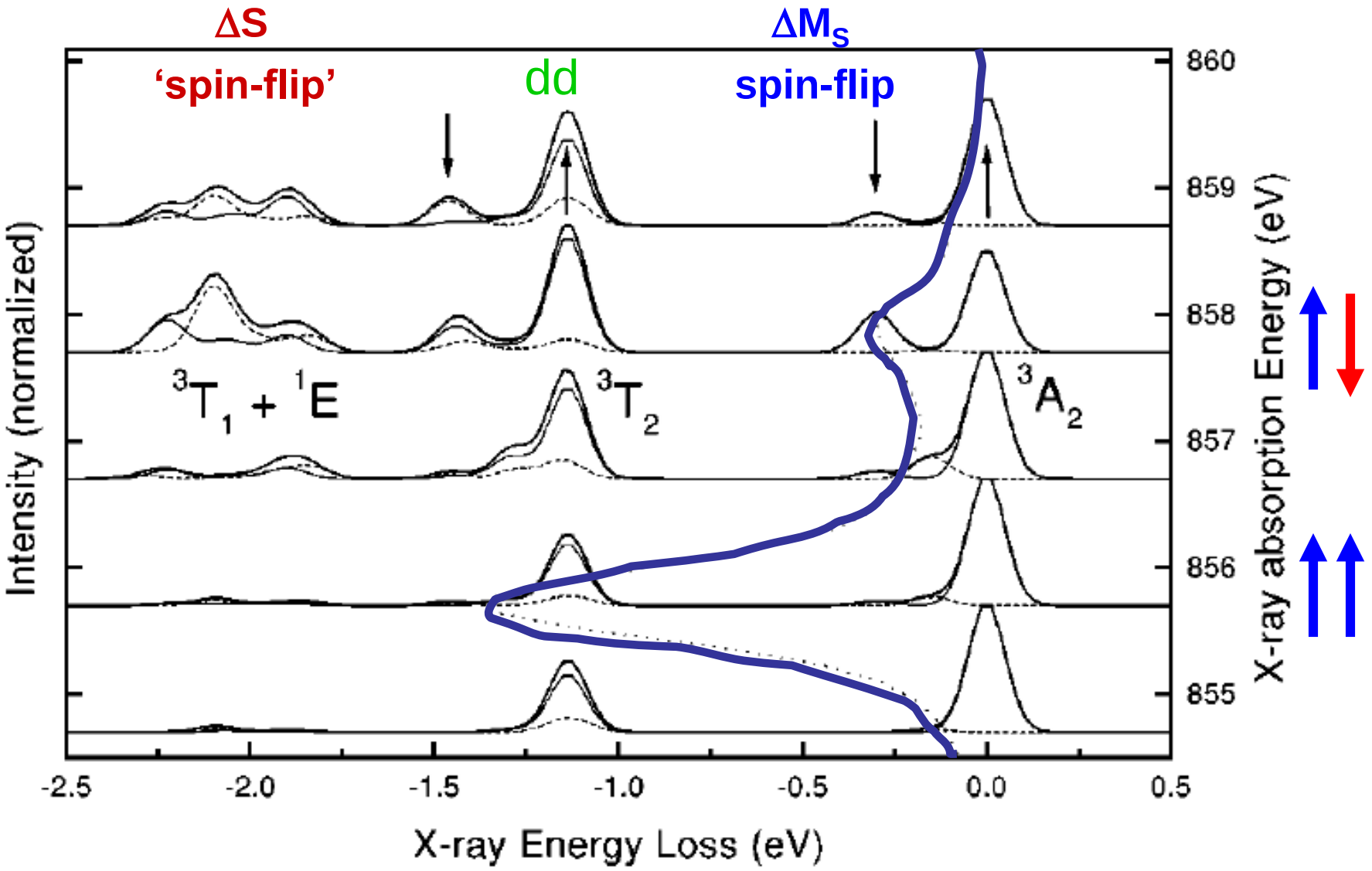
Chaix et. al., Phys. Rev. B. 97, 155144 (2018)

2p3d RIXS of NiO

Ni^{II} $3d^8$ [↑↑] → $2p^5 3d^9$[jj] → $3d^8$[↓↓]

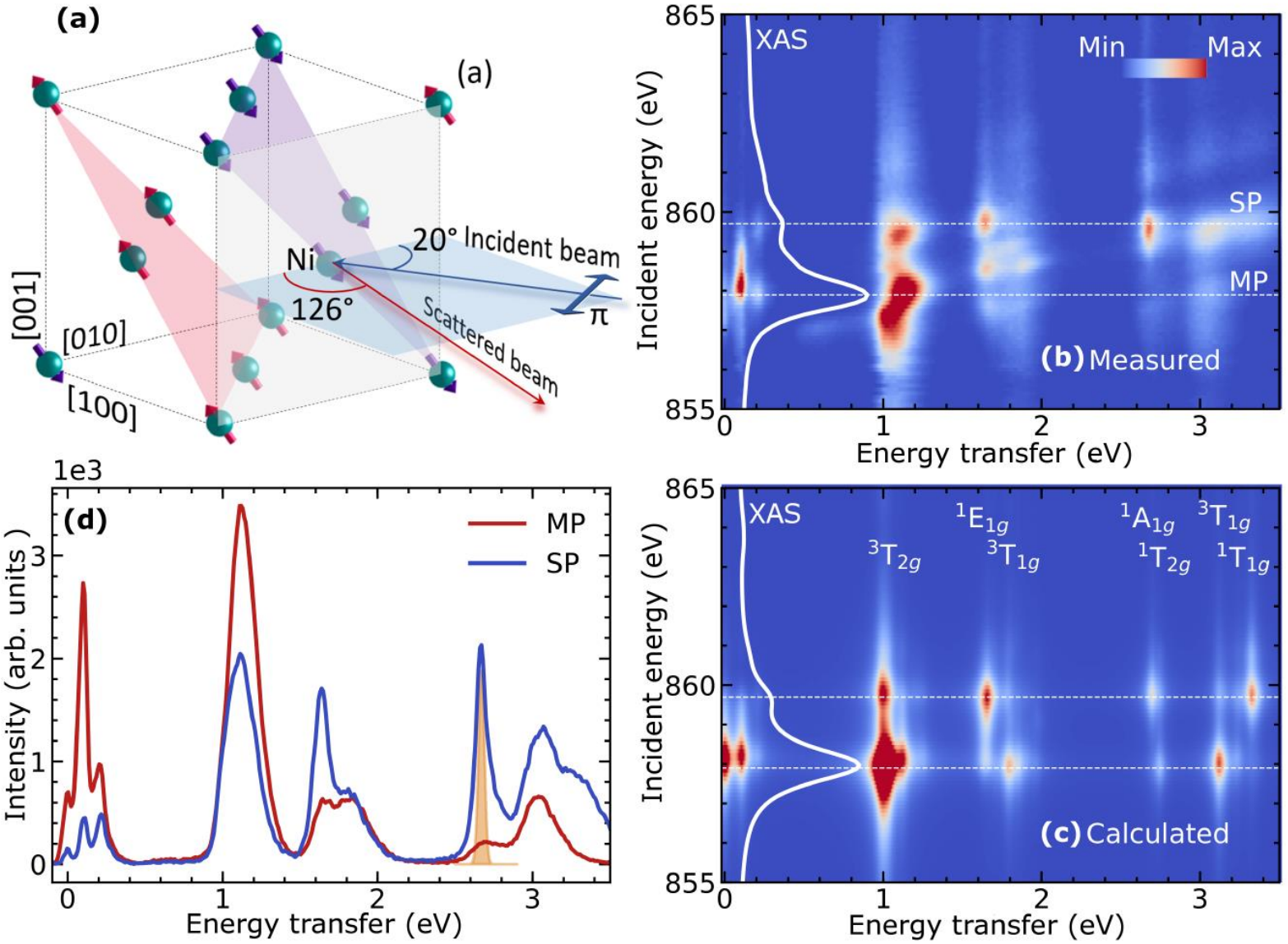


2p3d RIXS of NiO



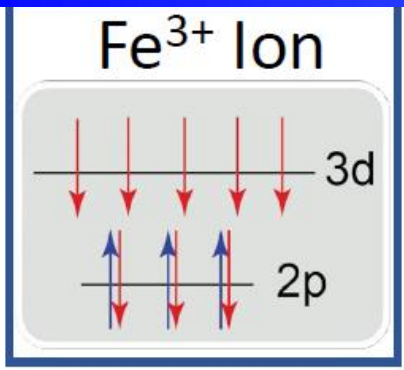
[Phys. Rev. B. 57, 14584 (1998)]

2p3d RIXS of NiO



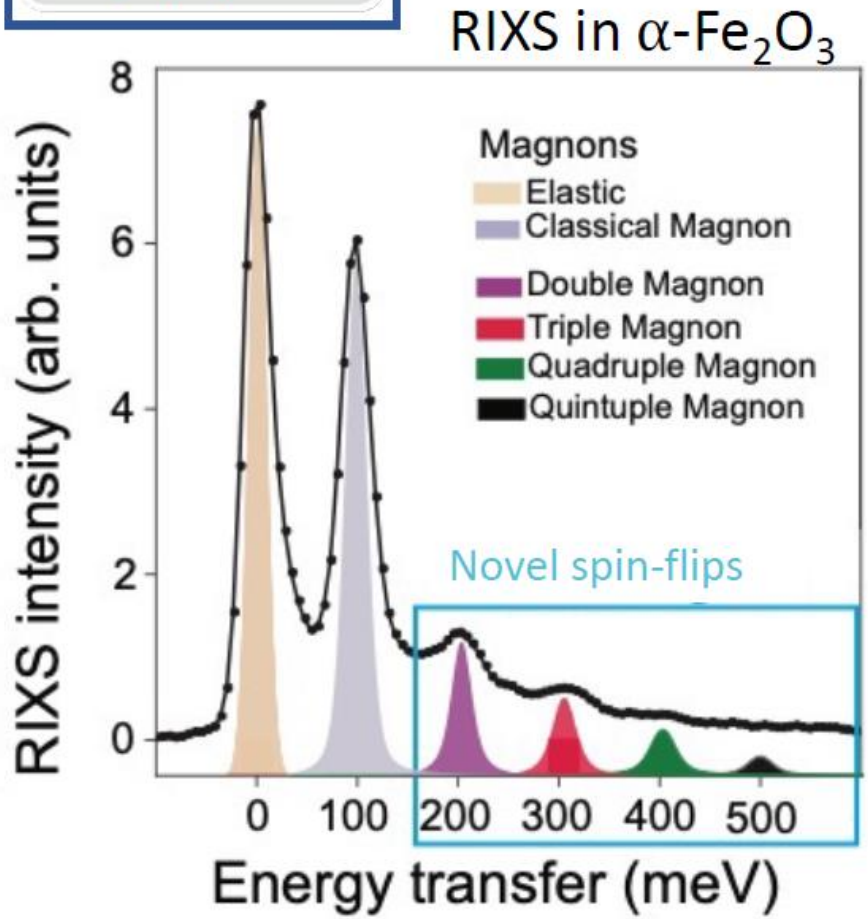
[Nag, Phys. Rev. Lett. 124, 067202 (2020)]

2p3d RIXS of Fe2O3

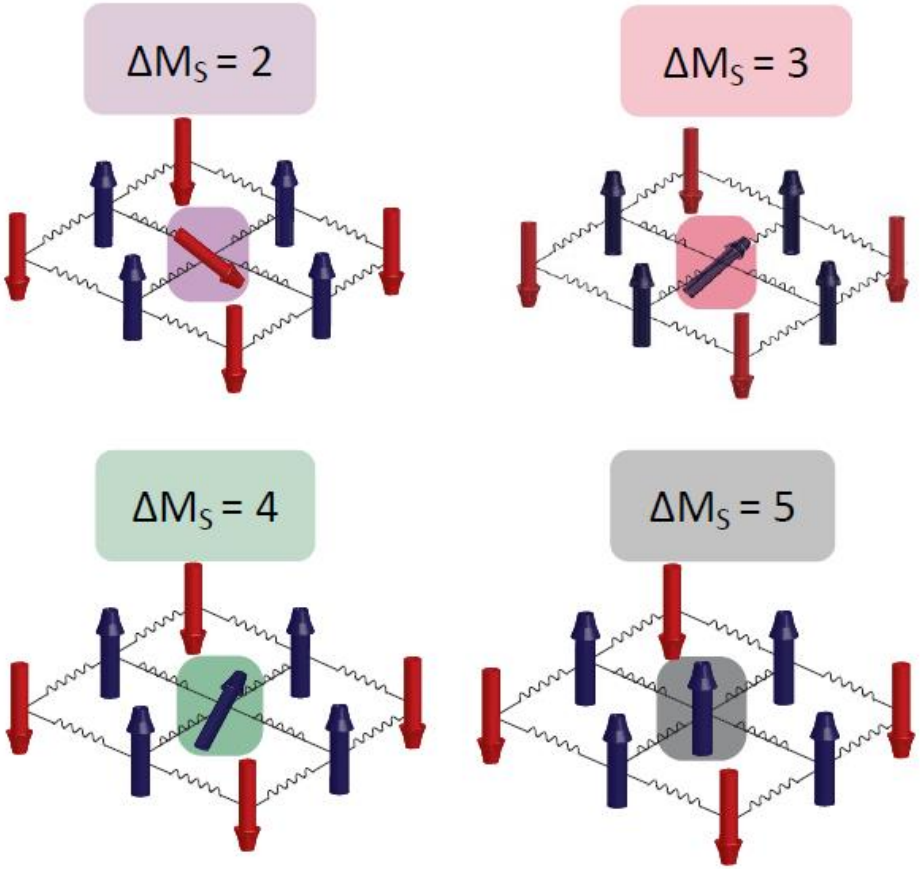


Ground State:

- $3d^5$
- $S_z = 5/2$

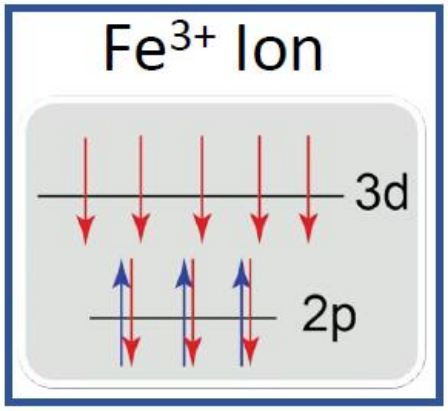


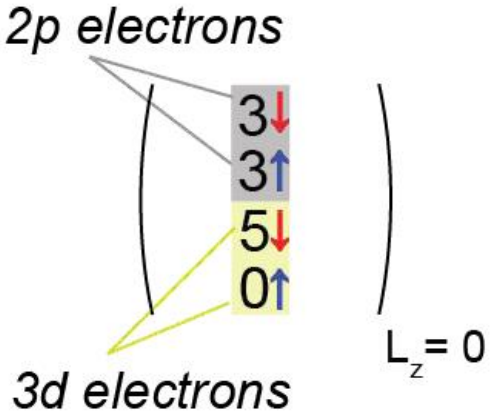
Novel Magnetic Excitations



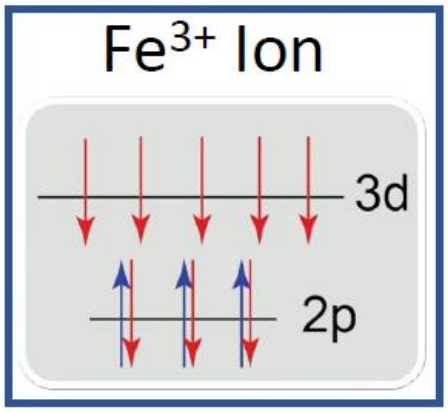
Elnaggar et. al., arXiv preprint arXiv:2208.03198

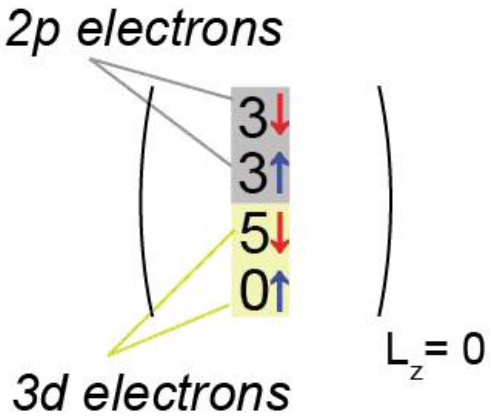
0,1 and 2-magnons in 2p3d RIXS of Fe2O3



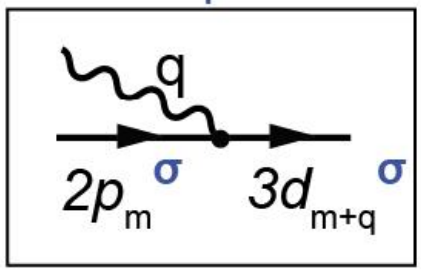


0,1 and 2-magnons in 2p3d RIXS of Fe2O3

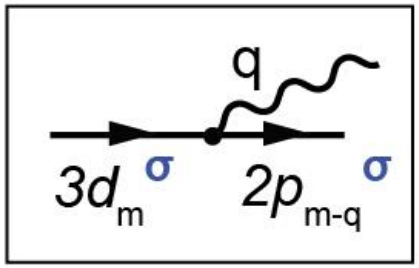




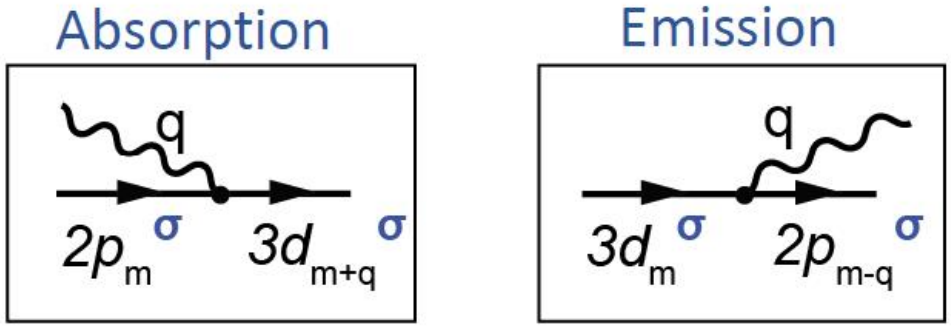
Absorption

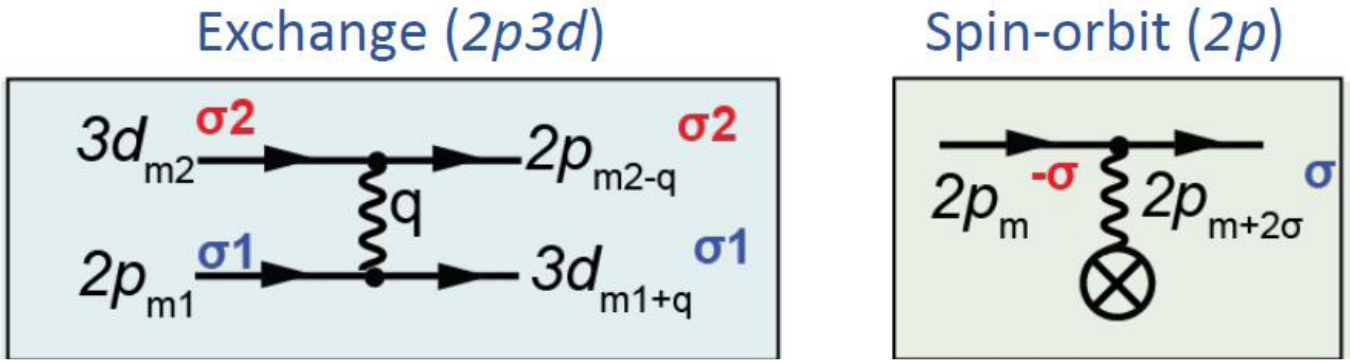


Emission

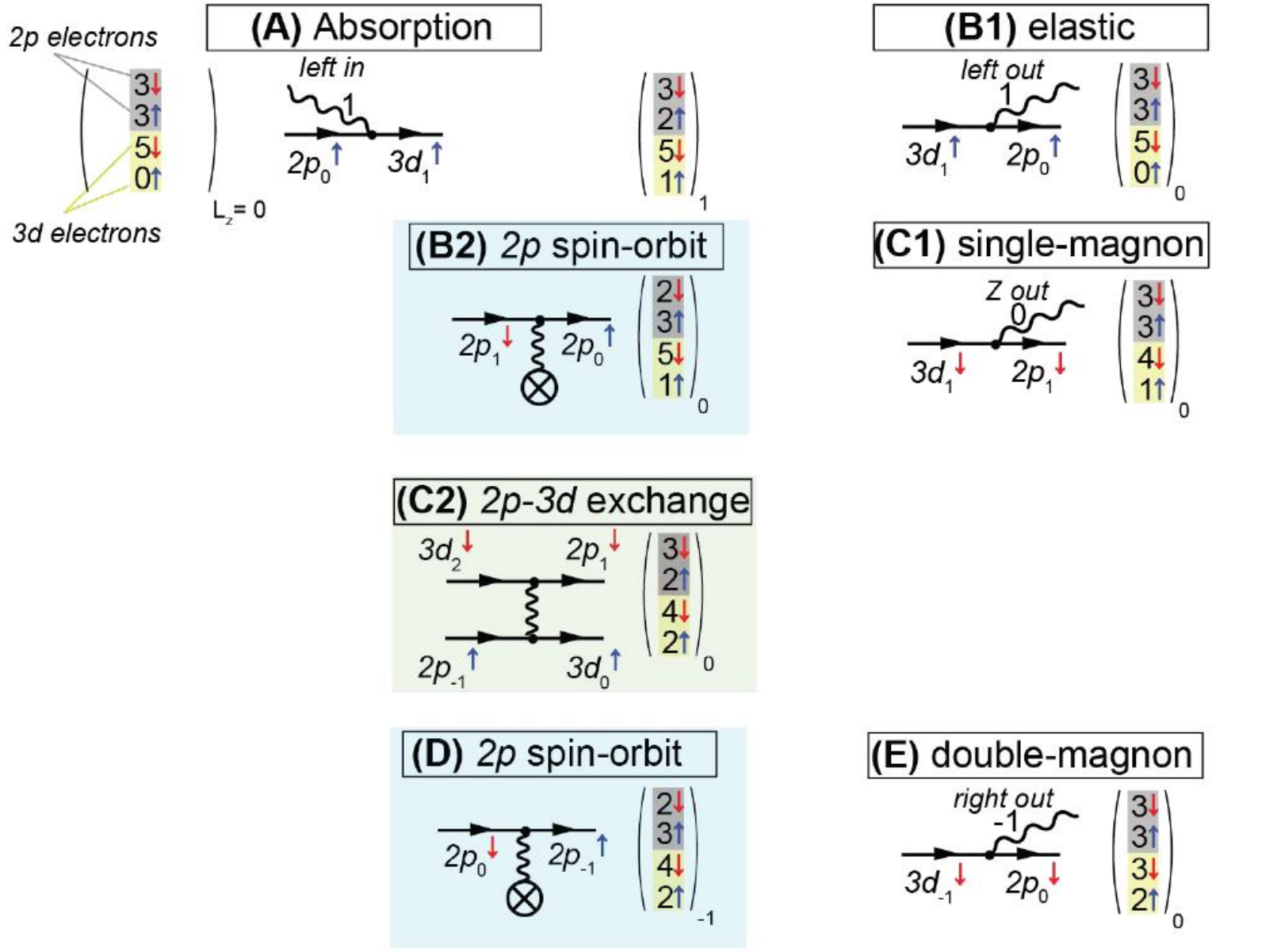


0,1 and 2-magnons in 2p3d RIXS of Fe2O3

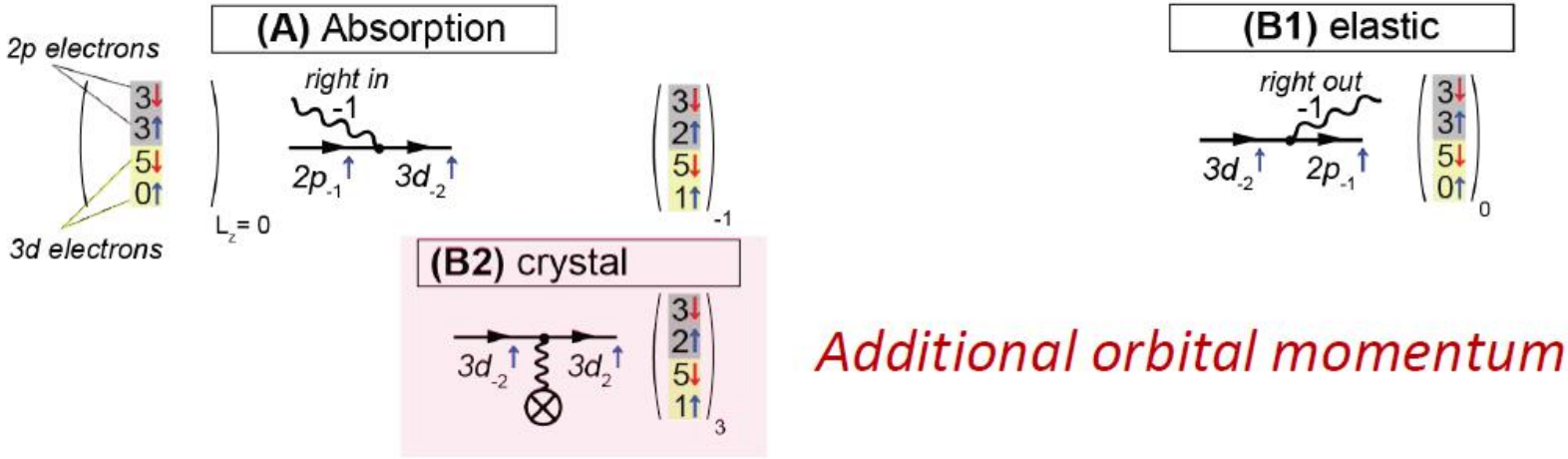




0,1 and 2-magnons in 2p3d RIXS of Fe2O3

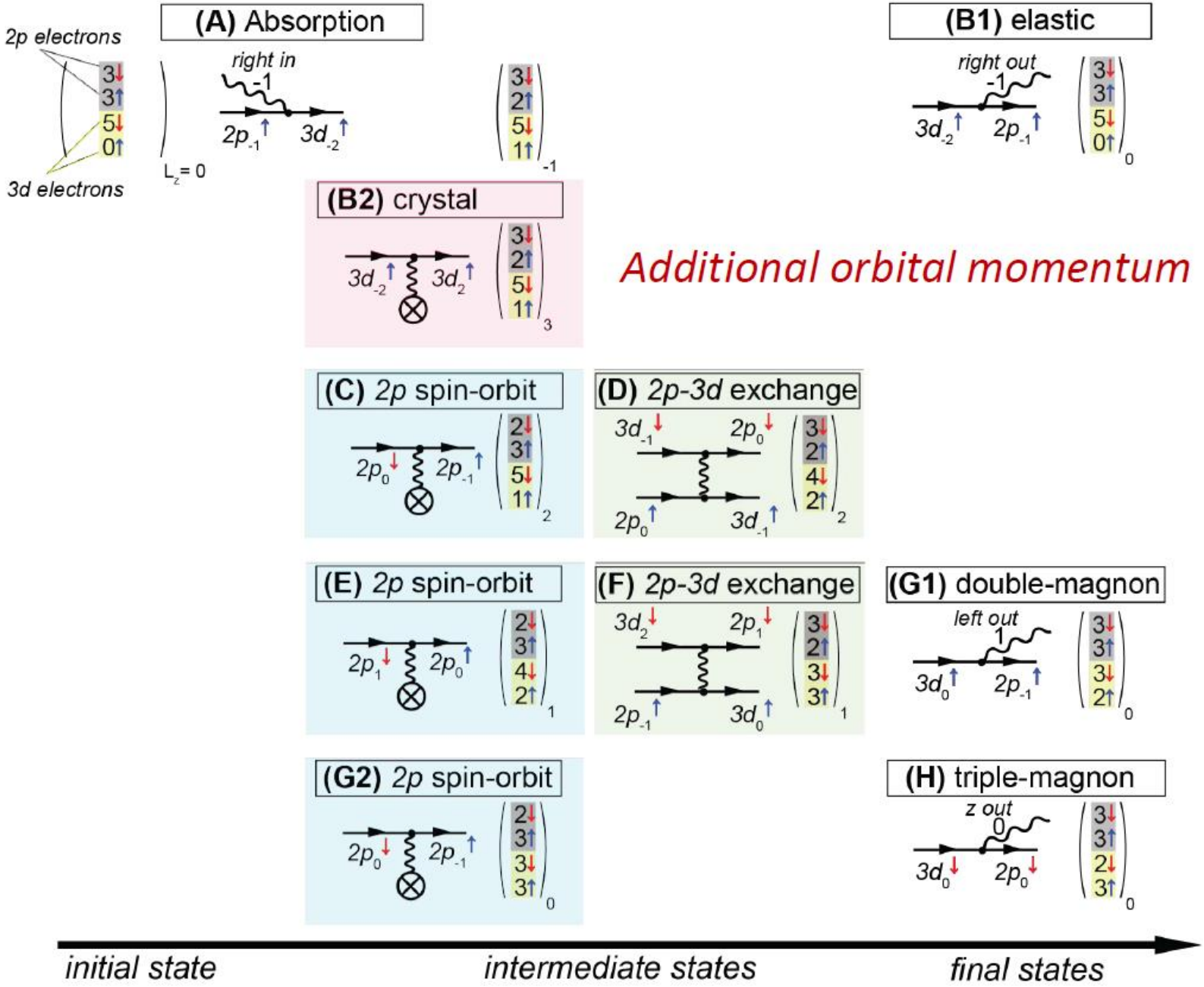


3-magnons in 2p3d RIXS of Fe2O3



Additional orbital momentum

3-magnons in 2p3d RIXS of Fe2O3



2p3d RIXS

polarization, angles
(in, sample, out)

eV
electron-electron
crystal field
charge transfer

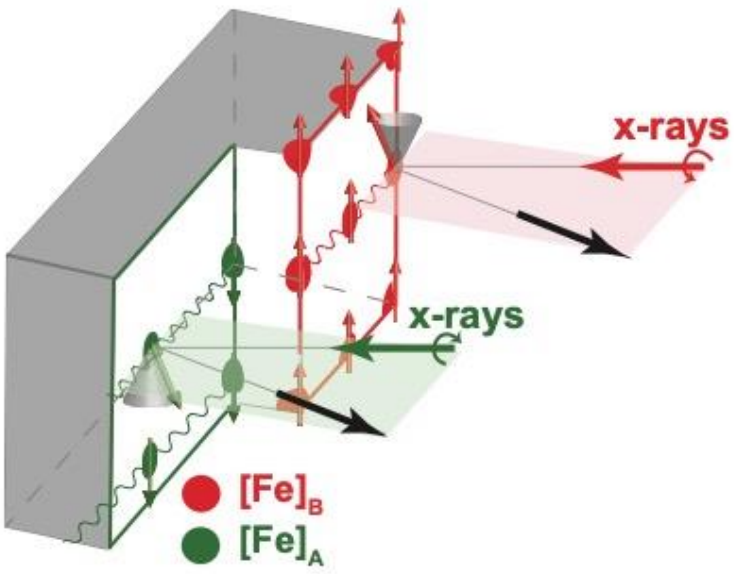
meV
spin-orbit, magnetic
distortions
vibrations

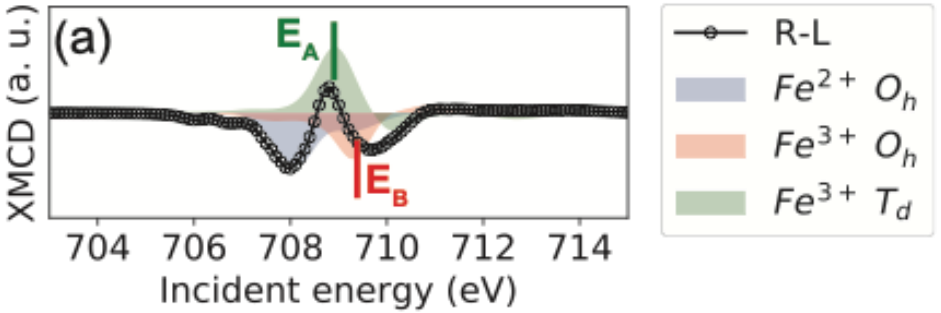
RIXS1998:
500 meV

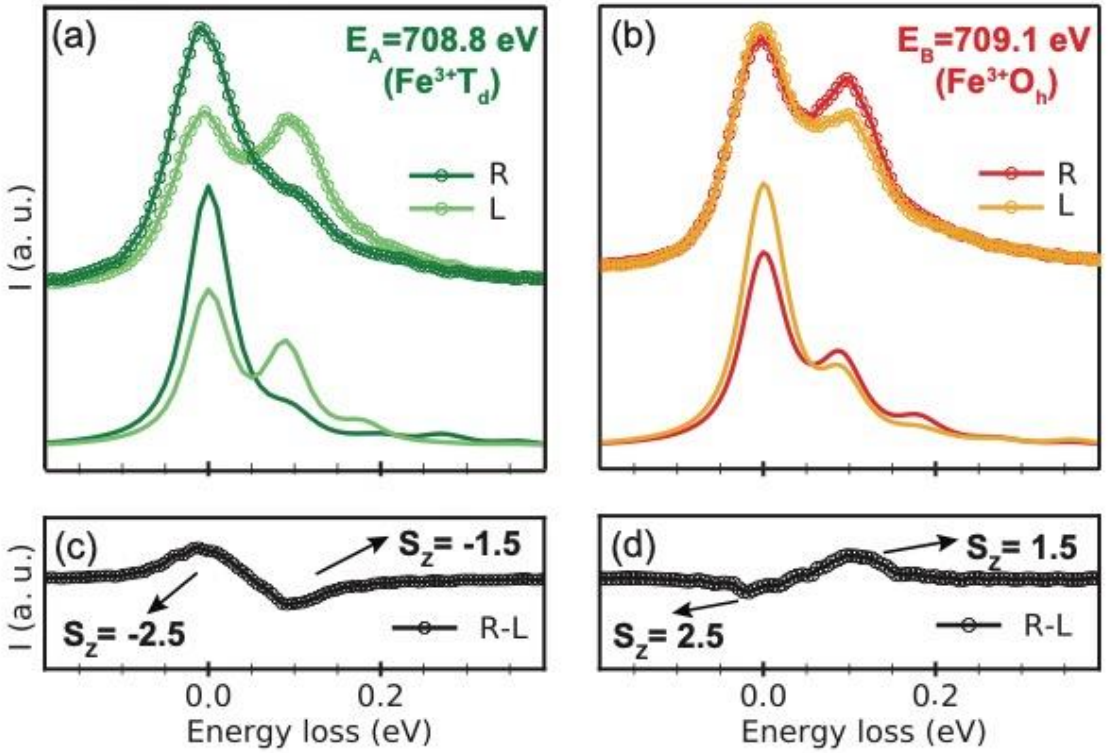
RIXS 2019:
20 meV

Disentangling the A and B sites

2p3d RIXS-MCD



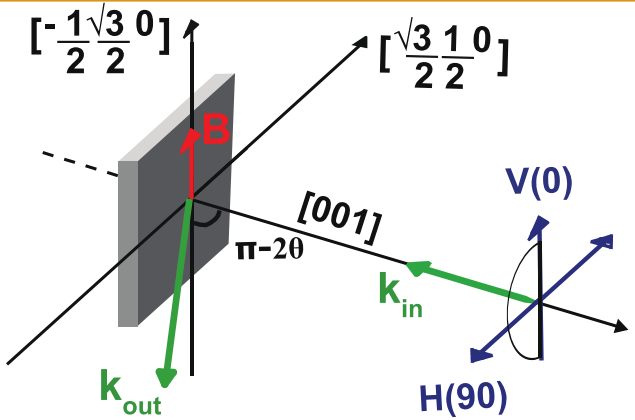


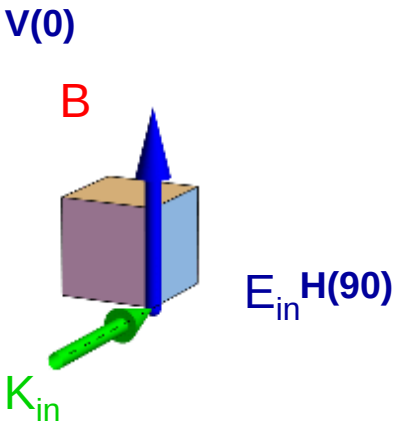


J_{eff} = 90 meV

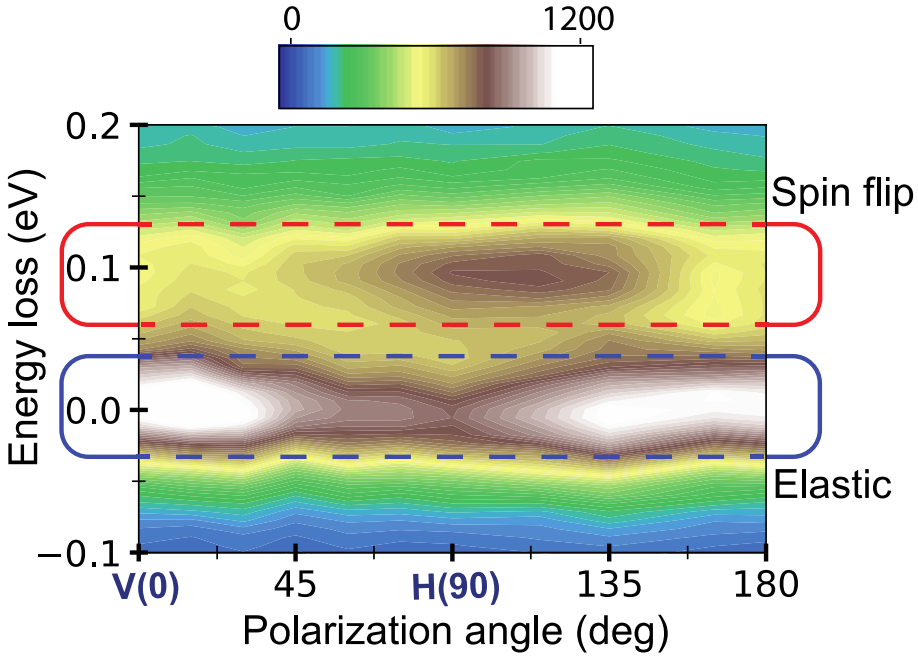
[Elnaggar et al. ACS Appl. Mat & Interf. (2019)]

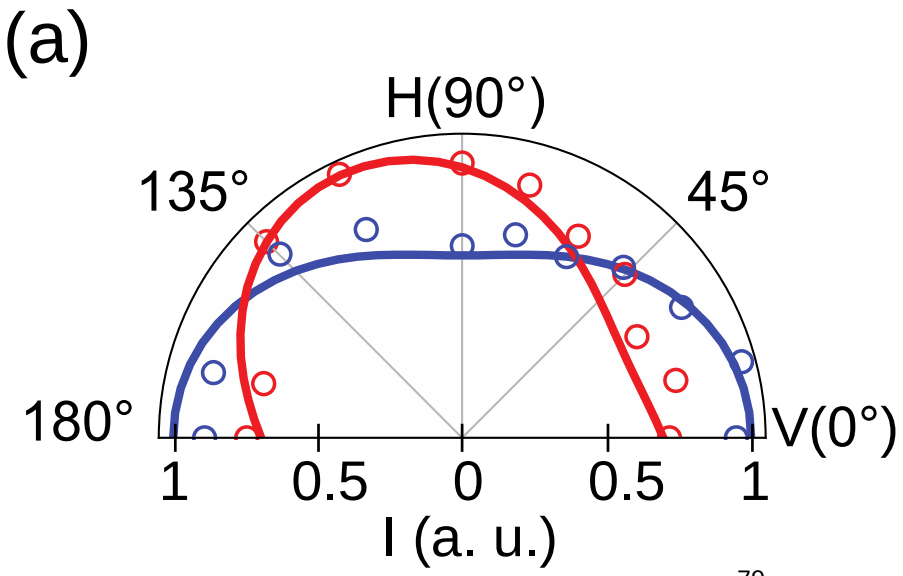
RIXS magnetic angular distribution





Fe^{3+}_A





[Elnaggar et al. PRM 4, 024415 (2020)/PRL 123, 207210 (2019) / PRB 101, 085107 (2020)

Soft x-ray RIXS

dd-excitations (20 meV resolution)

- detailed electronic structure
- dispersion of dd-excitations
- separate different valences
- distortions & spin-orbit coupling

magnons

- dispersion of magnons
- multi-magnons

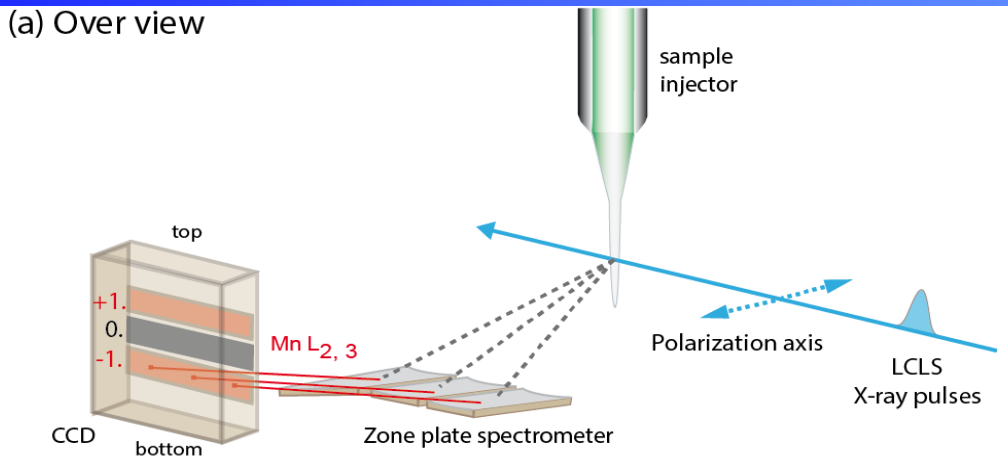
polarization analysis

- detailed moment analysis (Lz, Sz, site specific)
- RIXS-MCD

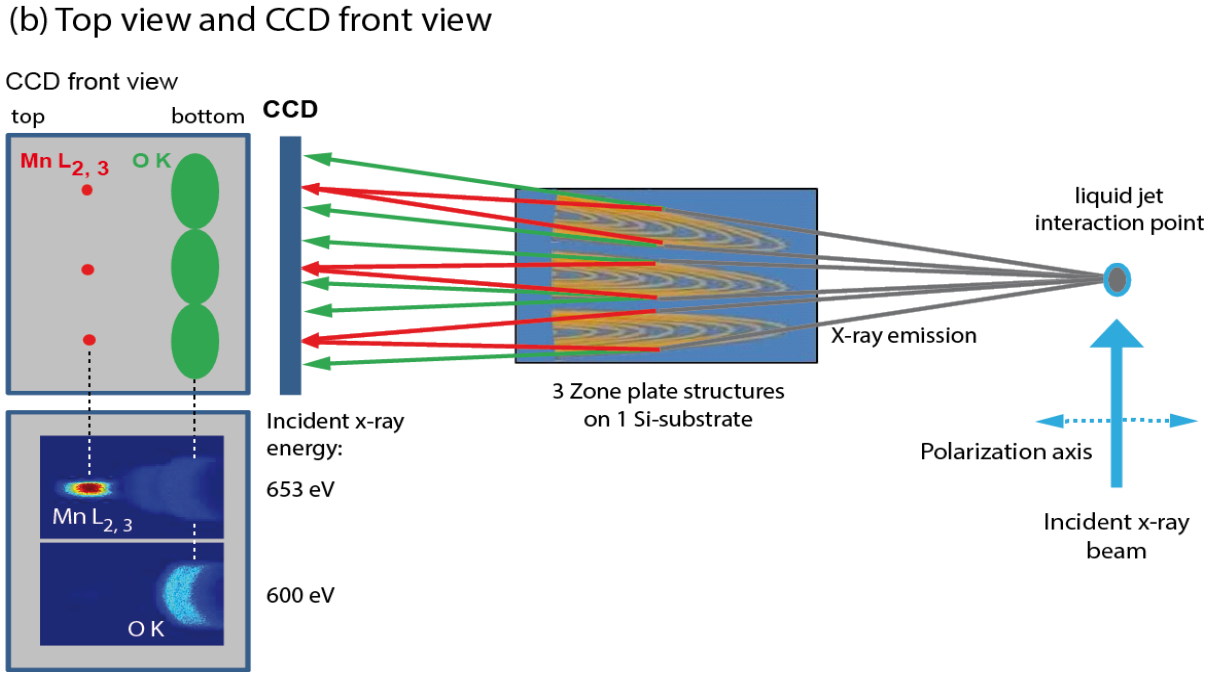
time: experiments with 100 fs (or better)

XAS distortions in FY

FY-XAS of radiation sensitive sample

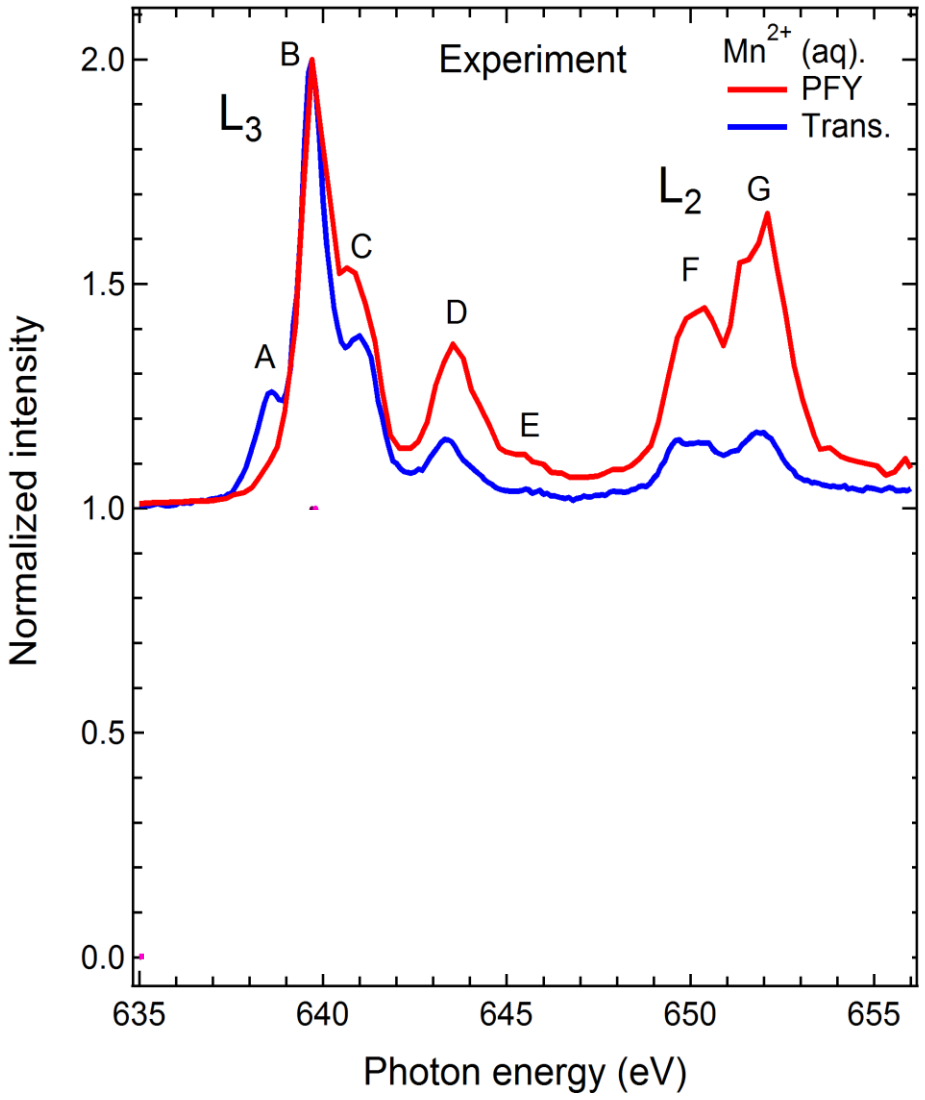


Single synchrotron pulselength is too long



Mitzner et al, J. Phys. Chem. Lett. 4, 3641 (2013)

FY-XAS of radiation sensitive sample

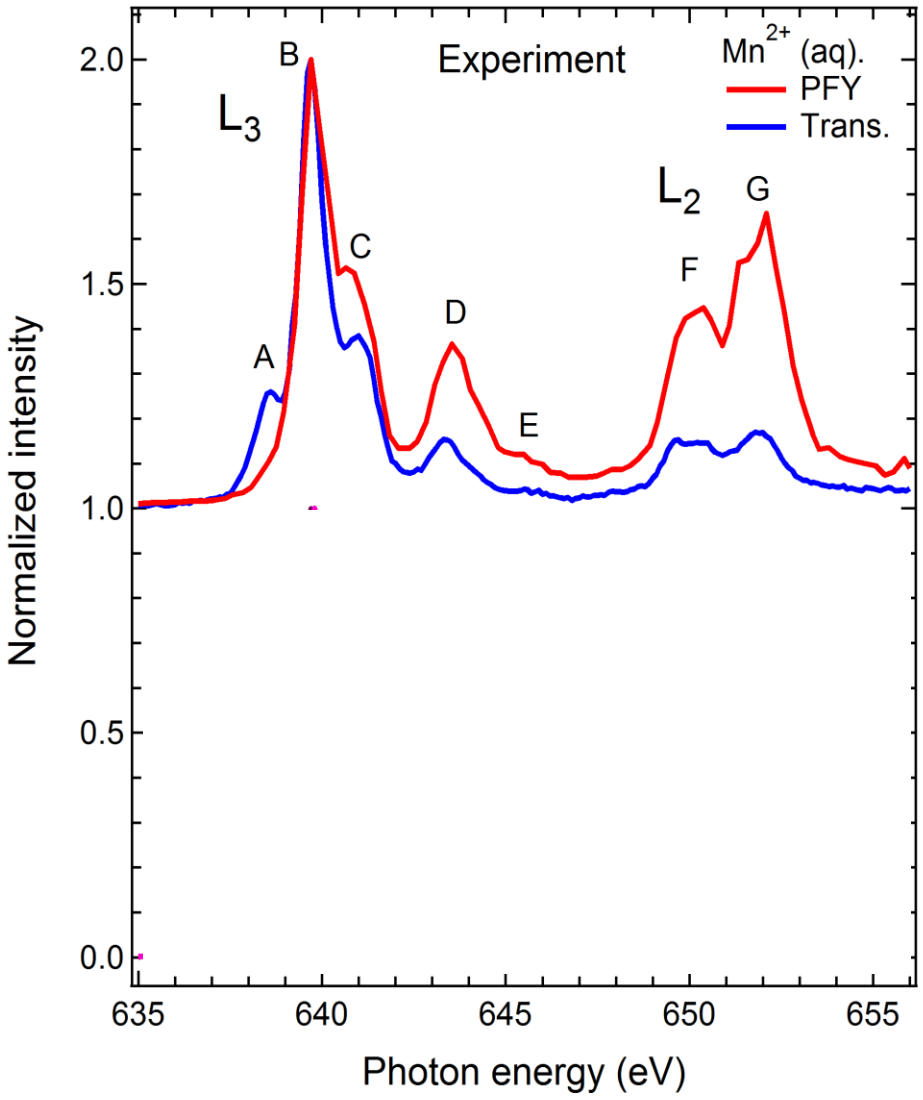


Fluorescence does not measure XAS spectrum

- Saturation ?

Mitzner et al, J. Phys. Chem. Lett. 4, 3641 (2013)

FY-XAS of radiation sensitive sample



Fluorescence does not measure XAS spectrum

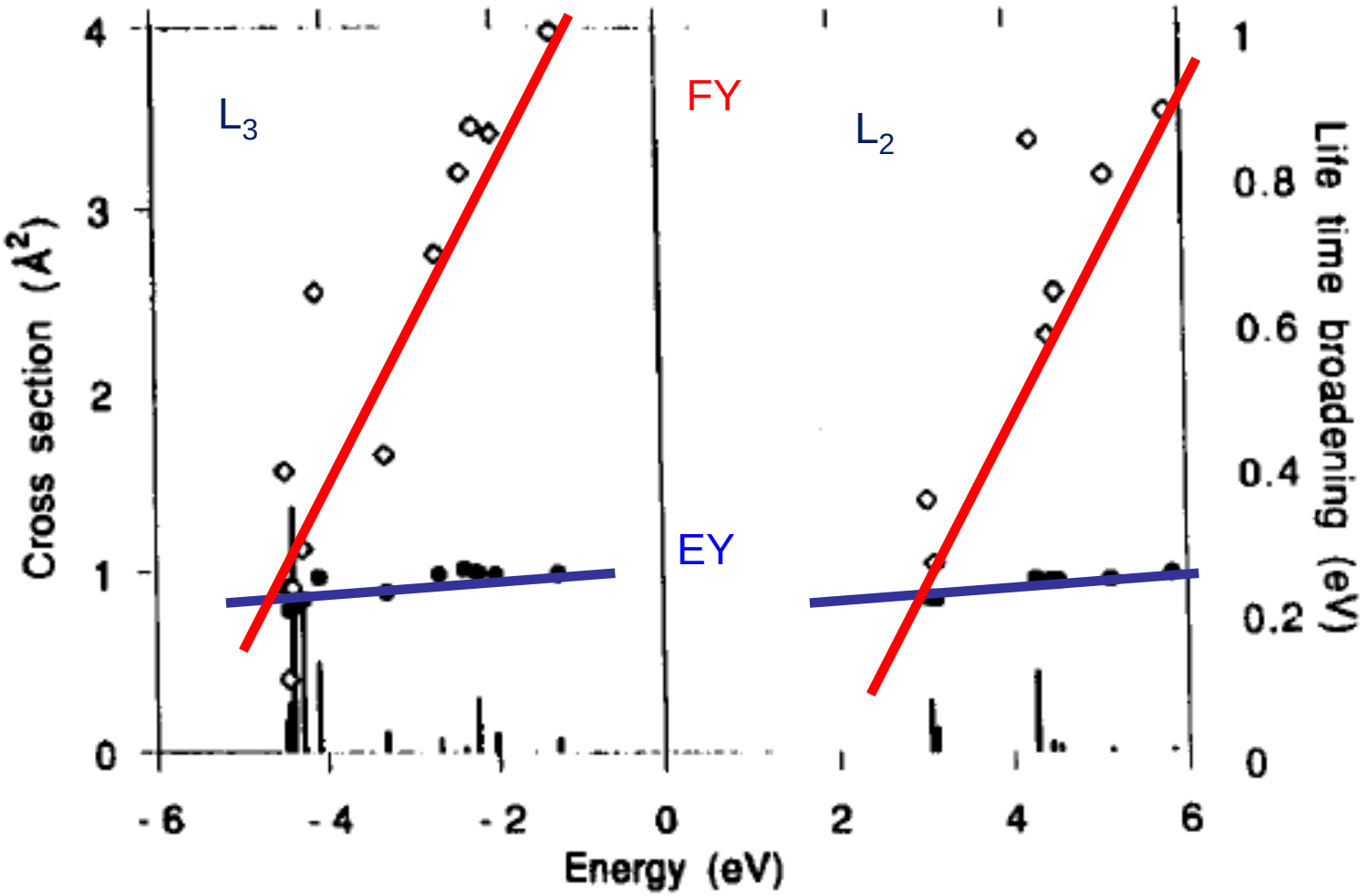
- NO Saturation
- State-dependent decay

Mitzner et al, J. Phys. Chem. Lett. 4, 3641 (2013)

FY detection: State dependent decay

- Yield methods assume a constant ratio between radiative and non-radiative decay
- If this ratio is state (= energy) dependent then the related yield methods do not measure XAS.

FY detection: State dependent decay



Solid State Comm. 92, 991 (1994)

FY detection: State dependent decay

- The dominant yield method is not visibly affected, thus for soft X-rays only FY is affected, not electron yield.

FY detection (state-dependent, dilute)

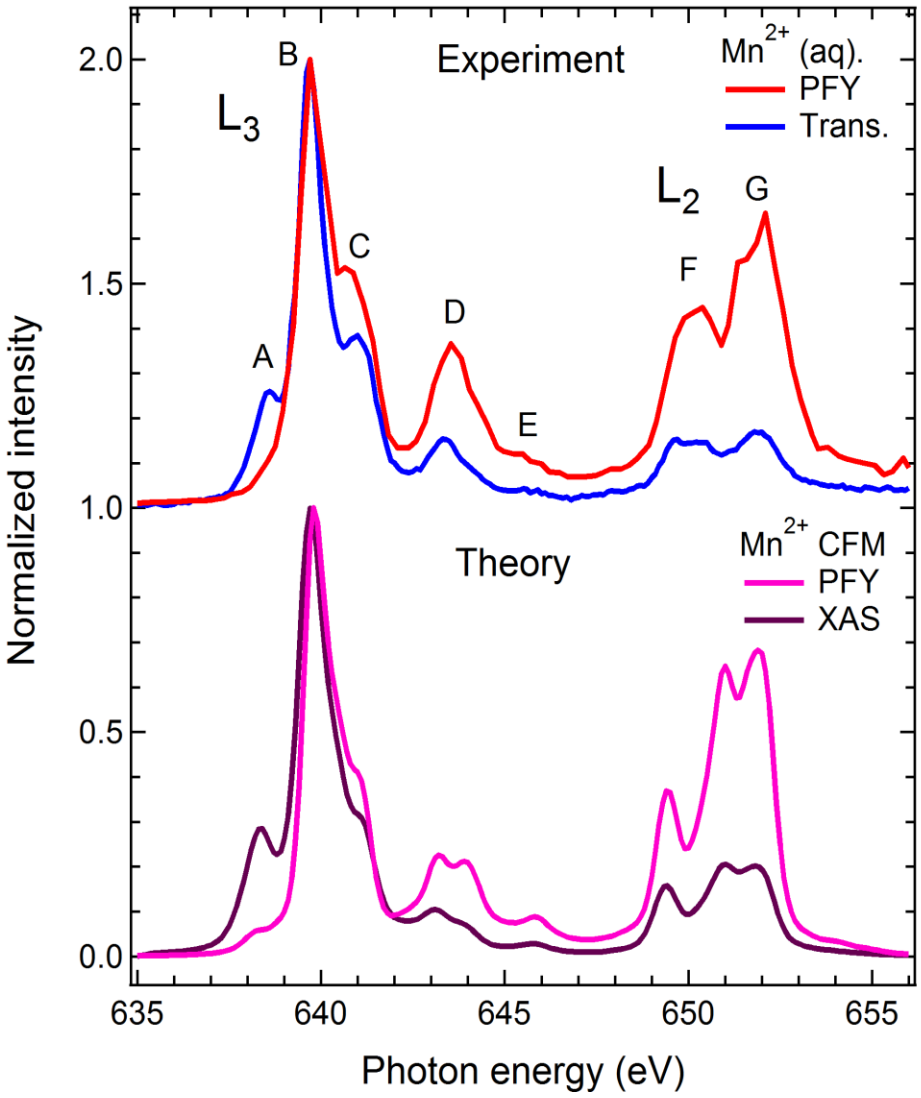
$$I_{TFY} \sim \frac{\mu(\omega)*\sigma}{\mu(\omega)+\mu B} + \frac{\mu B*\sigma B}{\mu(\omega)+\mu B}$$

$$I_{TFY} \sim \frac{\mu(\omega)*\sigma(\omega)}{\mu B}$$

- Main decay of 2p core hole is 2p3d RIXS
- Integrate RIXS spectrum to 2p3d PFY
- TFY ~ 2p3d PFY

- NOTE: “RIXS” has angular dependence effects

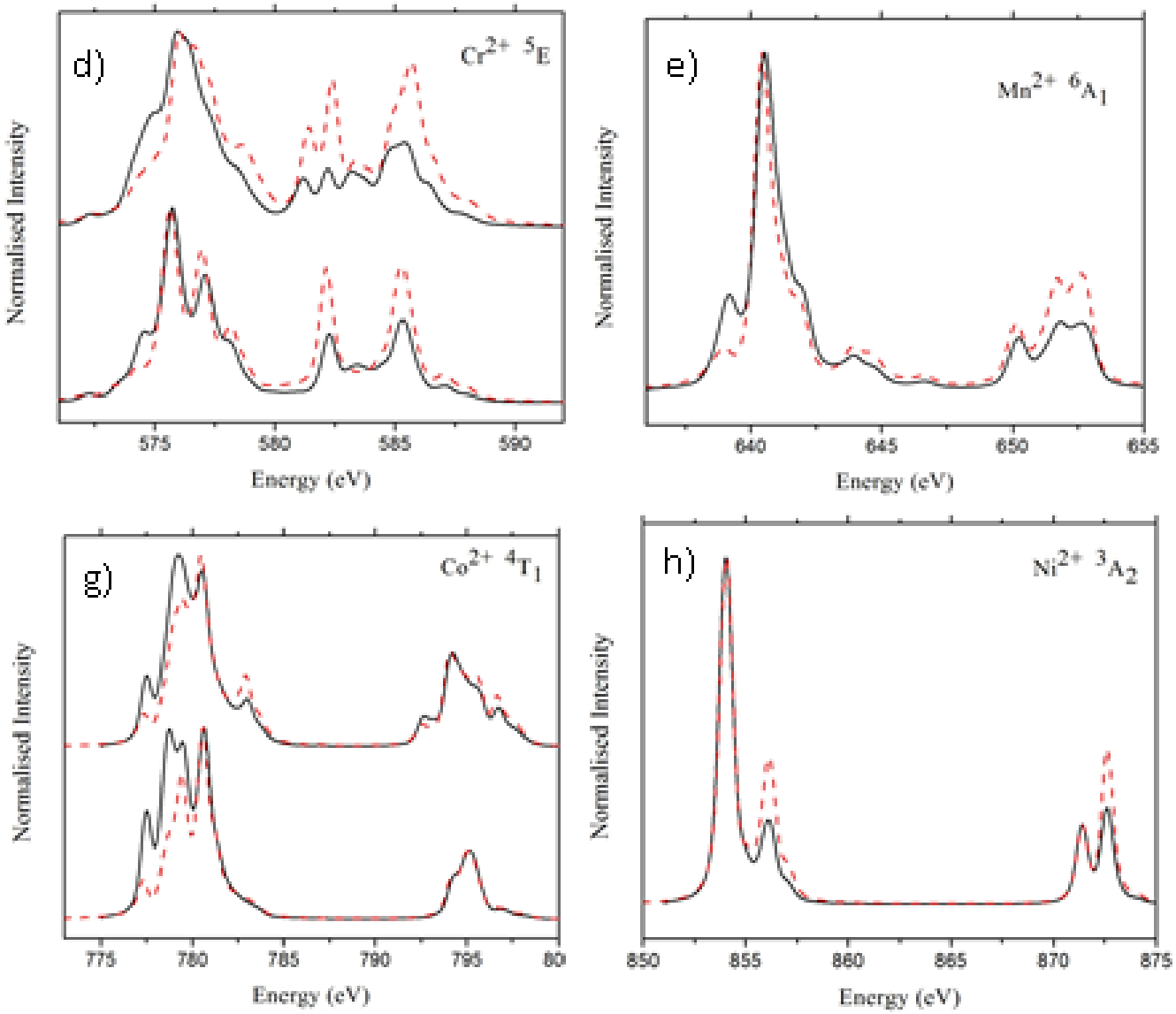
XAS: transmission & FY



Mitzner et al, J. Phys. Chem. Lett. 4, 3641 (2013)

Fluorescence Yield detection

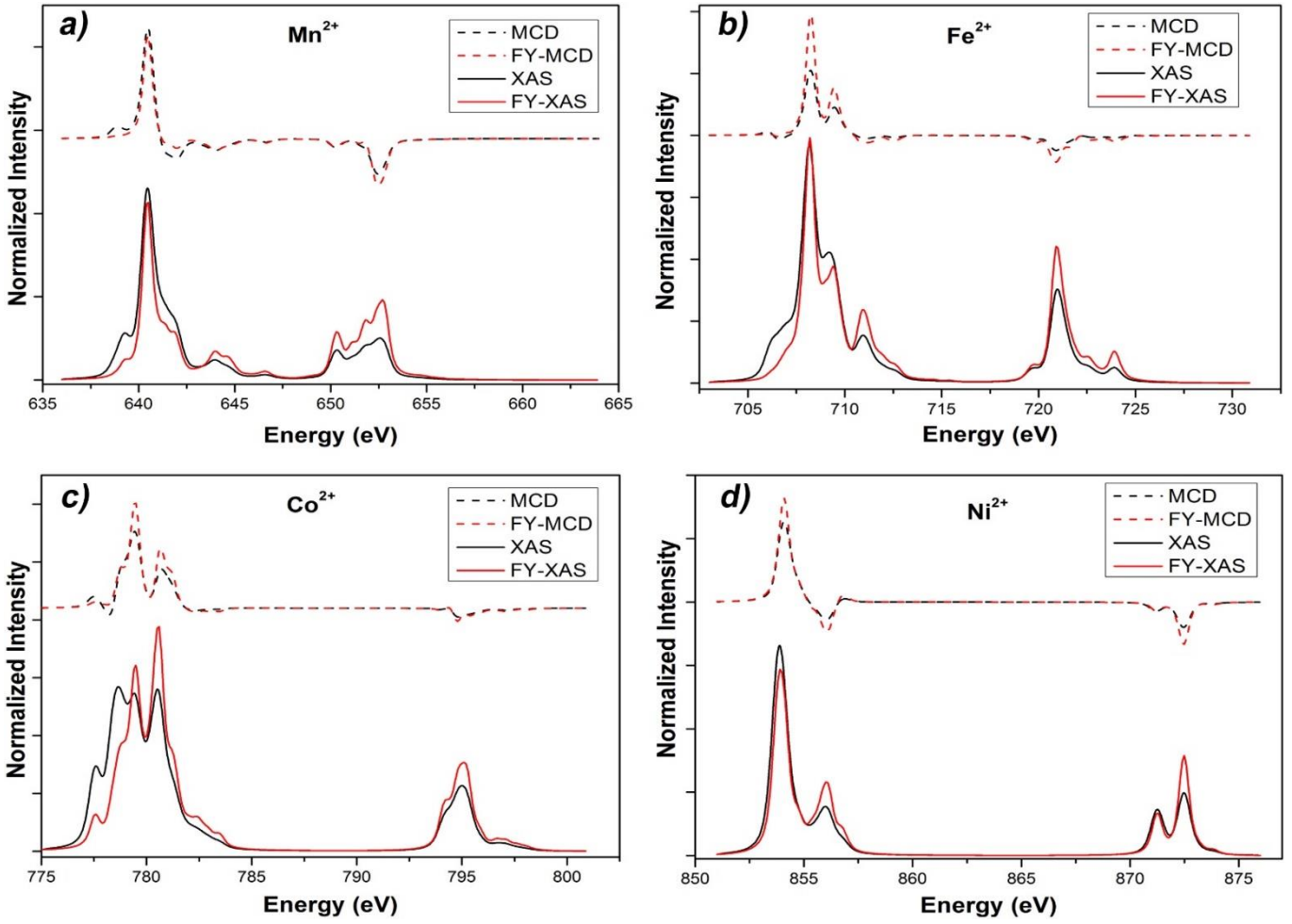
FY-XAS ≠ XAS L_2 edge increases High-energies increase



Kurian J. Phys. Cond. Matt. 24, 435602 (2012)

Fluorescence Yield XMCD

- XMCD sum rules break down
- Ni/Co 20%, Fe 30%, Mn > 100% error



Liu, Phys. Rev. B. 96, 054446 (2017)

RIXS with hard x-rays

1s2p RIXS of transition metal ions

10^{-10}

10^{-8}

$.5 \times 10^{-6}$

10^{-5}

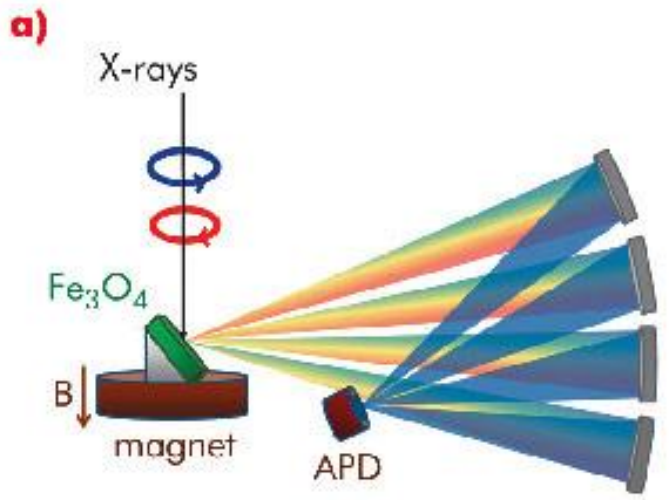
1s

2p

electronic
dd, CT

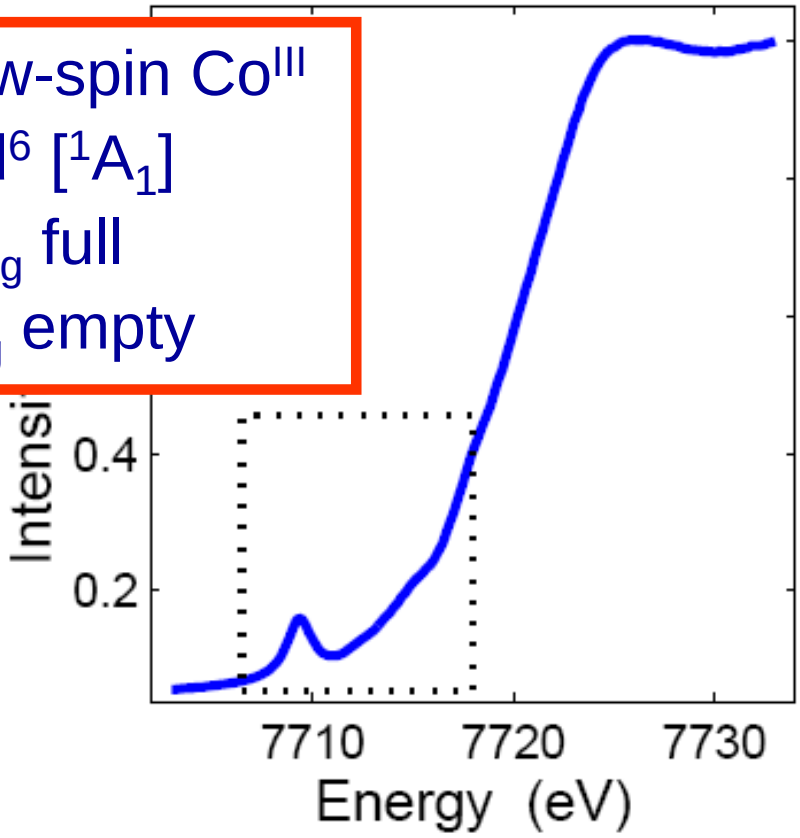
magnon
vibrations

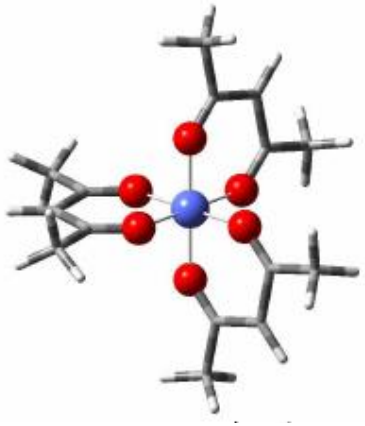
Ψ_0



1s2p RIXS of transition metal ions

low-spin Co^{III}
$3d^6$ [$^1A_1$]
T_{2g} full
E_g empty

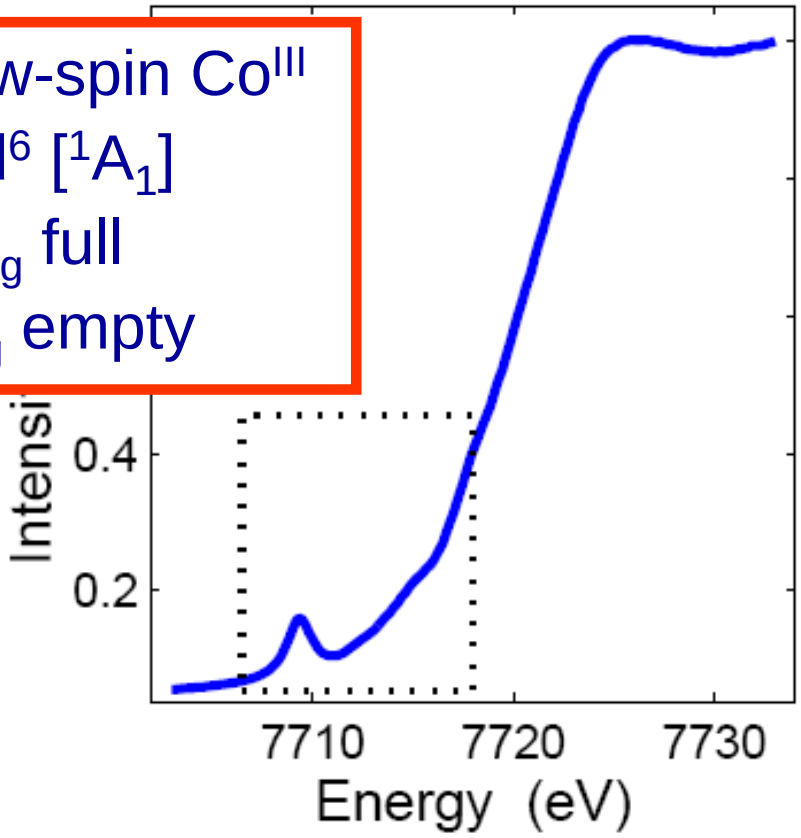


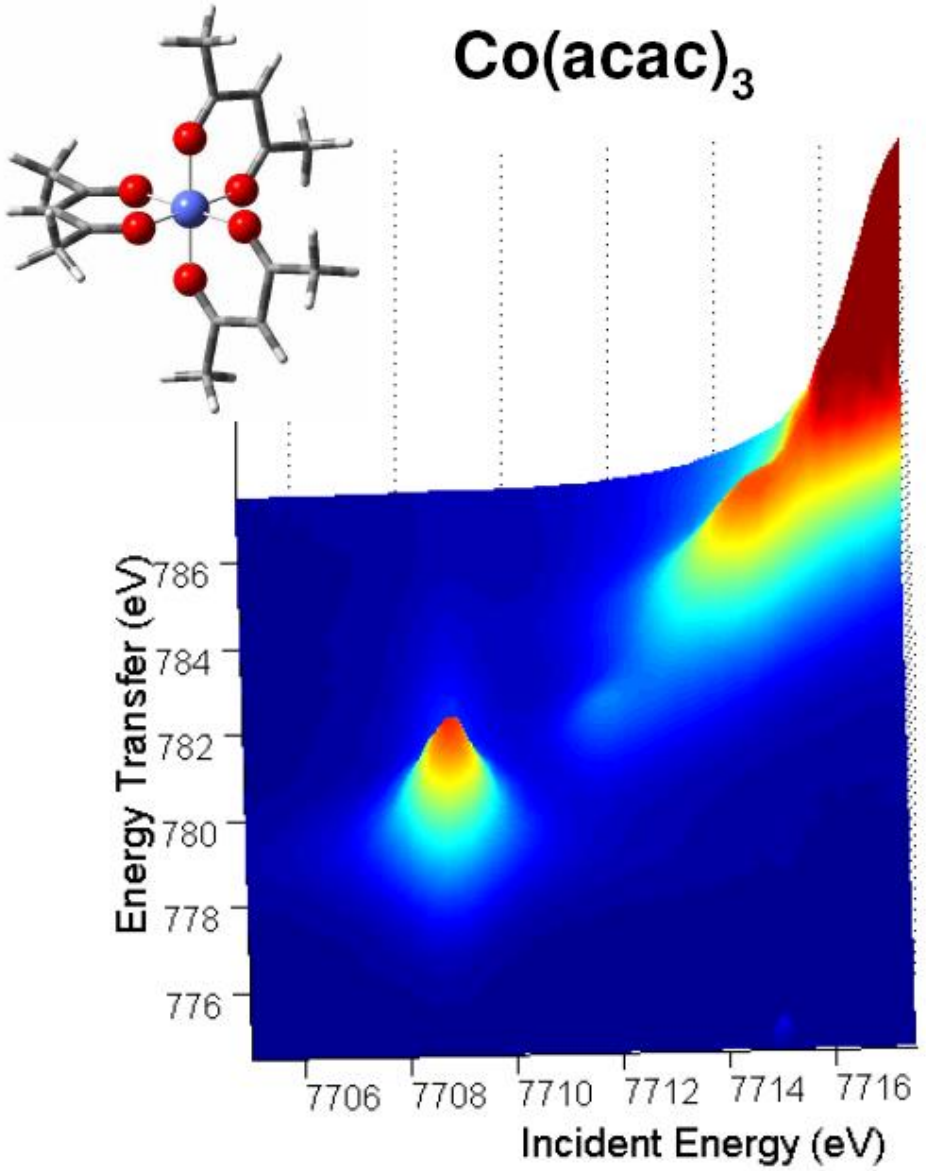


$Co(acac)_3$

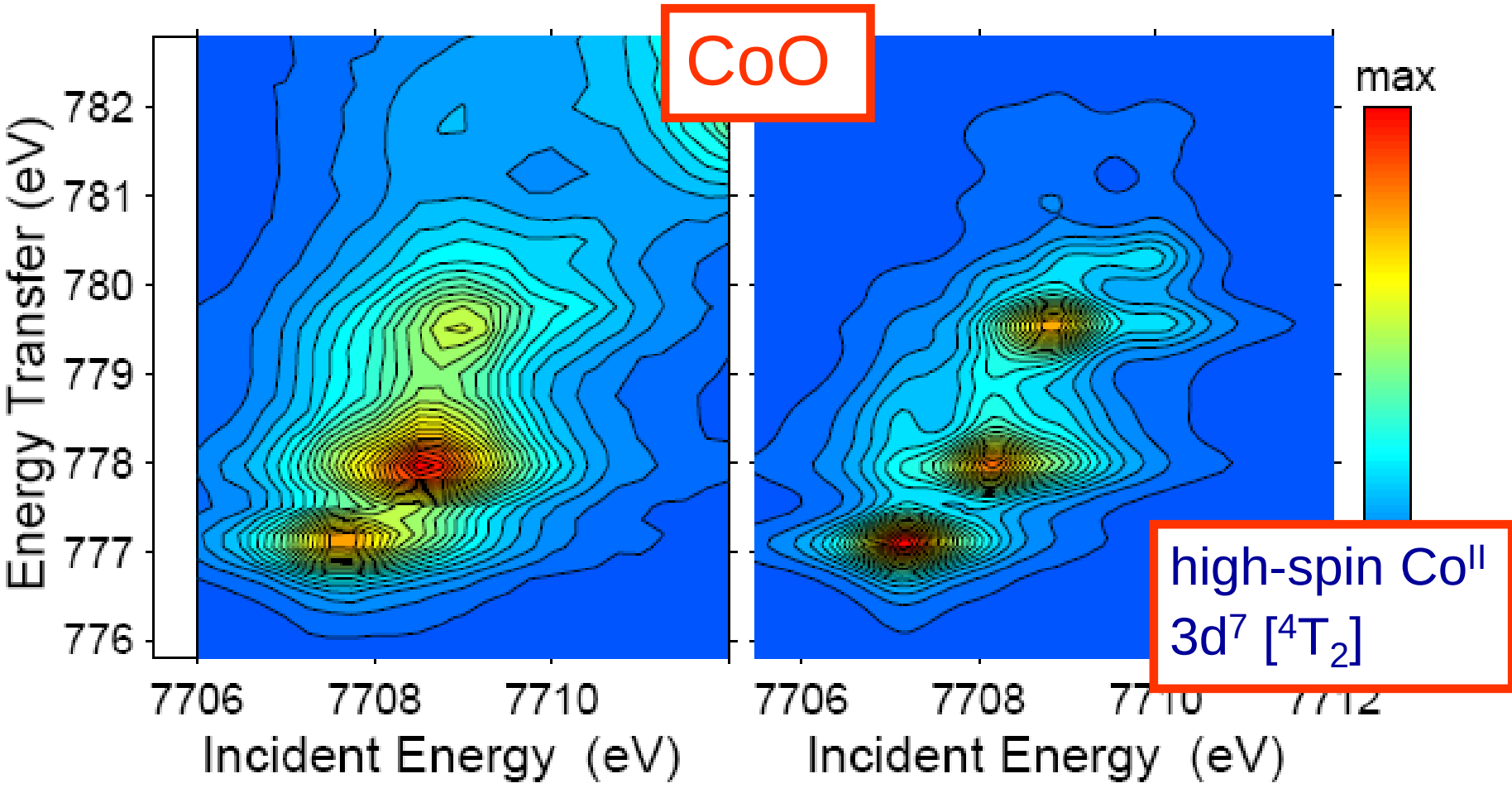
1s2p RIXS of transition metal ions

low-spin Co^{III}
$3d^6$ [$^1A_1$]
T_{2g} full
E_g empty





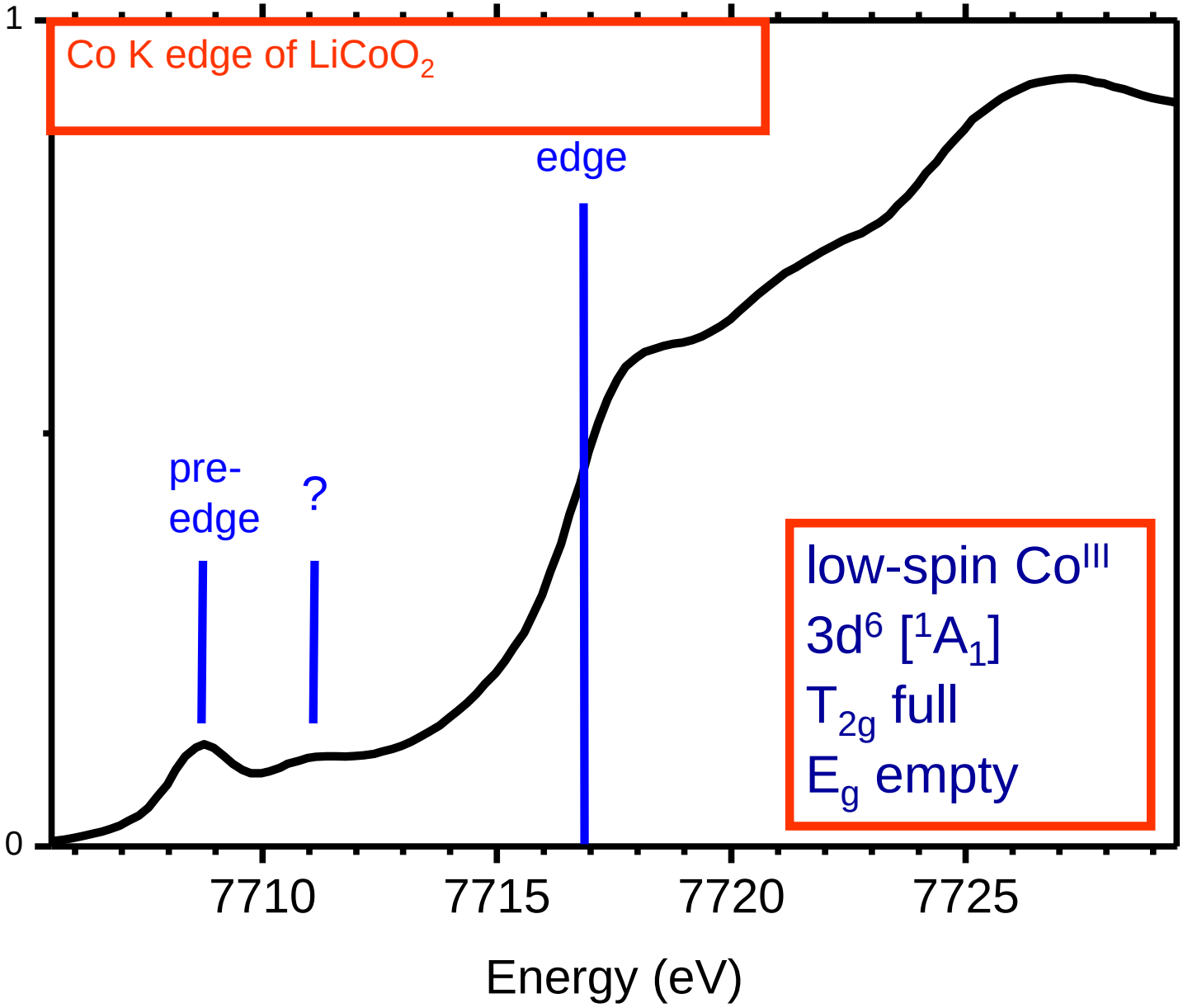
Sharper pre-edge structures in 1s XAS



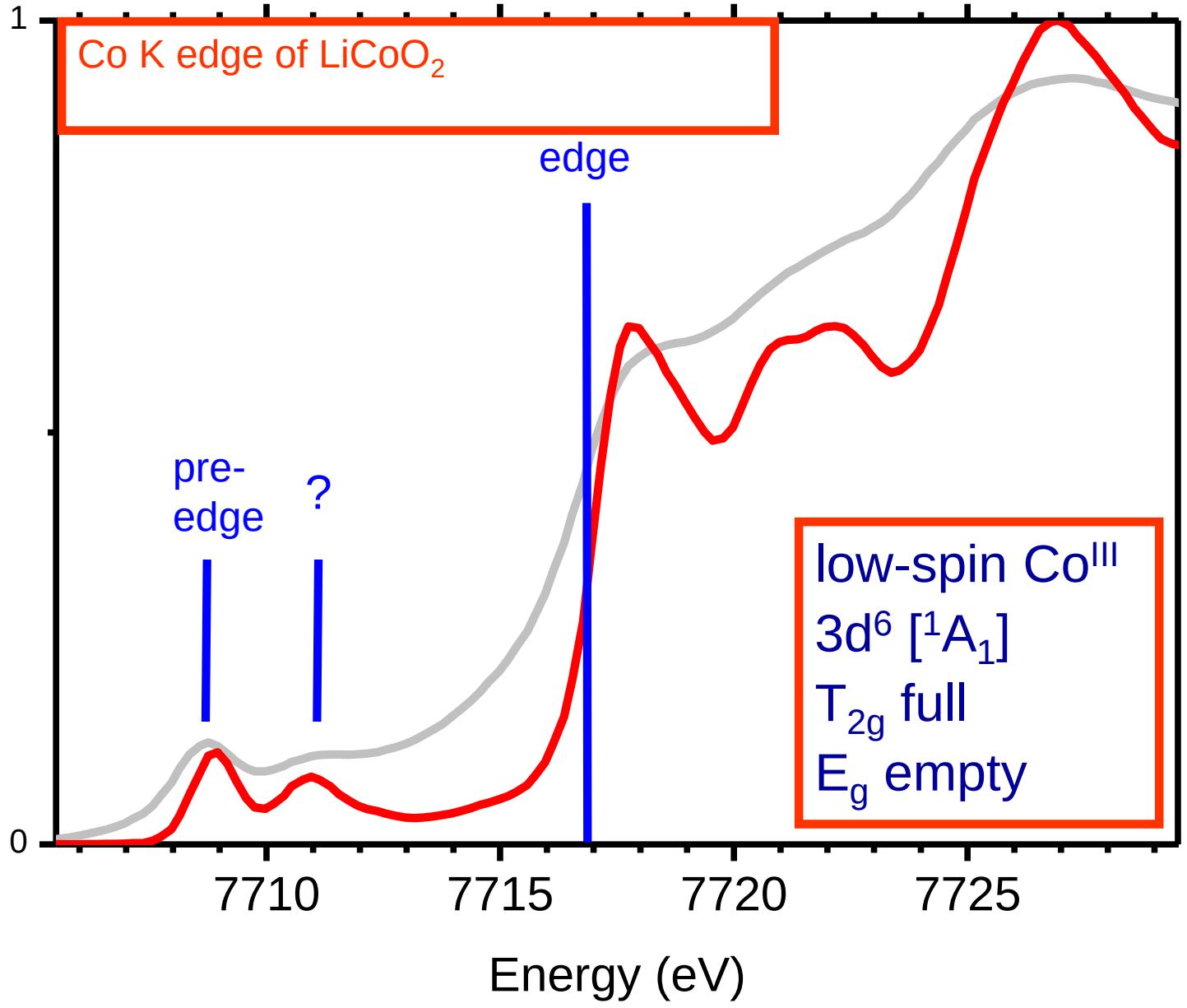
Only quadrupole peaks visible

$3d^7 \rightarrow 1s^1 3d^8 \rightarrow 2p^5 3d^8$

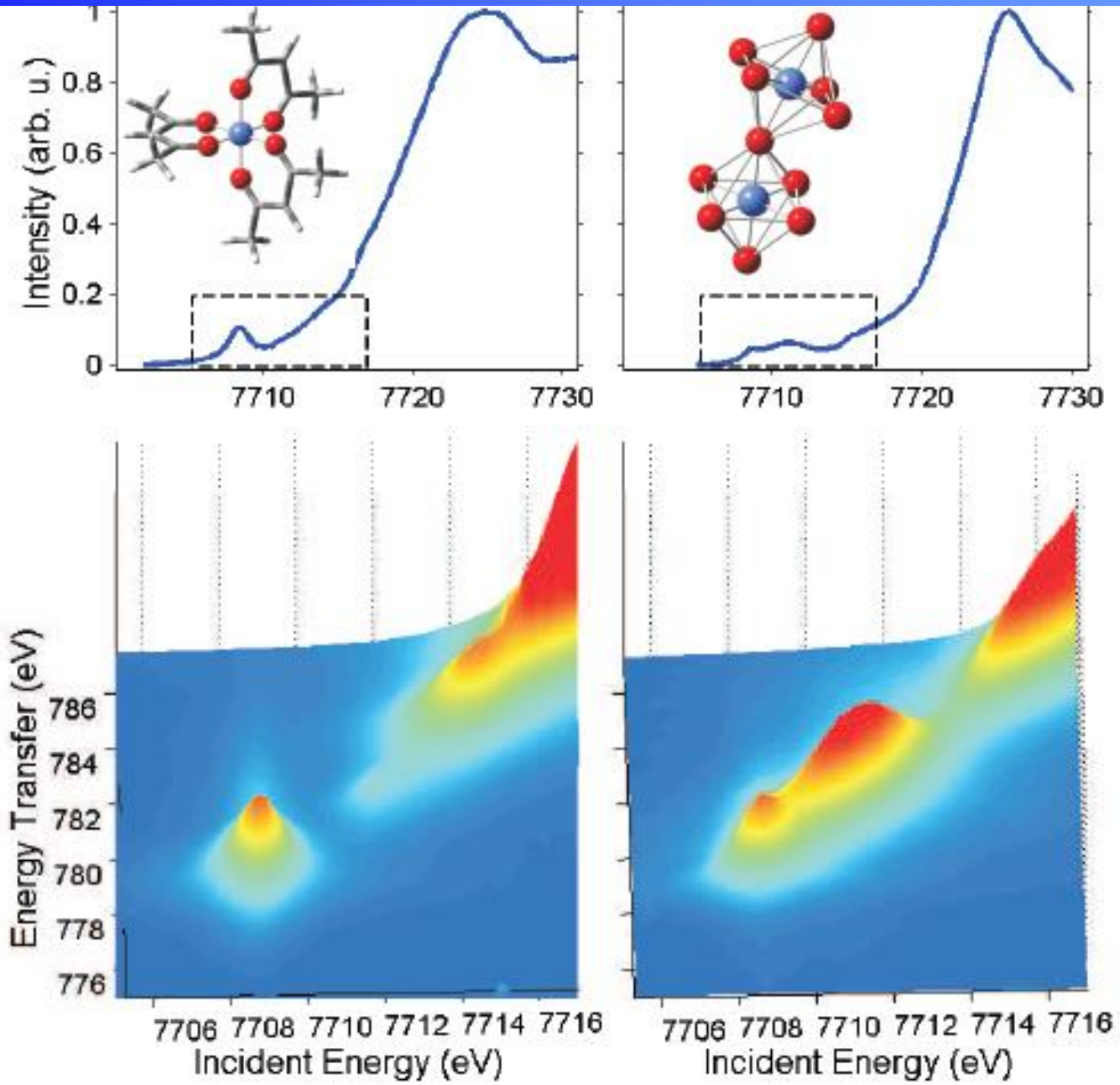
Pre-edges structures in 1s XAS



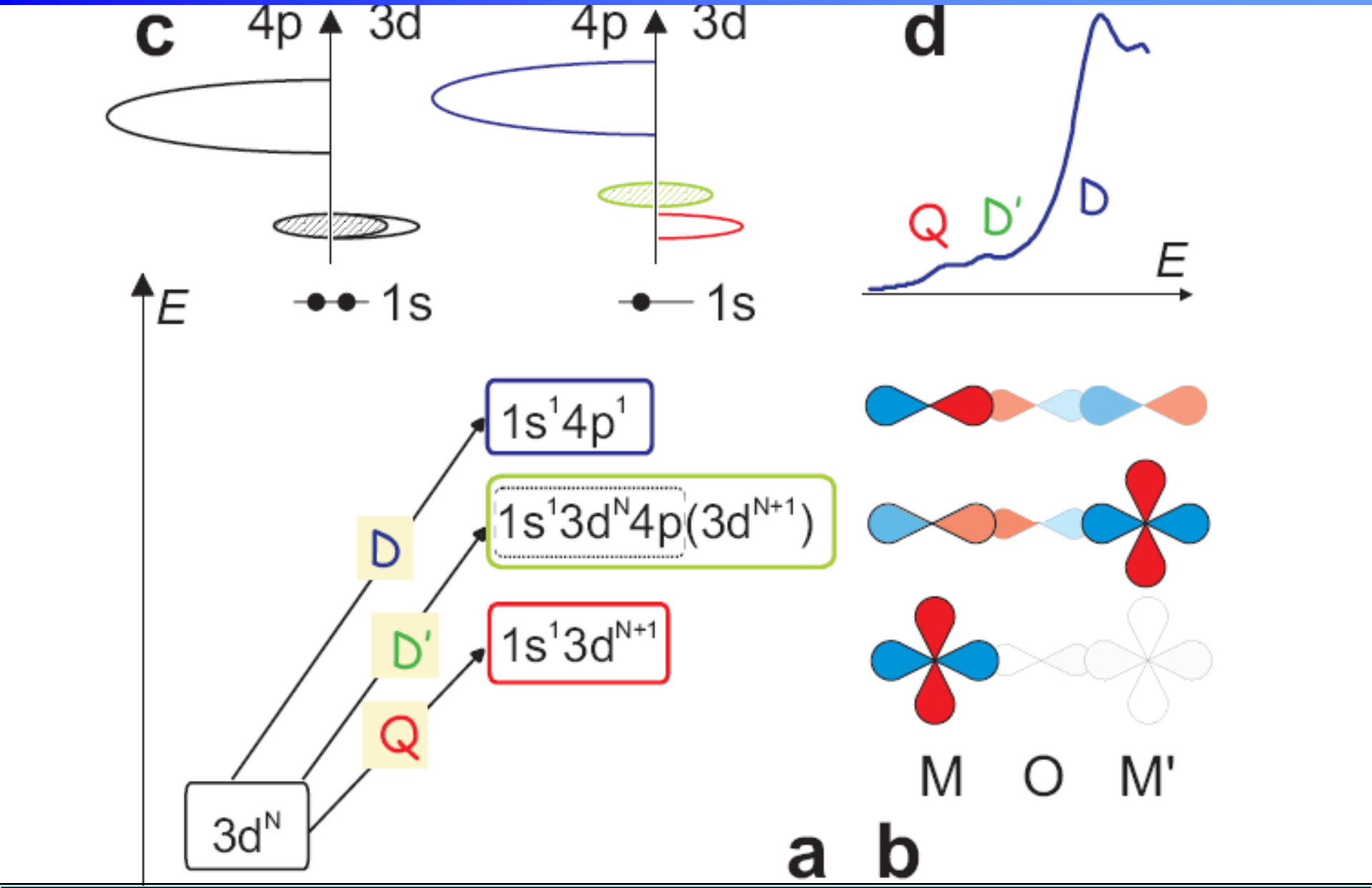
Pre-edges structures in 1s XAS



Pre-edges structures in 1s XAS

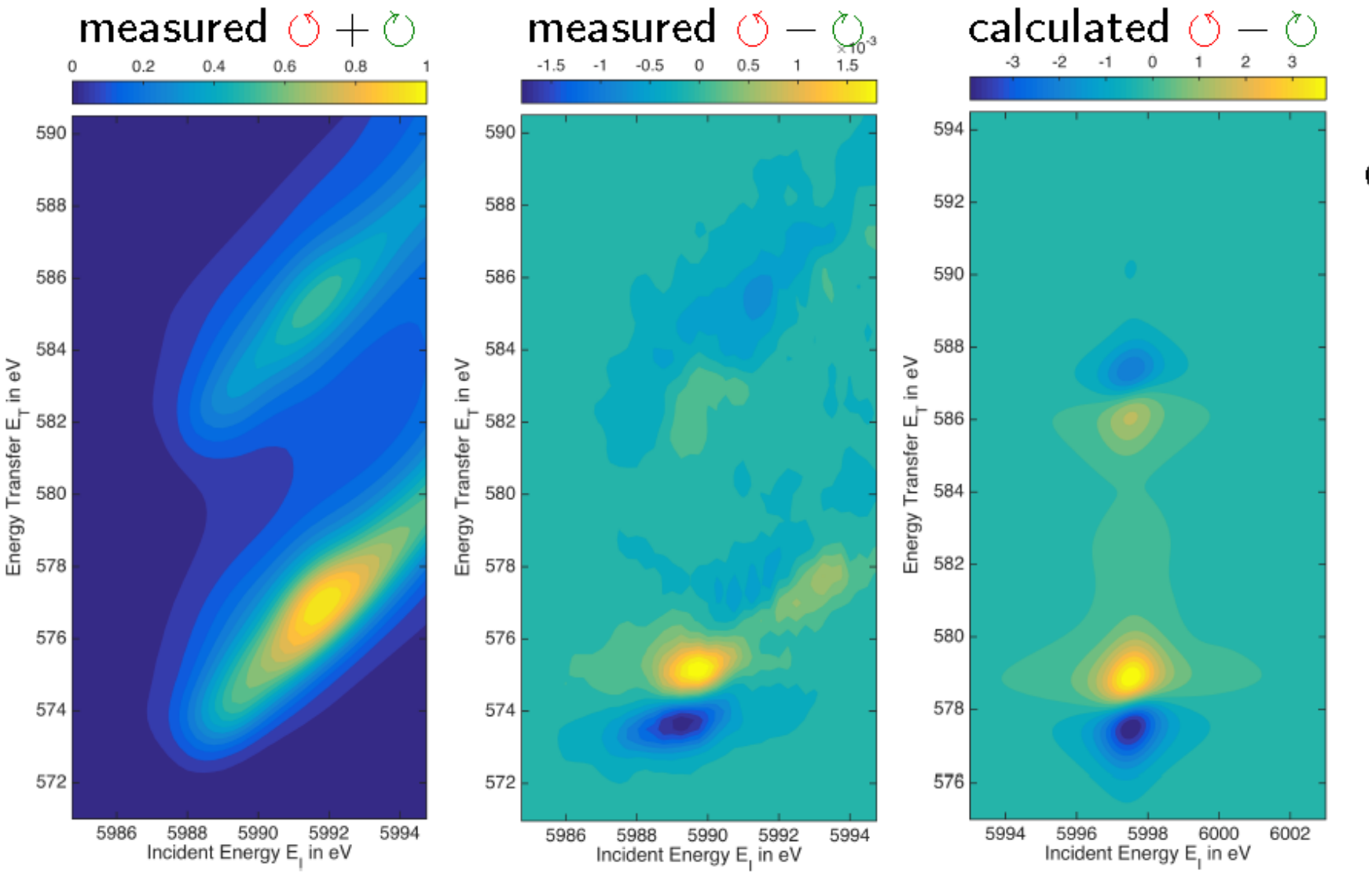


Pre-edges structures in 1s XAS



J. Phys. Cond. Matt. 21, 104207 (2009); Phys. Rev. B. 81, 115115 (2010)

RIXS-MCD of CrO_2

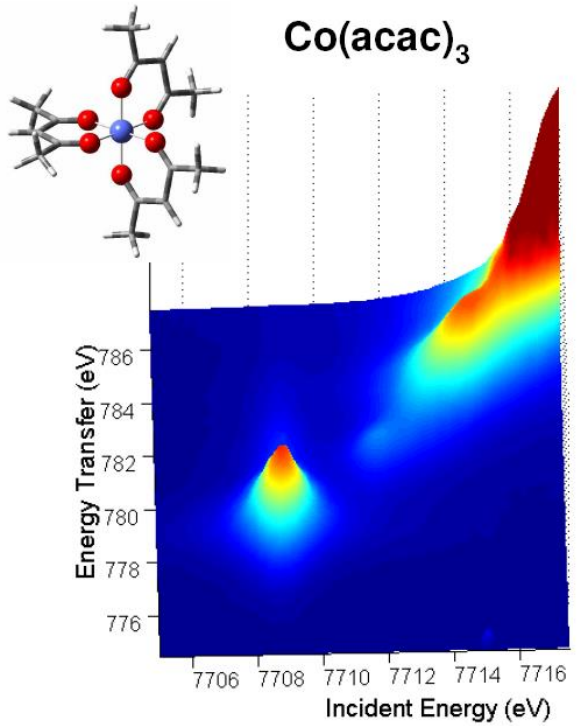


[Zimmermann et al. J. Elec. Spec (2017)]

Hard x-ray RIXS

- Reduce lifetime from 1.5 to 0.2 eV (HERFD XANES)
- Reveal new features at pre-edge

- Soft x-ray edges with hard x-rays
- Spin-polarized XAS
- Range extended EXAFS
- Background free FY for low conc.
- RIXS-MCD



resonant inelastic x-ray scattering

- X-ray absorption spectroscopy
- Multiplet calculations

  [let me know if you like to learn them]
- Resonant inelastic x-ay scattering