

POLITECNICO
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Inelastic x-ray scattering

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Outlook

Inelastic x-ray scattering

- scattering kinematics
- a bit of formalism

Non-resonant inelastic x-ray scattering

- examples

Resonant inelastic x-ray scattering

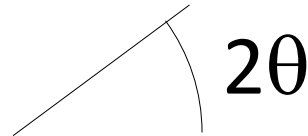
- examples

Instrumentation for (R)IXS

(Why inelastic x-ray scattering?)

Inelastic X-ray scattering

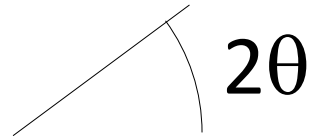
x-ray in – x-ray out process



$\lambda \sim 1-10 \text{ \AA}$: comparable to direct lattice spacing
($k \sim 0.1-1 \text{ \AA}^{-1}$: comparable to reciprocal lattice spacing)

Inelastic X-ray scattering

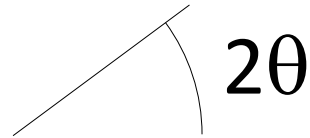
x-ray in – x-ray out process



$\omega = c|\mathbf{k}| \sim 1\text{-}10 \text{ keV}$: access core-levels

Inelastic X-ray scattering

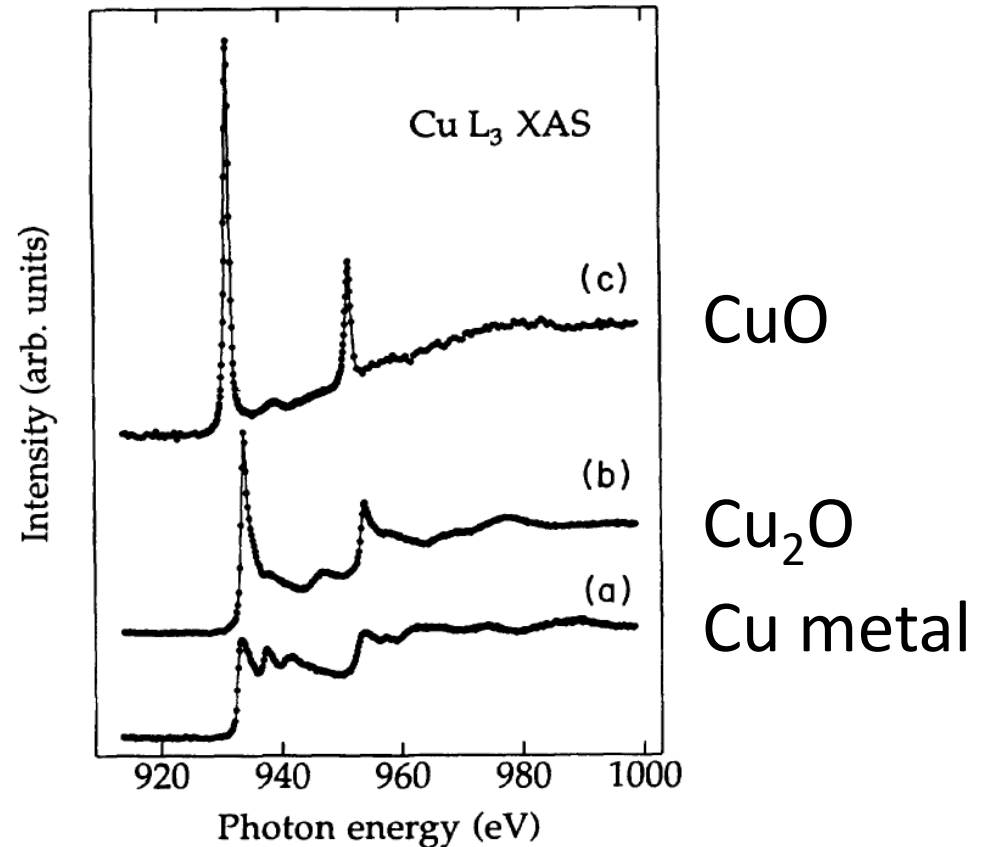
x-ray in – x-ray out process



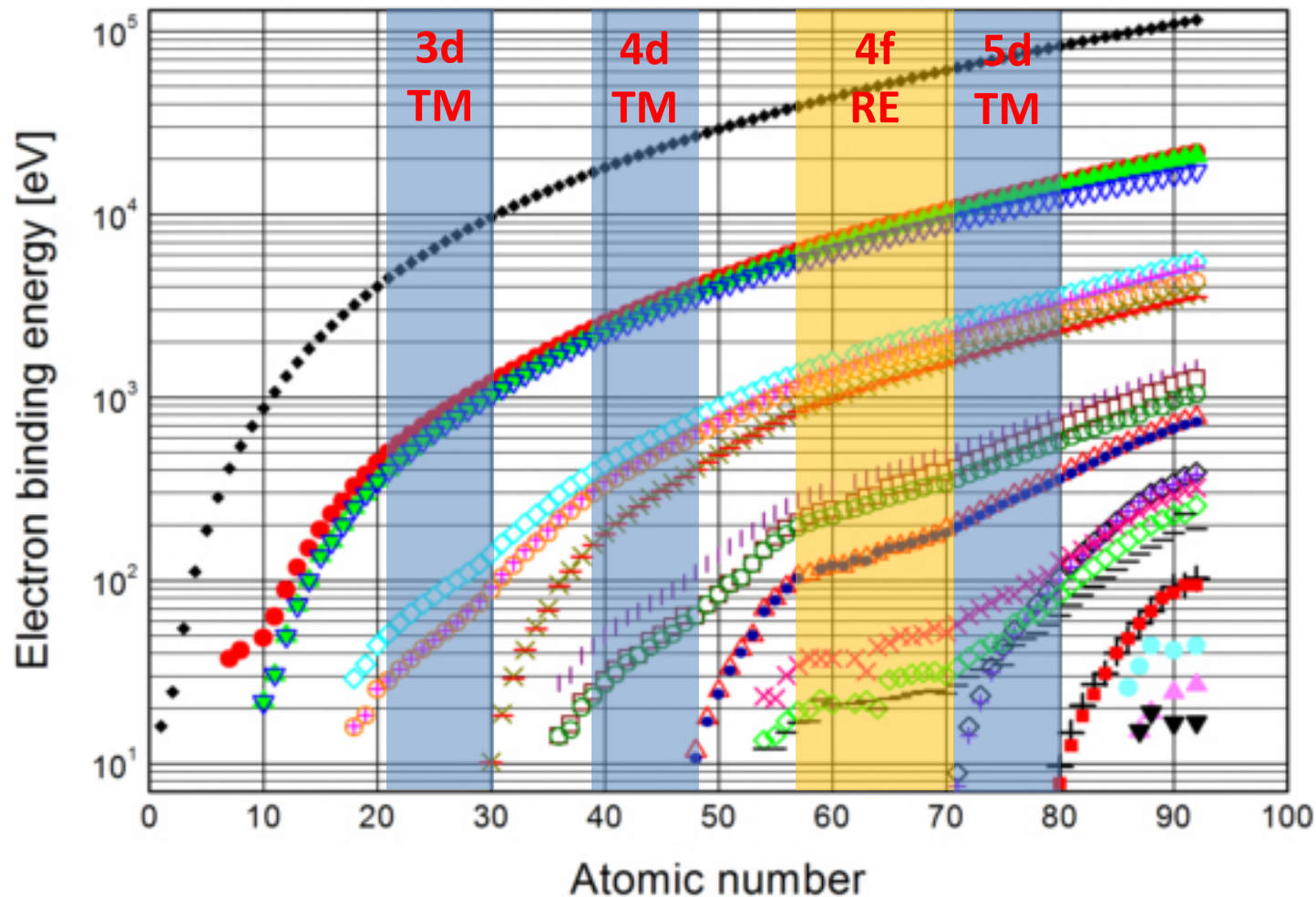
(non) trivial polarization dependence

Inelastic X-ray scattering

ω_i close to an absorption edge? Resonant vs. non-resonant



Inelastic X-ray scattering



K (n=1)

L (n=2)

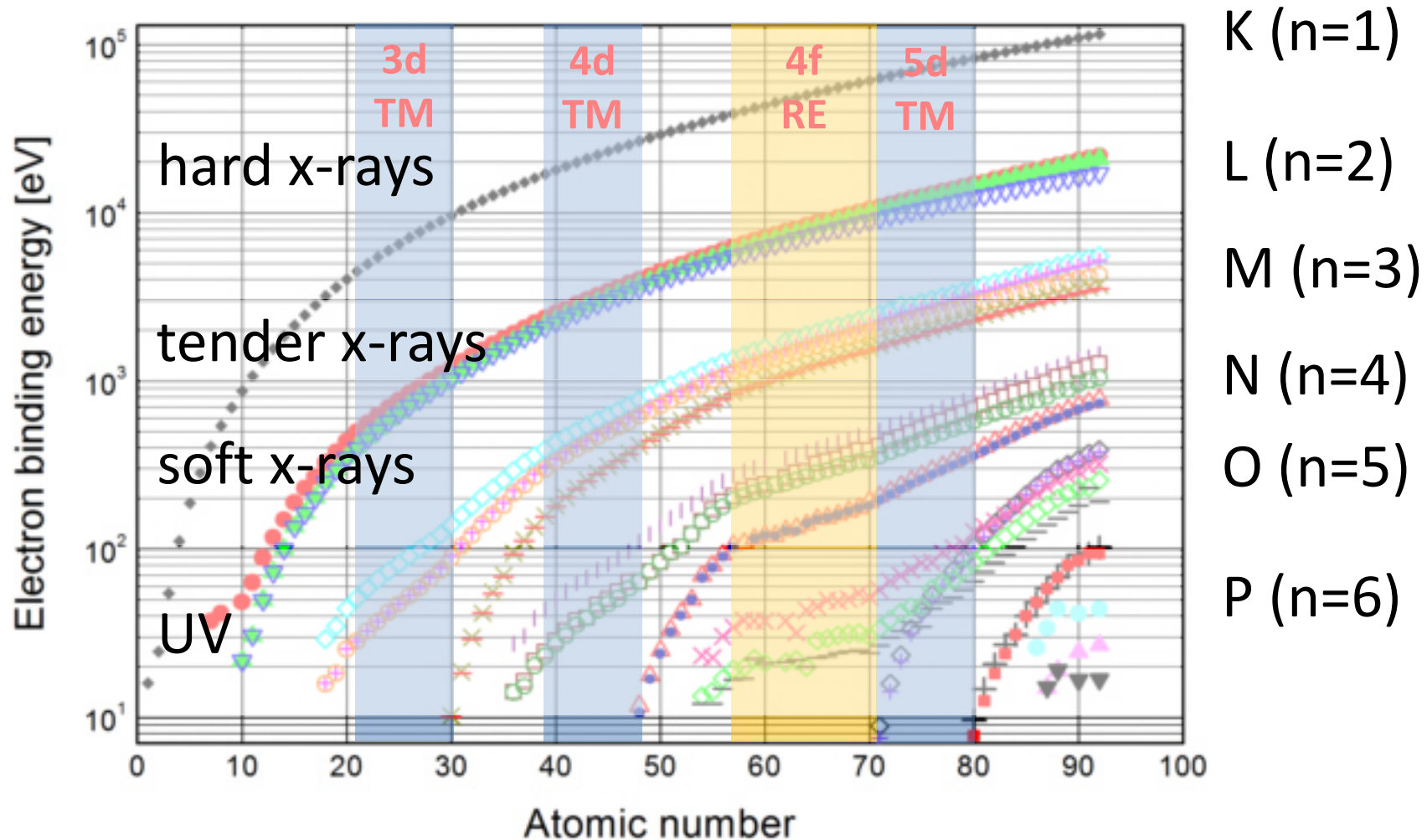
M (n=3)

N (n=4)

O (n=5)

P (n=6)

Inelastic X-ray scattering



Inelastic X-ray scattering

Distinction based on ω_i and/or ω_o (or $\omega = \omega_i - \omega_o$)

	non-resonant	resonant
$\omega = 0$	X-ray diffraction, X-ray reflectivity, SAXS, WAXS, XPCS, ...	
$\omega \neq 0$		

Inelastic X-ray scattering

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$\omega \neq 0$	(N)IXS, X-ray Raman scattering, Compton scattering, XES, XRF	

Inelastic X-ray scattering

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Inelastic X-ray scattering

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$\omega \neq 0$	(N)IXS, X-ray Raman scattering, Compton scattering, XES, XRF	Resonant inelastic x- ray scattering, resonant x-ray emission

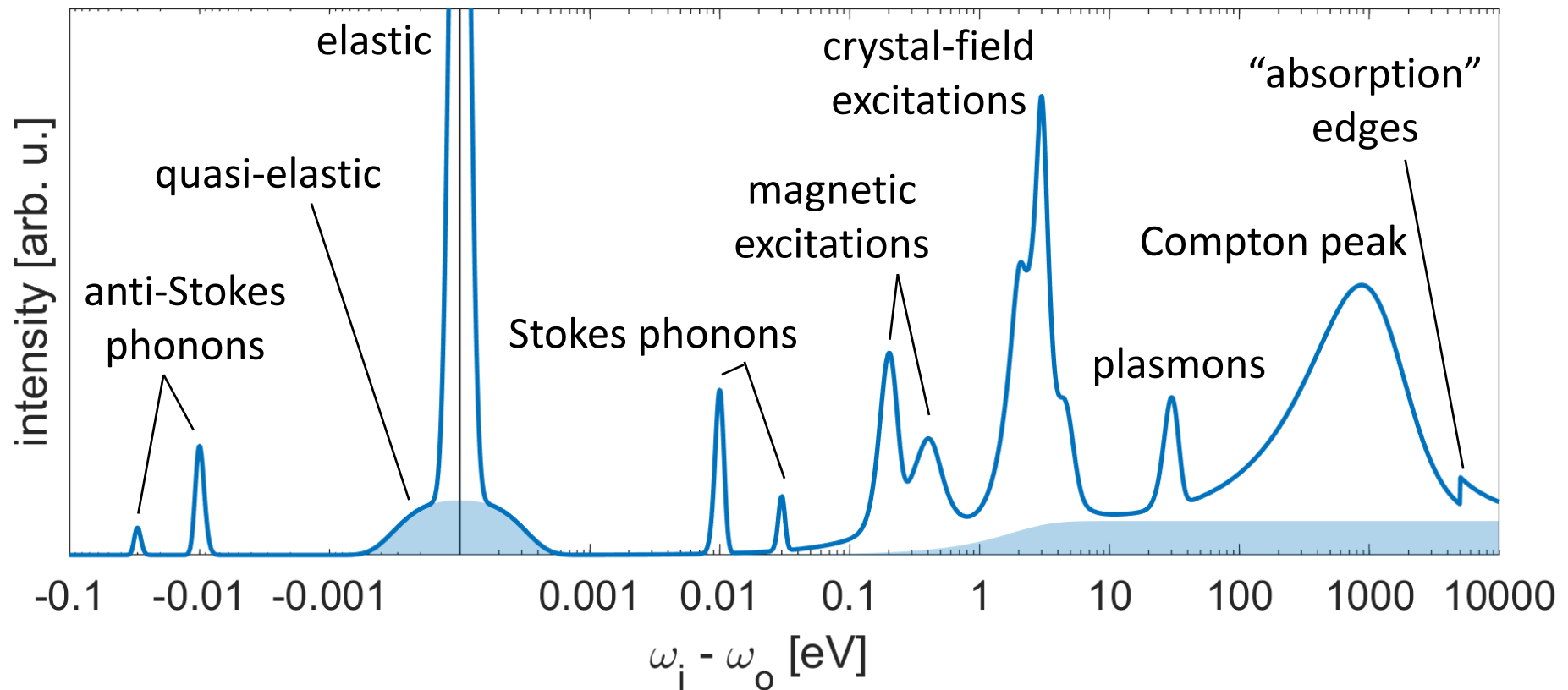
Inelastic X-ray scattering

Distinction based on ω_i and/or ω_o (or $\omega = \omega_i - \omega_o$)

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$\omega \neq 0$	(N)IXS, X-ray Raman scattering, Compton scattering, XES, XRF	Resonant inelastic x- ray scattering, resonant x-ray emission

Inelastic X-ray scattering

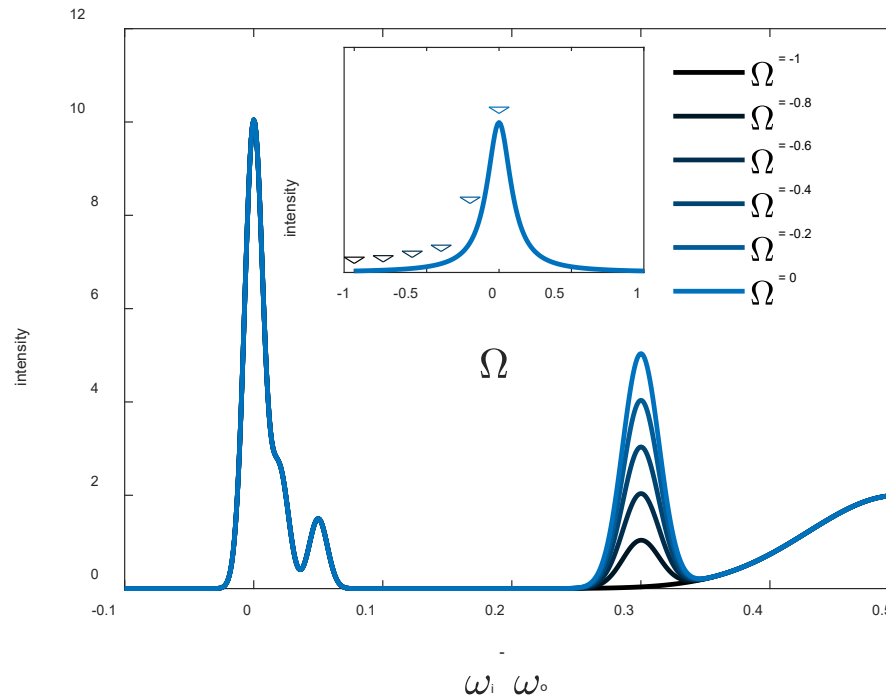
Various excitations over an extended energy gain/loss range



Inelastic X-ray scattering

Intrinsic IXS “parameters” (ω_i , $\mathbf{q}$, ε)

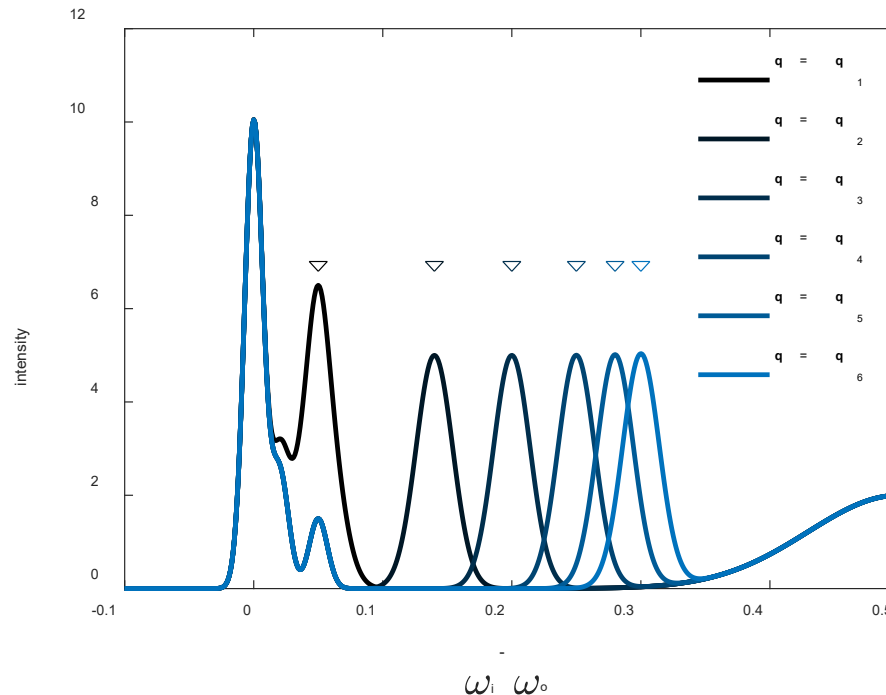
ω_i : resonant vs. non-resonant, Raman vs. fluorescence



Inelastic X-ray scattering

Intrinsic IXS “parameters” (ω_i , $\mathbf{q}$, ε)

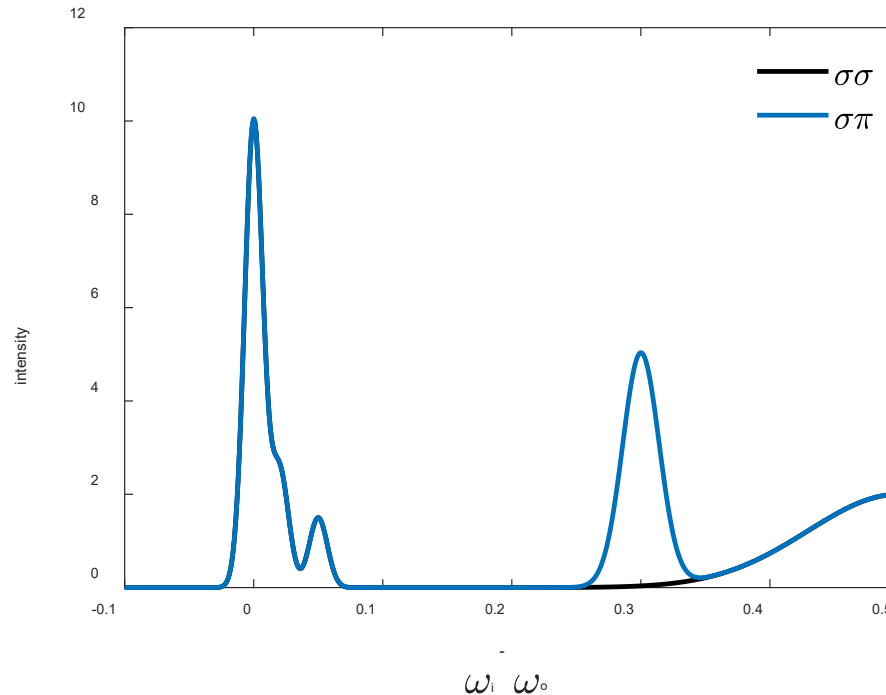
$\mathbf{q}$: interference effects (diffraction), local vs. collective excitations, multipole expansion contributions, ...



Inelastic X-ray scattering

Intrinsic IXS “parameters” (ω_i , $\mathbf{q}$, ϵ)

(ϵ_i, ϵ_o) : symmetry, nature of excitations (e.g. spin vs. charge)



Inelastic X-ray scattering

(R)IXS cross-section from light – matter interaction...

$$\begin{aligned}\mathcal{H} &= \sum_i^N \frac{[\mathbf{p}_i + e\mathbf{A}(\mathbf{r}_i)]^2}{2m} + \dots = \sum_i^N \frac{\mathbf{p}_i^2 + 2e\mathbf{p}_i \cdot \mathbf{A}(\mathbf{r}_i) + e^2\mathbf{A}(\mathbf{r}_i)^2}{2m} + \dots \\ &= \sum_i^N \frac{\mathbf{p}_i^2}{2m} + \mathcal{H}' + \dots = \mathcal{H}_0 + \mathcal{H}'\end{aligned}$$

Inelastic X-ray scattering

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...in second order perturbation theory

$$w = \frac{2\pi}{\hbar} \sum_f \left| \langle f | \mathcal{H}' | g \rangle + \sum_n \frac{\langle f | \mathcal{H}' | n \rangle \langle n | \mathcal{H}' | g \rangle}{E_g + \hbar\omega_i - E_n} \right|^2 \delta(E_f + \hbar\omega_o - E_g - \hbar\omega_i)$$

Inelastic X-ray scattering

(R)IXS cross-section from light – matter interaction...

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non-resonant

resonant

Non-resonant inelastic X-ray scattering

Dynamic structure factor

$$w \approx \frac{2\pi}{\hbar} \sum_f \left| \frac{e^2}{2m} \sum_i^N \langle f | \mathbf{A}(\mathbf{r}_i)^2 | g \rangle \right|^2 \delta(E_f + \hbar\omega_o - E_g - \hbar\omega_i) =$$
$$\sim \sum_f \left| \sum_i^N \langle f | e^{i\mathbf{q}\cdot\mathbf{r}_i} | g \rangle \right|^2 \delta(E_f + \hbar\omega_o - E_g - \hbar\omega_i) = S(\mathbf{q}, \omega)$$

$$S(\mathbf{q}) = \int S(\mathbf{q}, \omega) d\omega \quad \text{(static) structure factor – e.g., XRD}$$

Non-resonant inelastic X-ray scattering

The fluctuation-dissipation theory connects the dynamic structure factor to the complex susceptibility

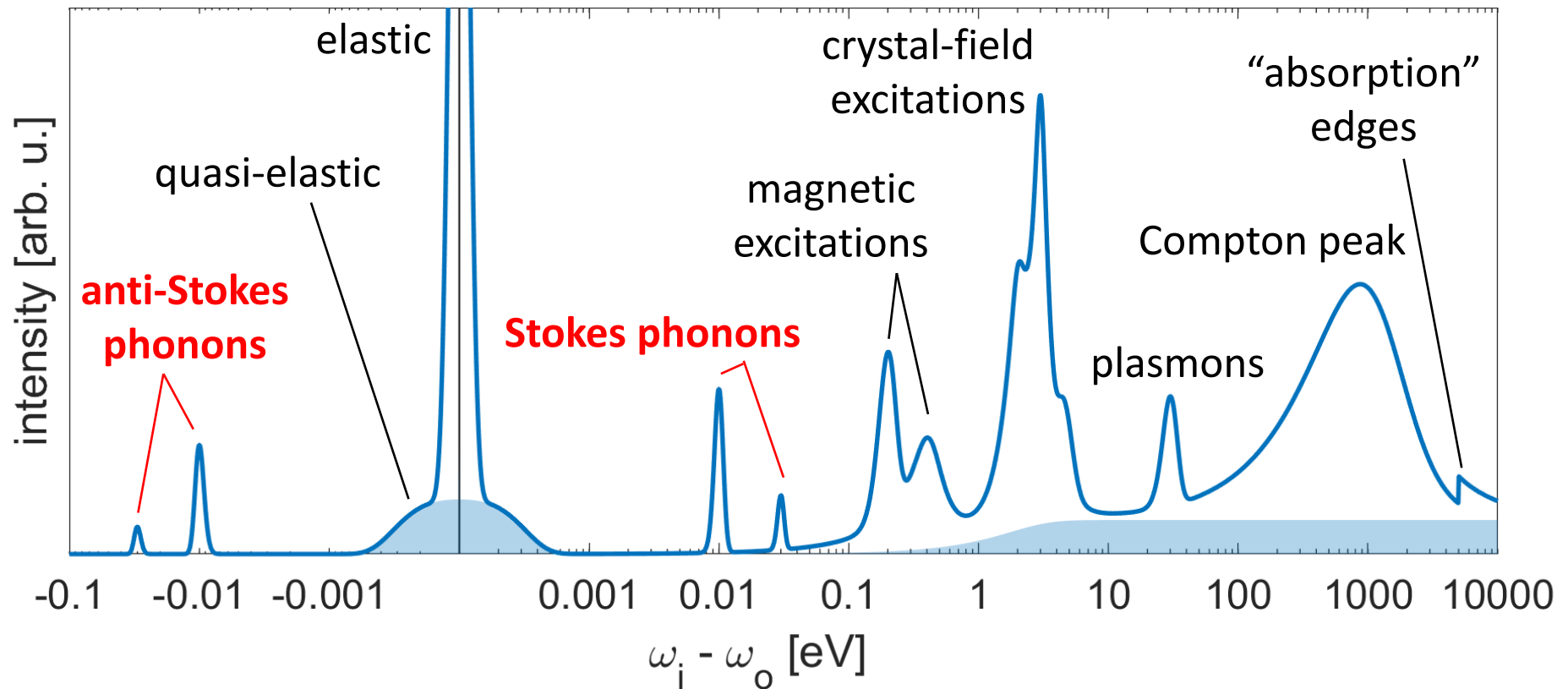
$$S(\mathbf{q}, \omega) = -\frac{1}{\pi} \frac{1}{1 - e^{-\omega/k_B T}} \text{Im}\{\chi(\mathbf{q}, \omega)\}$$

or to the complex dielectric function

$$S(\mathbf{q}, \omega) = \frac{1}{1 - e^{-\omega/k_B T}} \frac{q^2}{4\pi^2 e^2} \text{Im} \left\{ \frac{1}{\epsilon(\mathbf{q}, \omega)} \right\}$$

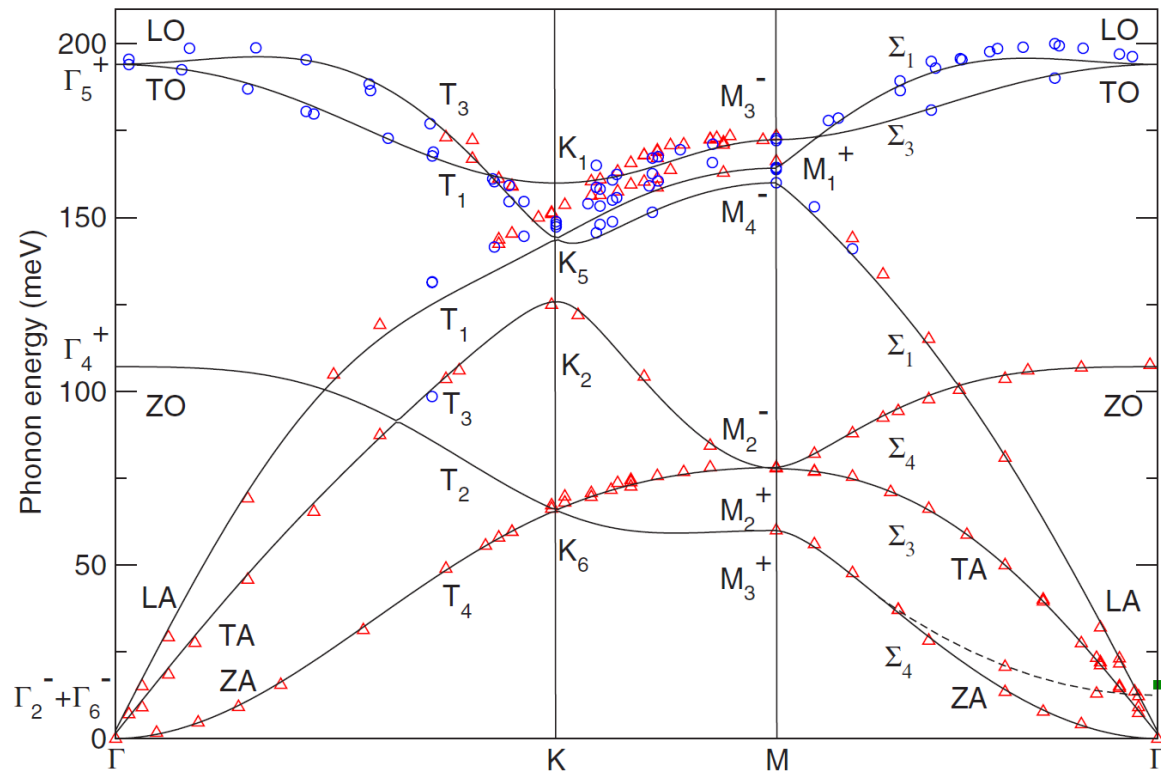
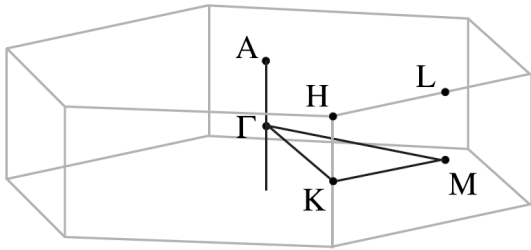
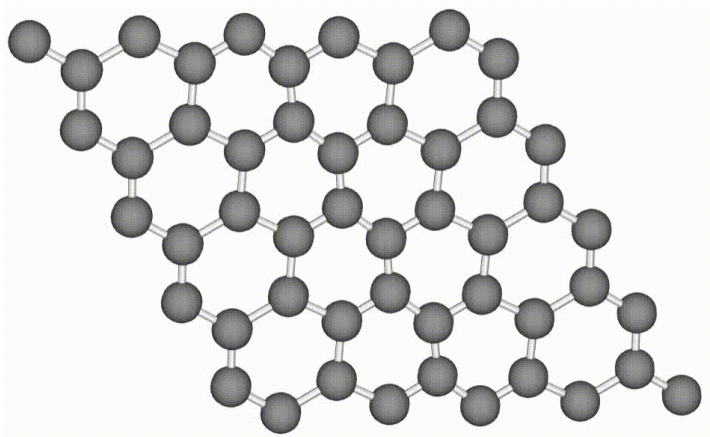
Non-resonant inelastic X-ray scattering

High resolution IXS of phonons



High resolution IXS of phonons

High resolution IXS of phonons



High resolution IXS of phonons

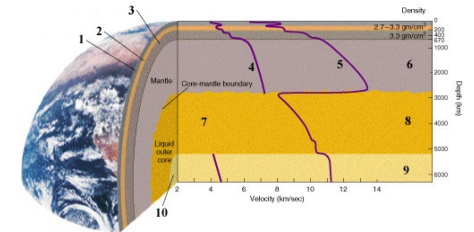
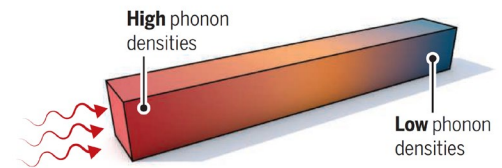
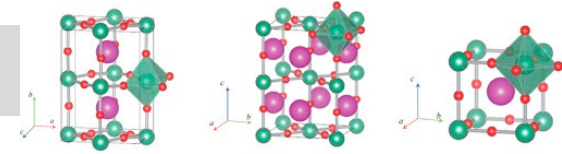
Relevance of phonons

structural properties (phase transitions, ...)

thermodynamic properties (specific heat, thermal conductivity, ...)

mechanical properties (elastic constants, sound velocity, ...)

transport properties (conductivity, superconductivity, ...)



High resolution IXS of phonons

Typical probes of phonons

infrared absorption

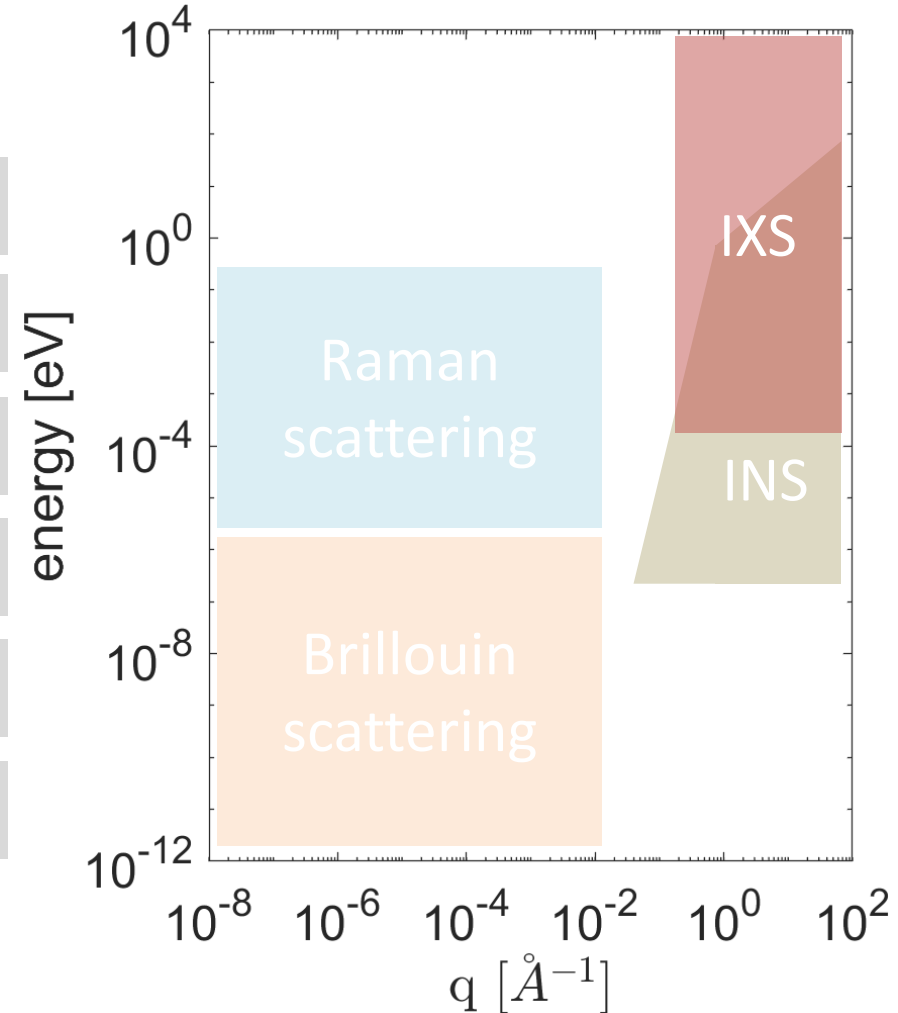
Brillouin and Raman scattering

nuclear inelastic scattering

thermal diffuse scattering

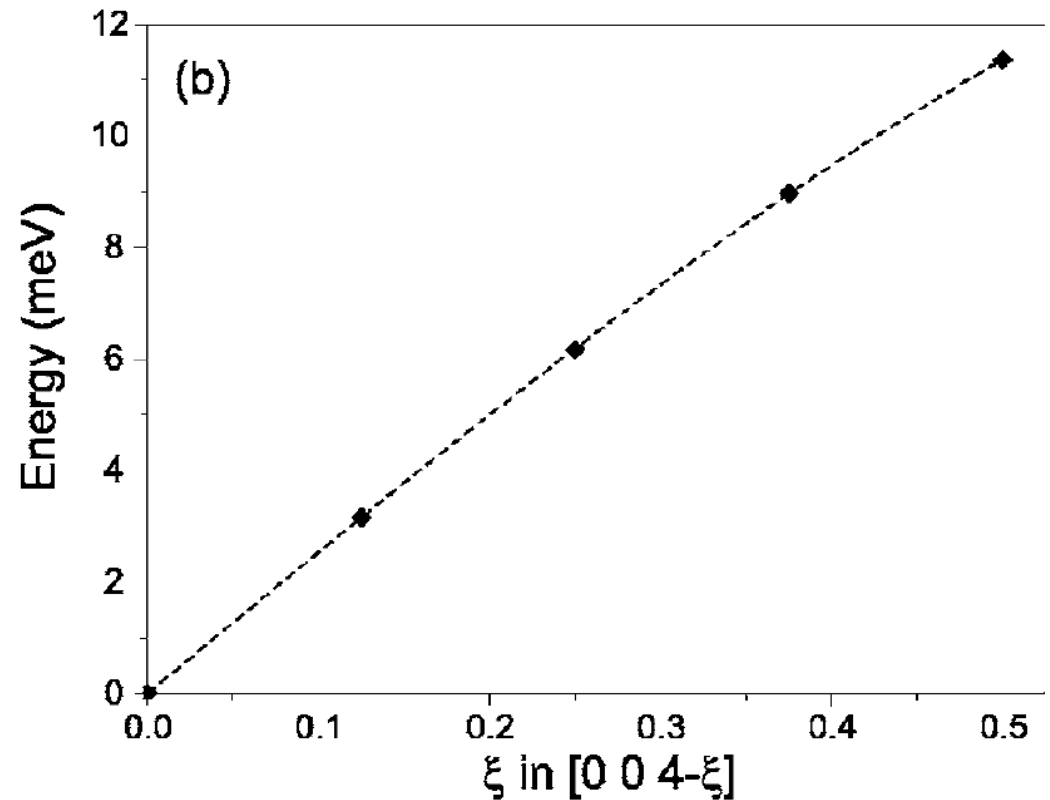
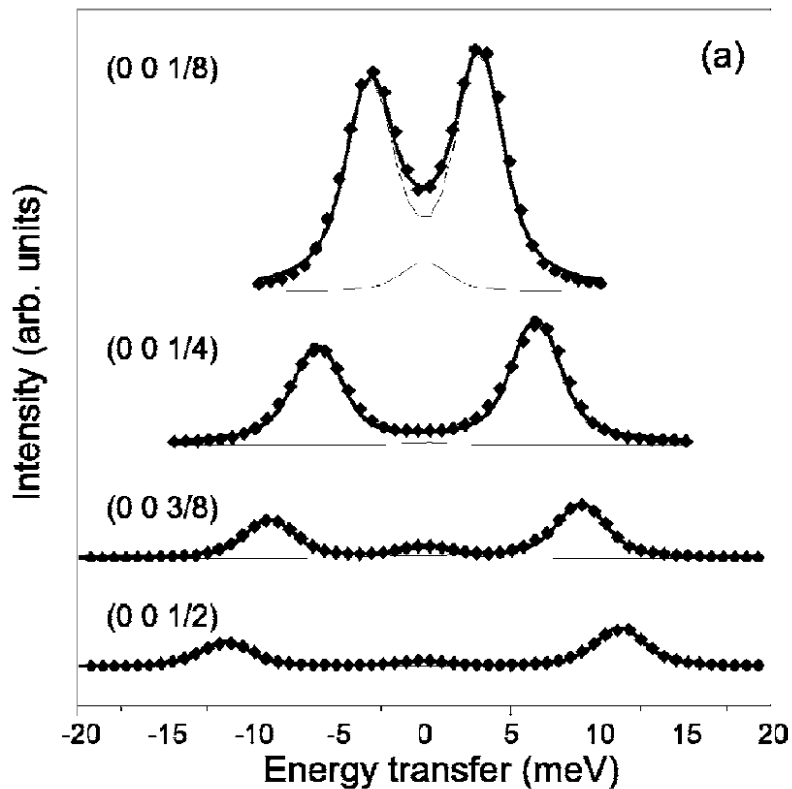
inelastic neutron scattering

electron energy loss



High resolution IXS of phonons

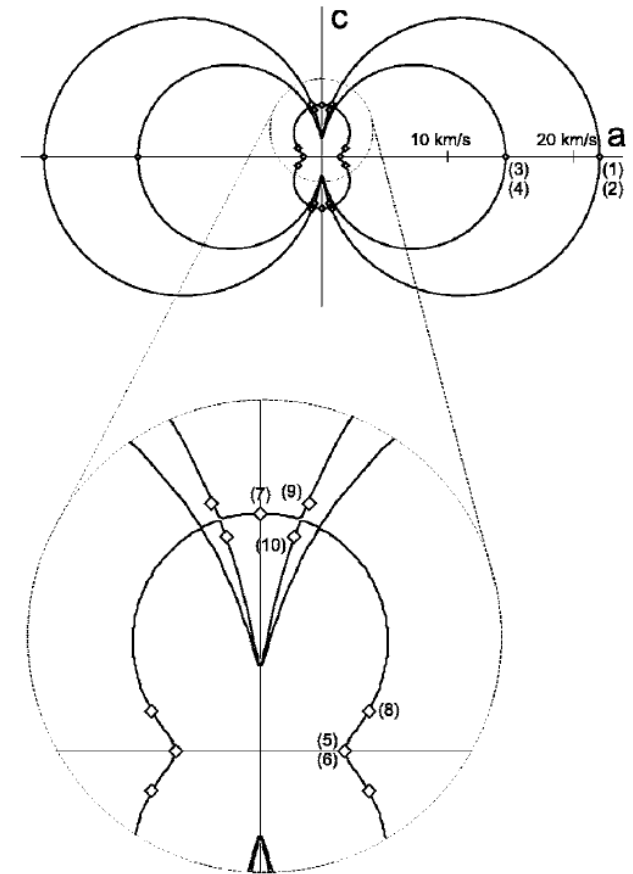
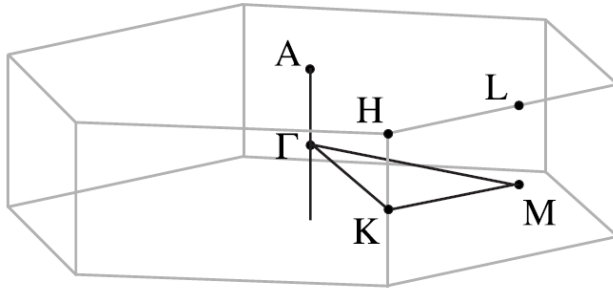
Sound velocity and elastic moduli in single-crystalline graphite



High resolution IXS of phonons

Sound velocity and elastic moduli in single-crystalline graphite

Notation	Momentum transfer	Propagation vector	Polarization vector	Velocity [km/s]
(1) LA[1 0 0]	$[1 + \xi \ 0 \ 0]$	$[1 \ 0 \ 0]$	$\langle 1 \ 0 \ 0 \rangle$	22.16(17)
(2) LA $\langle 1 \ 1 \ 0 \rangle$	$[1 + \xi \ 1 + \xi \ 0]$	$[1 \ 1 \ 0]$	$\langle 1 \ 1 \ 0 \rangle$	
(3) TA[1 0 0] $_{\langle 1-20 \rangle}$	$[1 - \xi \ 1 + \xi \ 0]$	$[1 \ -1 \ 0]$	$\langle 1 \ 1 \ 0 \rangle$	14.66(15)
(4) TA[1 1 0] $_{\langle 1-10 \rangle}$	$[1 - 2\xi \ 1 + \xi \ 0]$	$[-2 \ 1 \ 0]$	$\langle 0 \ 1 \ 0 \rangle$	
(5) TA[1 1 0] $_{\langle 001 \rangle}$	$[1 - \xi \ 1 - \xi \ 2]$	$[1 \ 1 \ 0]$	$\langle 0 \ 0 \ 1 \rangle$	1.48(6)
(6) TA[1 0 0] $_{\langle 001 \rangle}$	$[1 - \xi \ 0 \ 3]$	$[1 \ 0 \ 0]$	$\langle 0 \ 0 \ 1 \rangle$	
(7) LA[0 0 1]	$[0 \ 0 \ 4 - \xi]$	$[0 \ 0 \ 1]$	$\langle 0 \ 0 \ 1 \rangle$	4.14(4)
(8) q-TA[1 1 2]	$[1 + \xi \ 1 + \xi \ 2 + 2\xi]$	$[1 \ 1 \ 2]$		2.02(2)
(9) q-LA[1 1 28]	$[1 + \xi \ 1 + \xi \ 2 + 28\xi]$	$[1 \ 1 \ 28]$		4.40(6)
(10) q-TA[1 1 35]	$[1 + \xi \ 1 + \xi \ 2 + 35\xi]$	$[1 \ 1 \ 35]$		3.77(4)



High resolution IXS of phonons

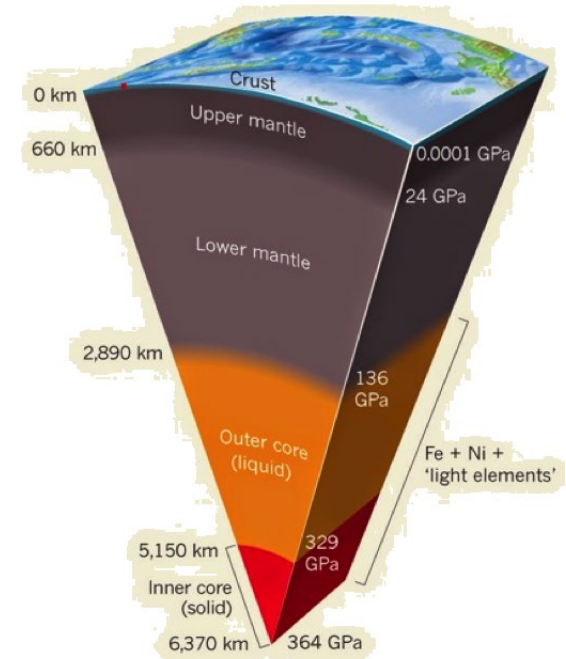
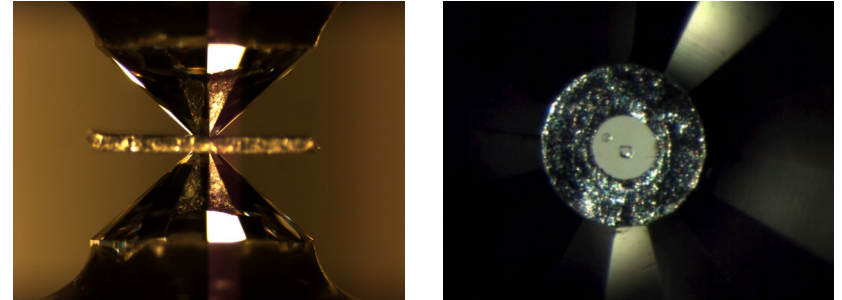
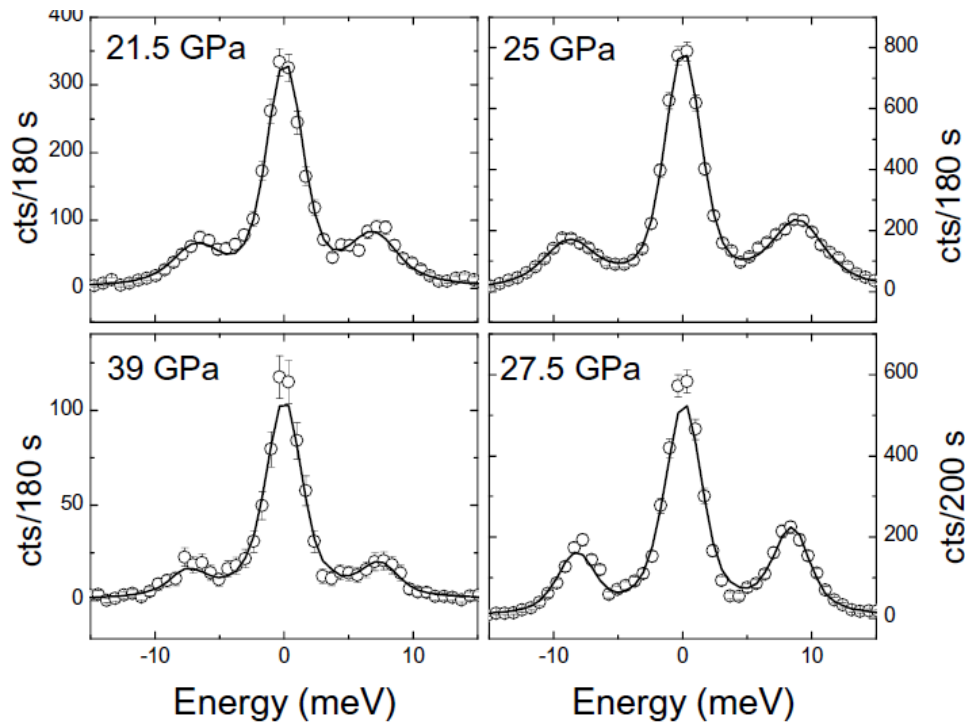
Sound velocity and elastic moduli in single-crystalline graphite

TABLE II. Comparison of our results with previous experiments and calculations. All values are in GPa.

	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	C_{66}	B
Present expt.	1109(16)	139(36)	0(3)	38.7(7)	5.0(3)	485(10)	36.4(11)
Previous expt.	1440(200) ^a 1060(20) ^d	180(20) ^d	15(5) ^d −51(6) ^d	37.1(5) ^a 36.5(10) ^d	4.6(2) ^a 5.05(35) ^b 4.0(4) ^d	460 ^a 440(20) ^d	33.8(30) ^c
Theory	$C_{11}+C_{12}=1280^e$, $C_{11}+C_{12}=1283, 976,$ 1235, 1230 ^f 1118, 1079 ^e		−0.5 ^e −2.8, −0.46, −4.6 ^g	40.8 ^e 29, 2.4, 1.9, 45, 29.5, 42.2 ^g 0.8, 30.4 ^h	4.5, 3.9 ^f		38.3 ^e 28.7 ^f 27.8, 2.4 1.9, 41.2 ^g

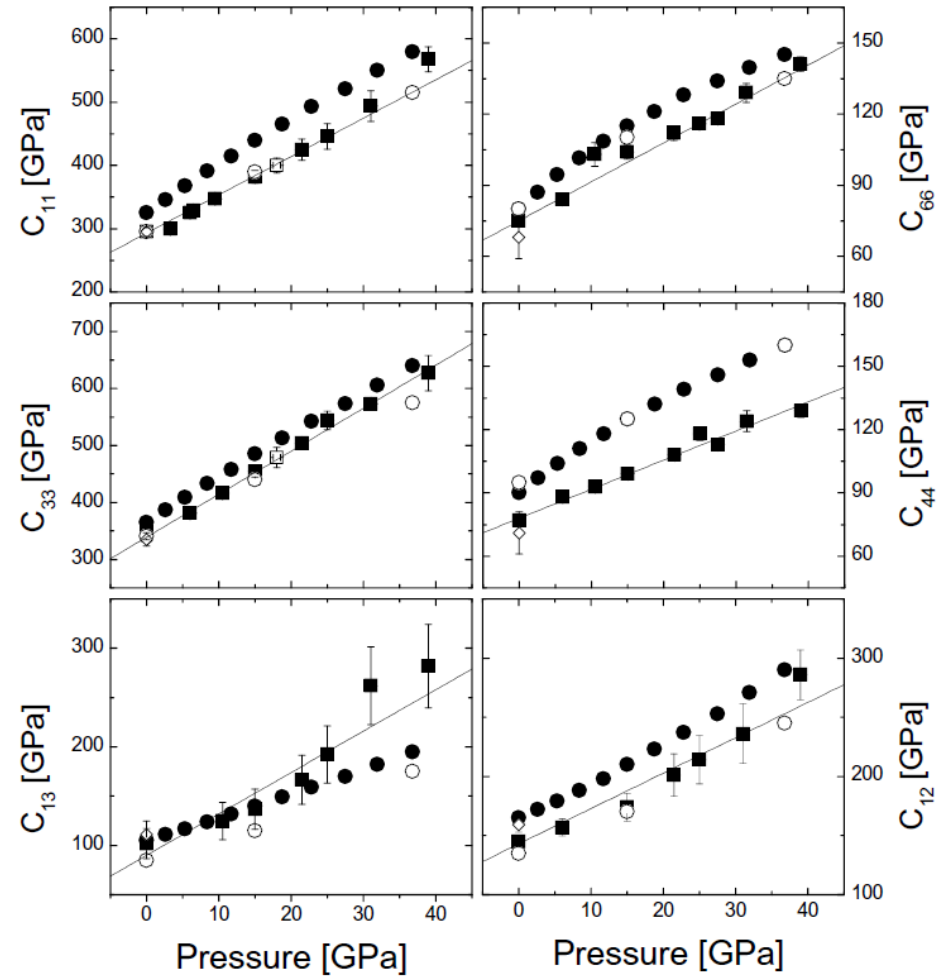
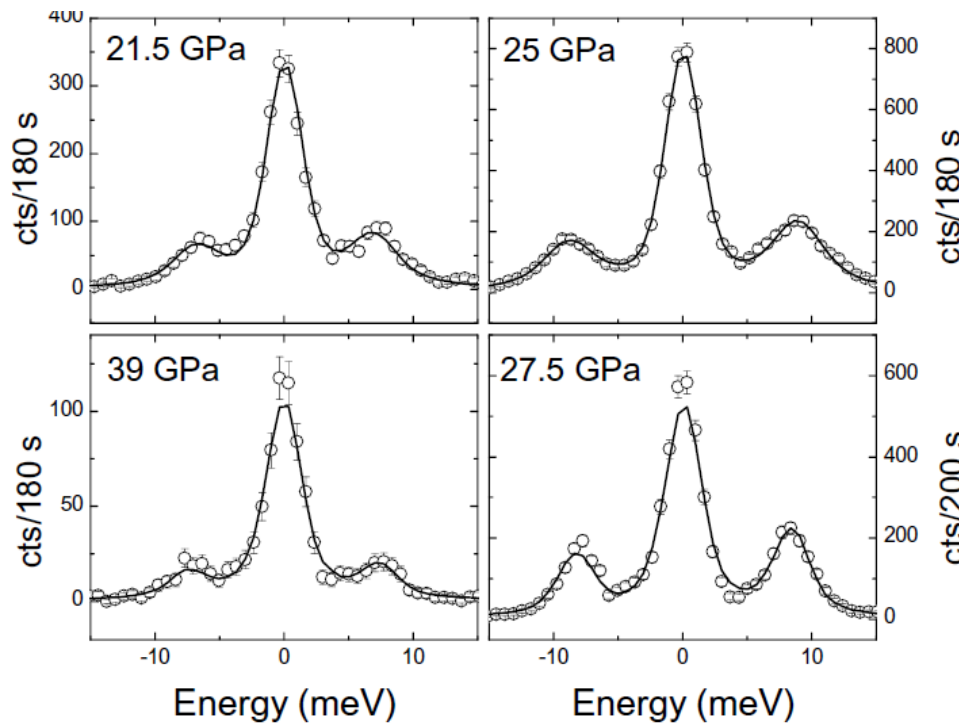
High resolution IXS of phonons

Elastic moduli in hcp cobalt at high pressure



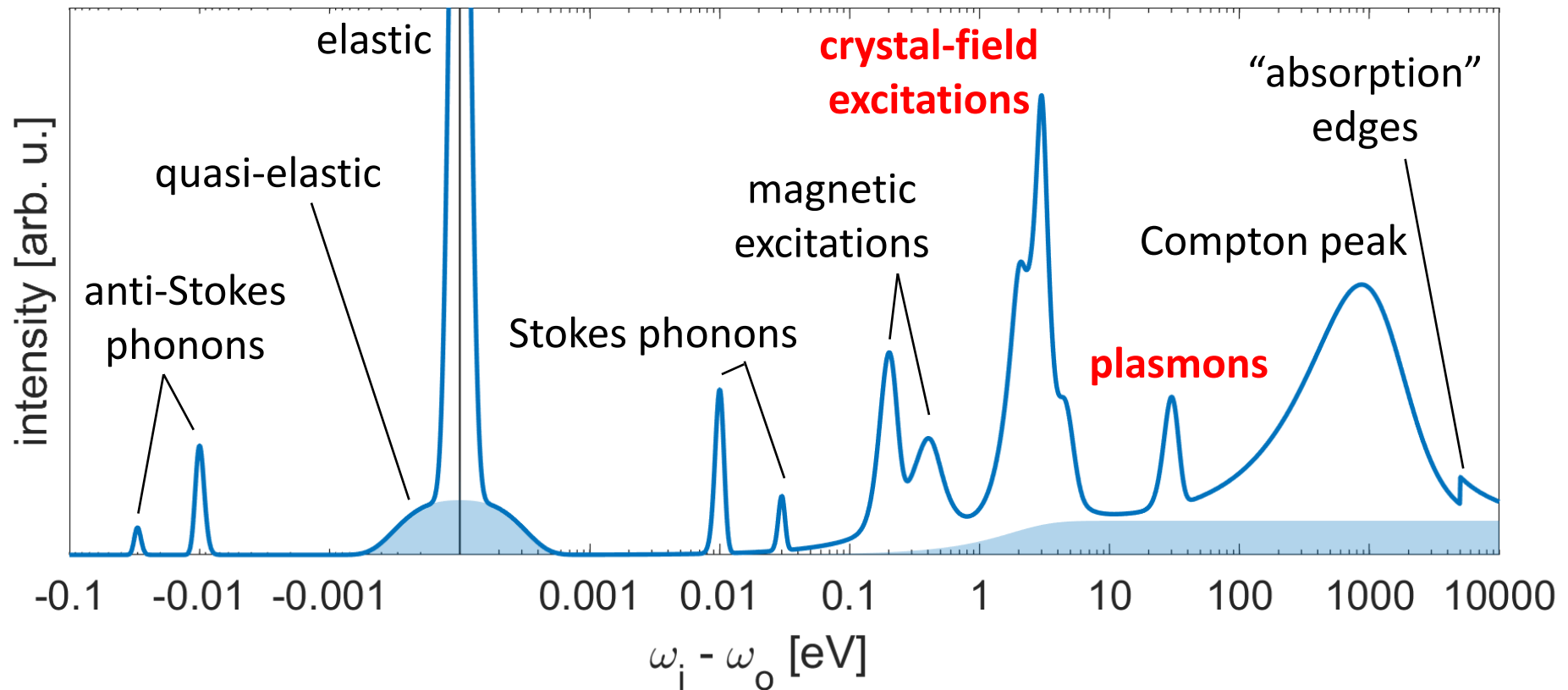
High resolution IXS of phonons

Elastic moduli in hcp cobalt at high pressure



Non-resonant inelastic X-ray scattering

(N)IXS of valence electron excitations



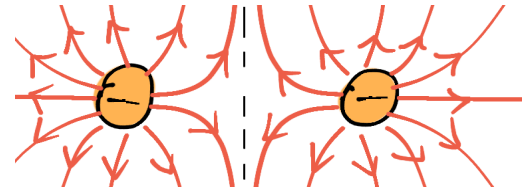
(N)IXS of valence electron excitations

Relevance of valence electron excitations

optical properties (reflectivity, absorption, dielectric function, ...)

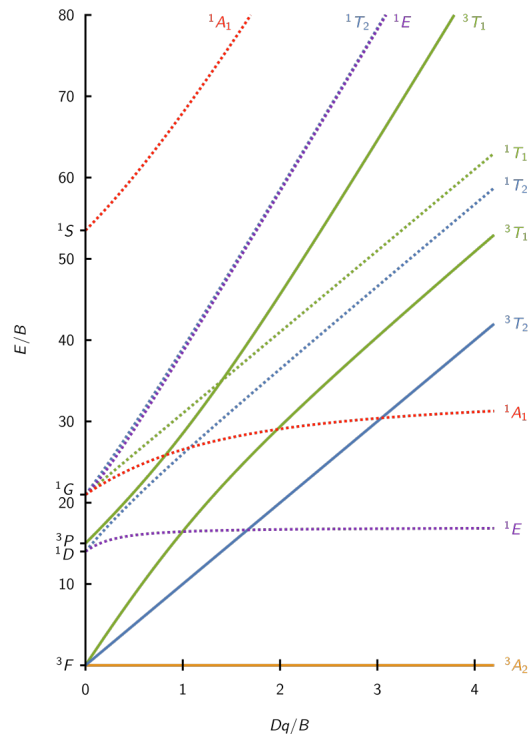


electronic properties (electron-electron correlations, crystal field splitting, SOC, ...)

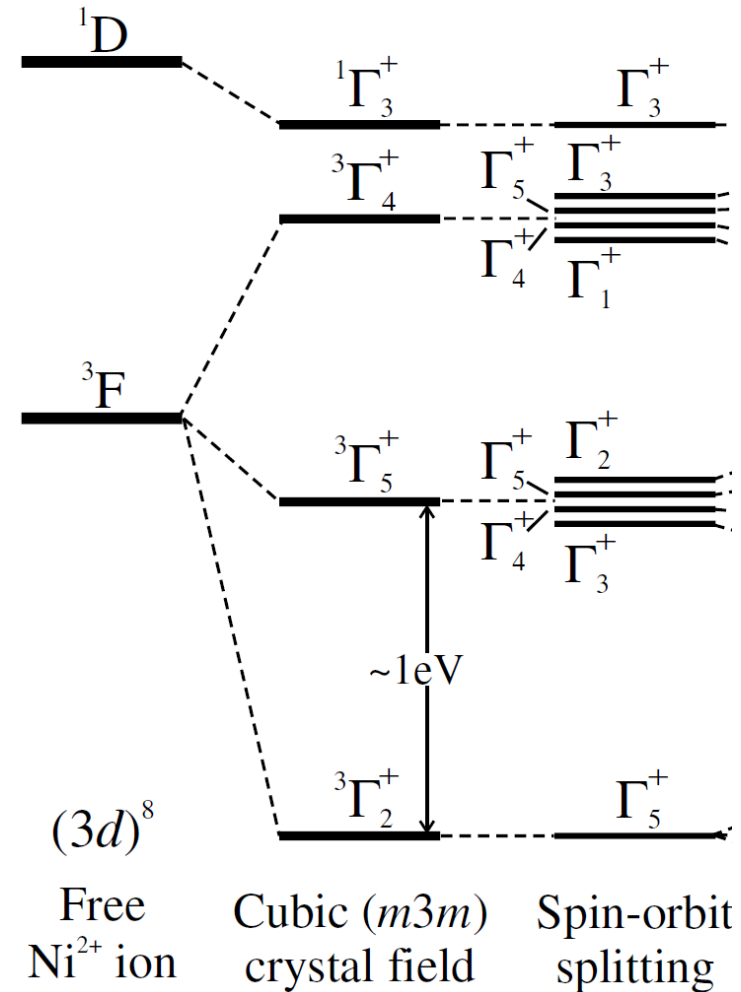


(N)IXS of valence electron excitations

E.g., crystal field excitations in NiO

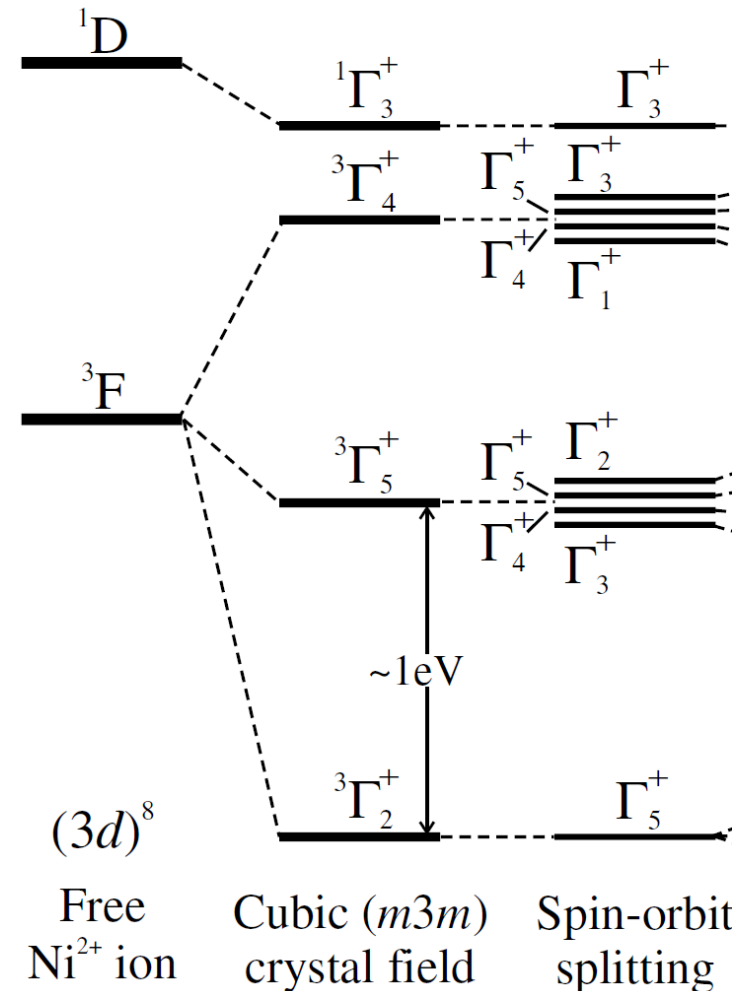
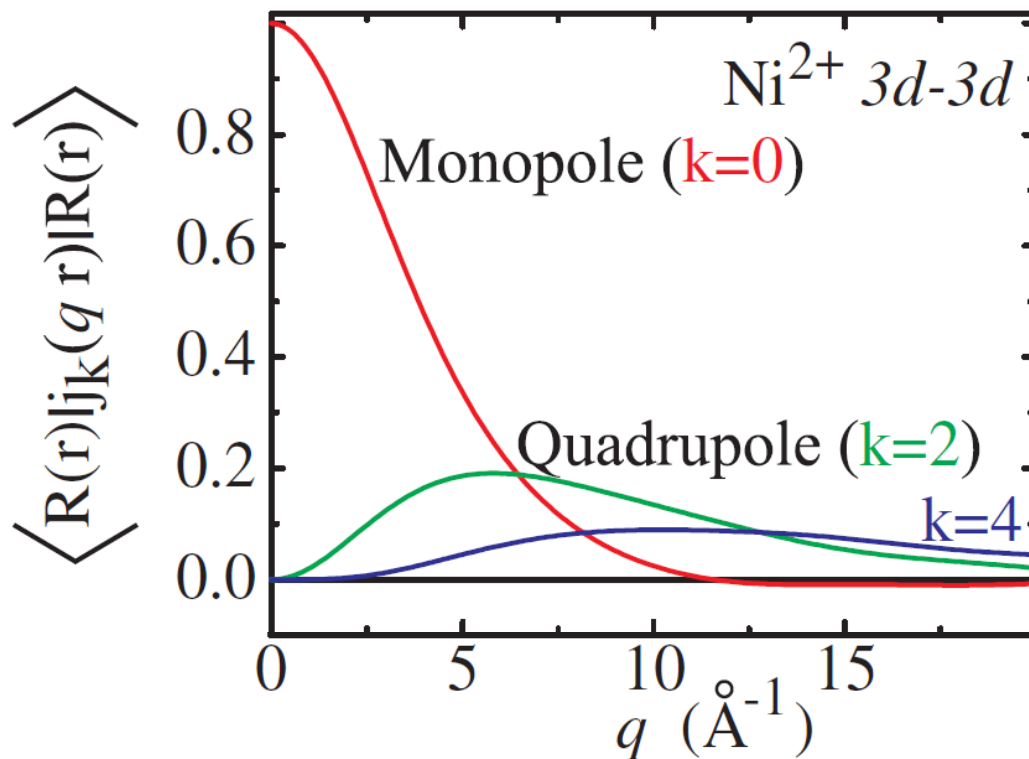


Sugano-Tanabe diagram for d^8



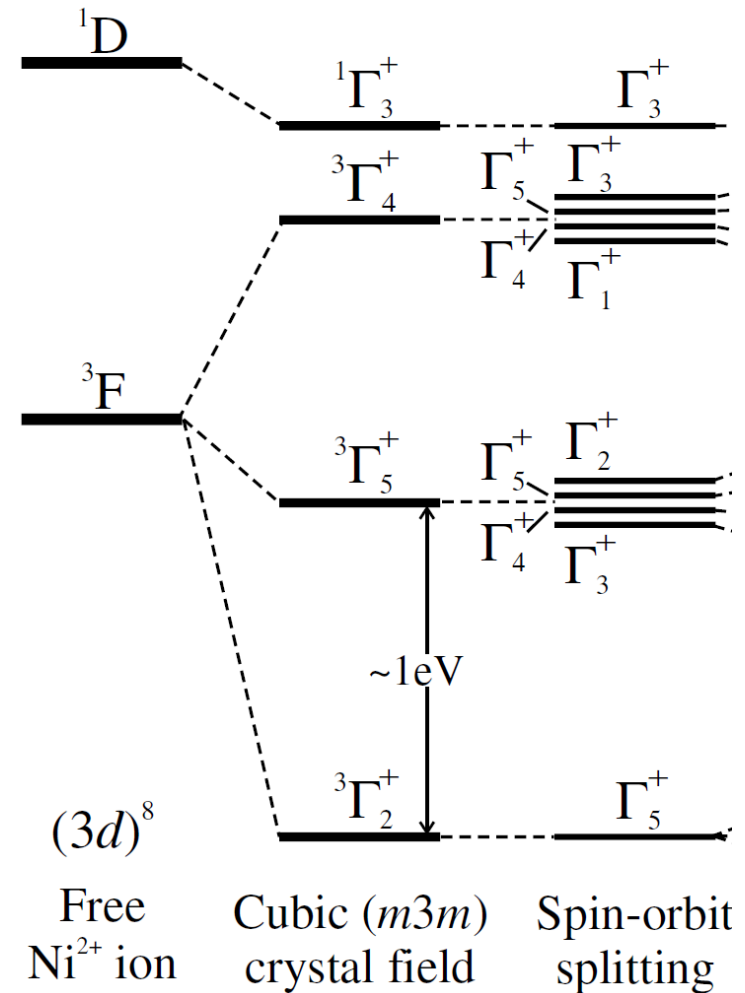
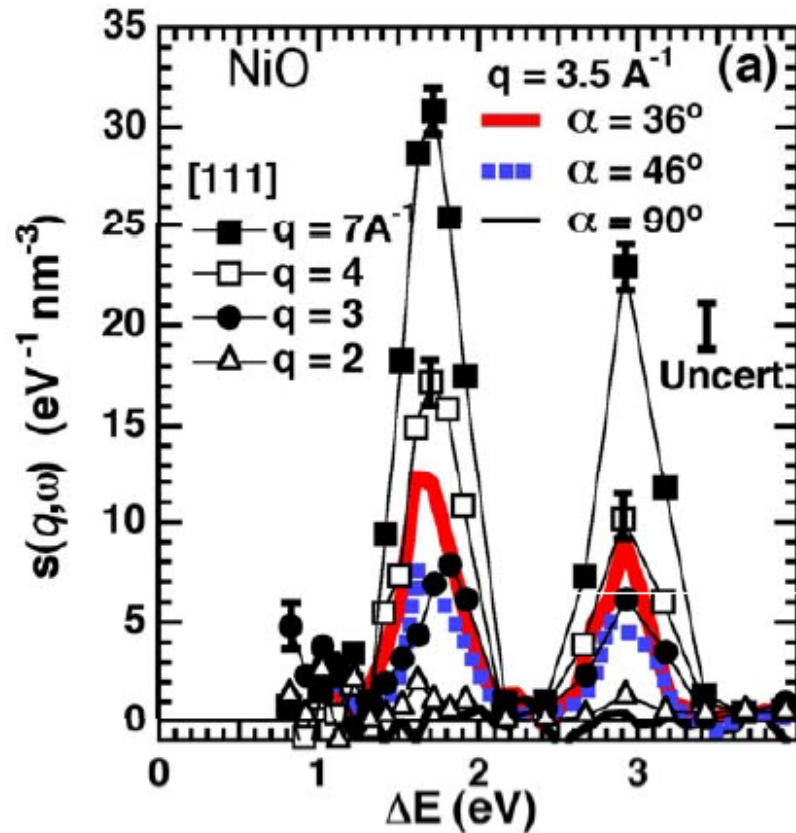
(N)IXS of valence electron excitations

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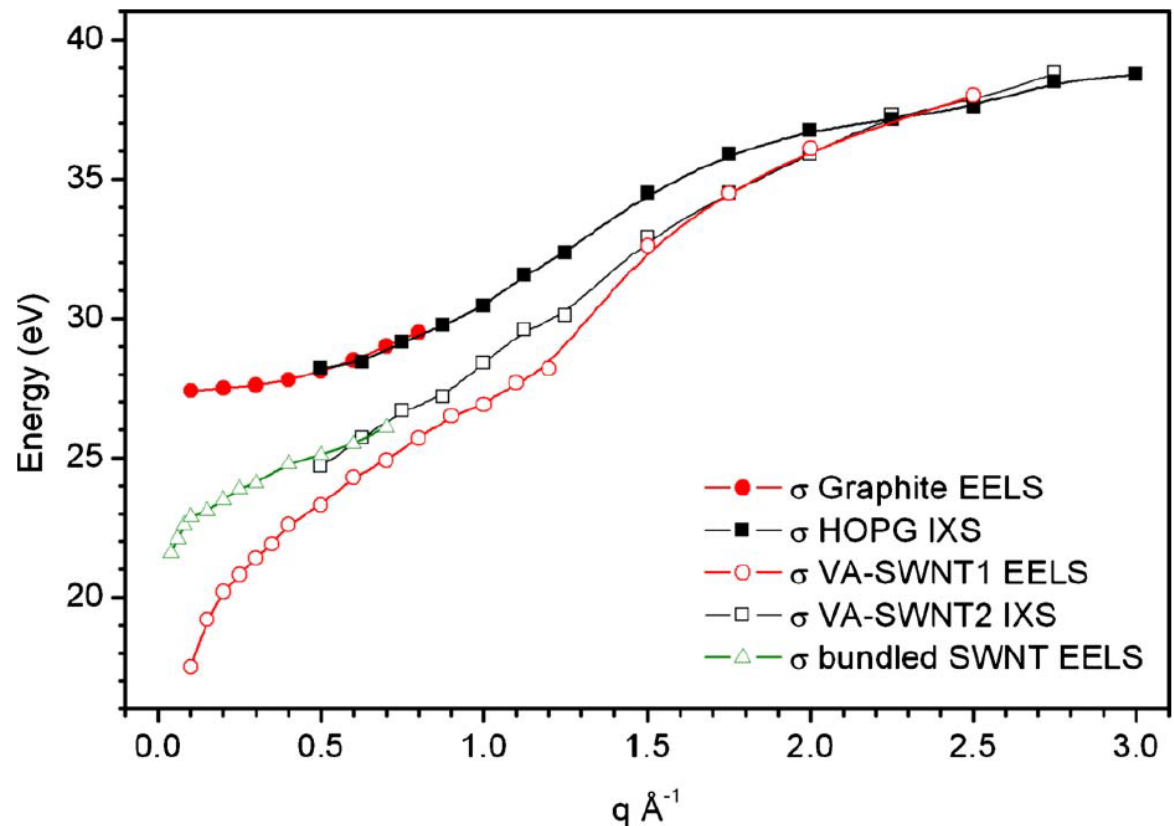
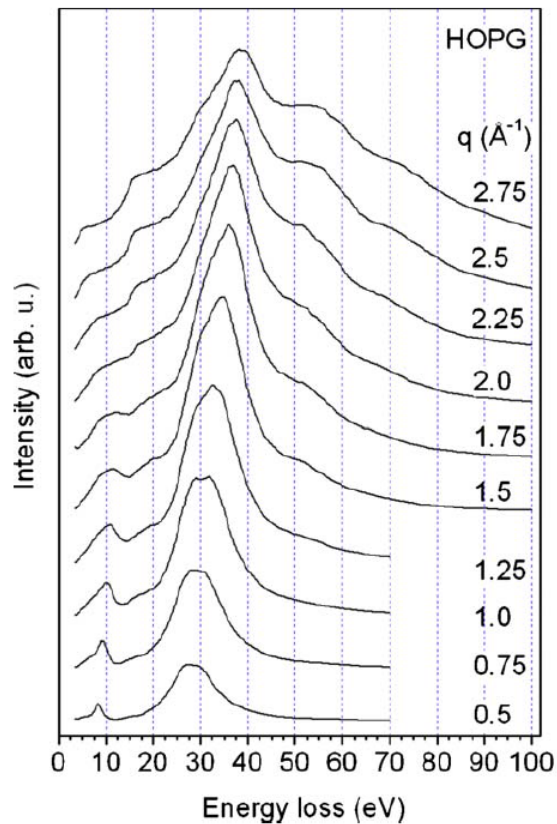
(N)IXS of valence electron excitations

E.g., crystal field excitations in NiO



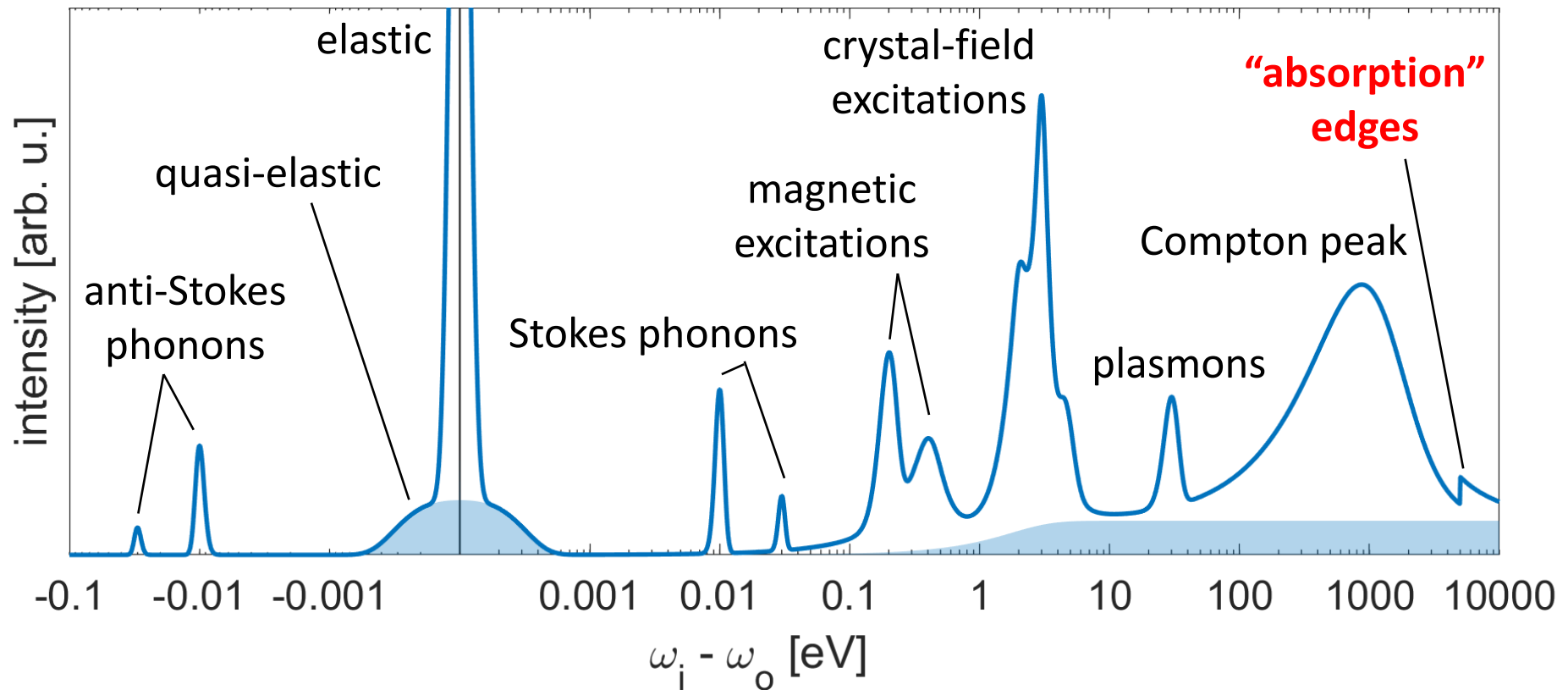
(N)IXS of valence electron excitations

E.g., plasmons in graphite and carbon nanotubes



Non-resonant inelastic X-ray scattering

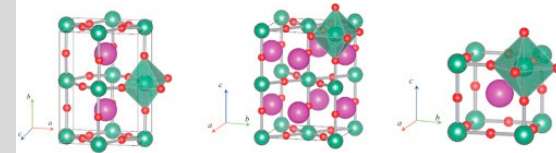
(N)IXS of core electron excitations – XRS



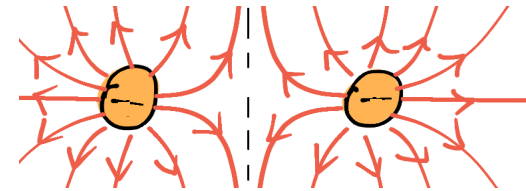
(N)IXS of core electron excitations – XRS

Relevance of core electron excitations

structural properties (phase transitions,
local coordination, ...)

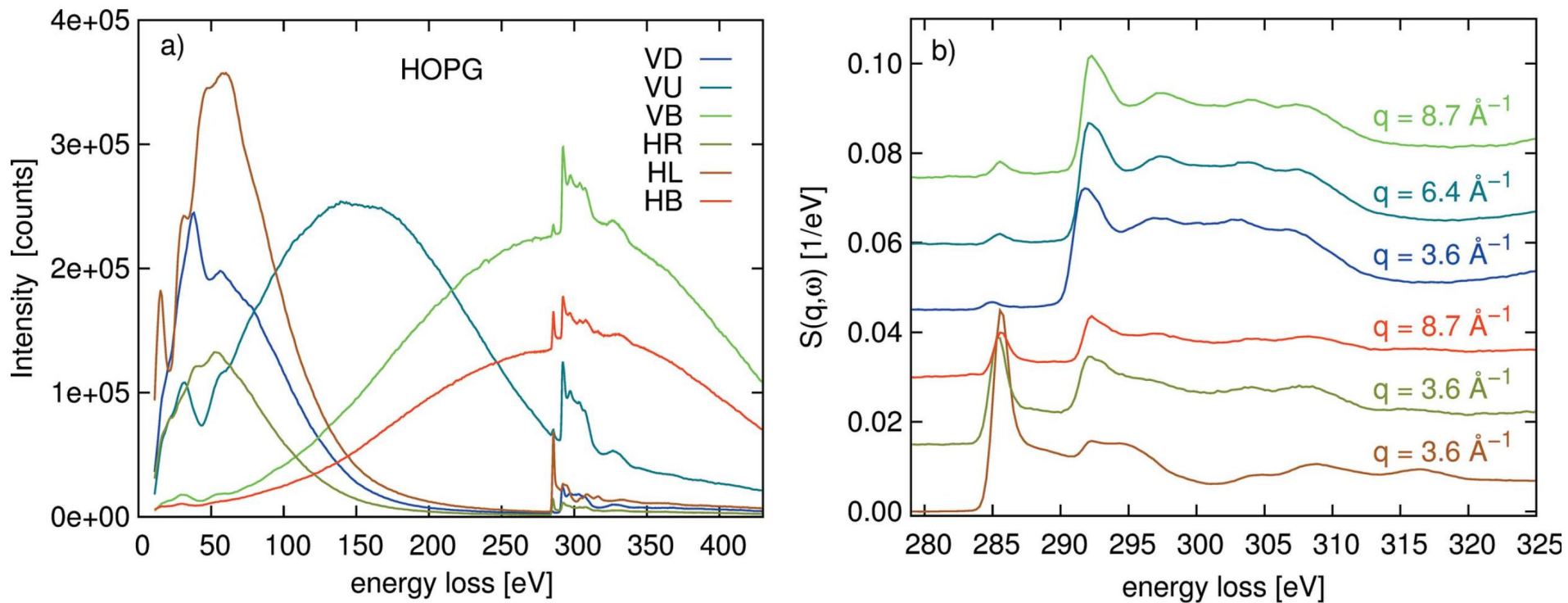


electronic properties (oxidation state,
crystal field splitting, ...)



Non-resonant inelastic X-ray scattering

Access to shallow (< 1keV) absorption edges



(N)IXS of core electron excitations – XRS



Similarity with soft XAS

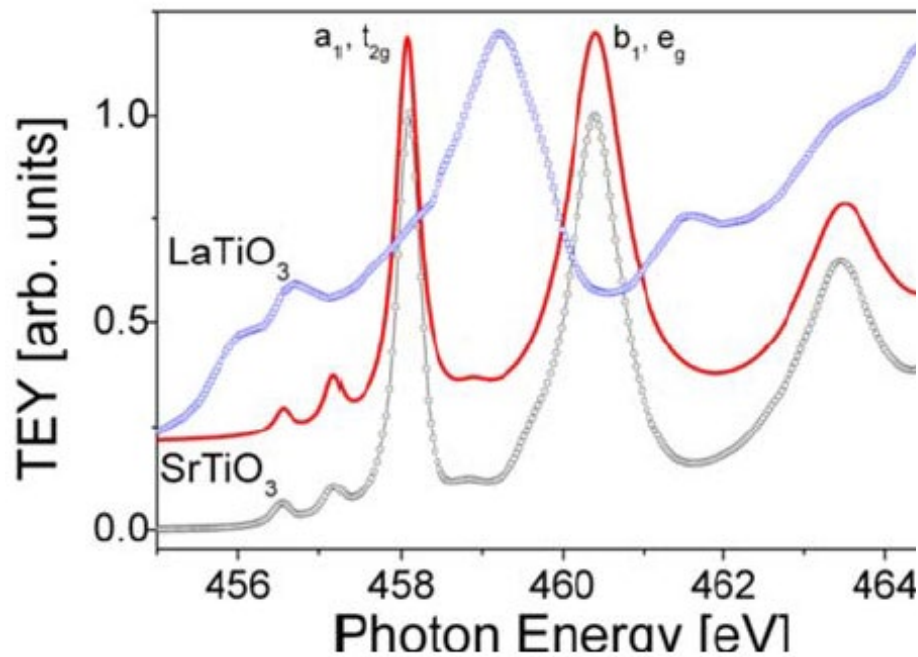
XAS

XRS

(N)IXS of core electron excitations – XRS

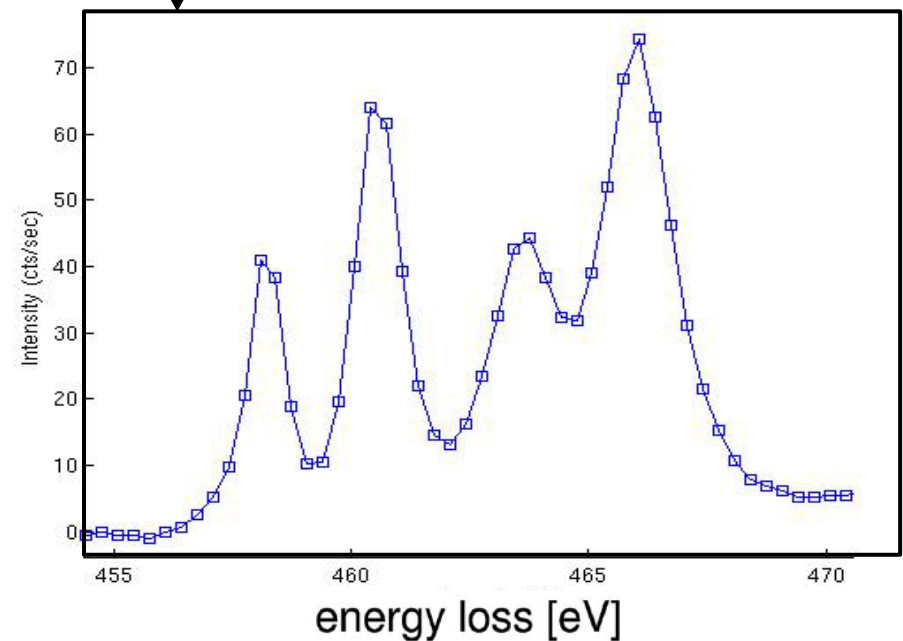
Similarity with soft XAS

XAS



$$456 \text{ eV} = 10148 \text{ eV} - 9692 \text{ eV}$$

XRS



(N)IXS of core electron excitations – XRS

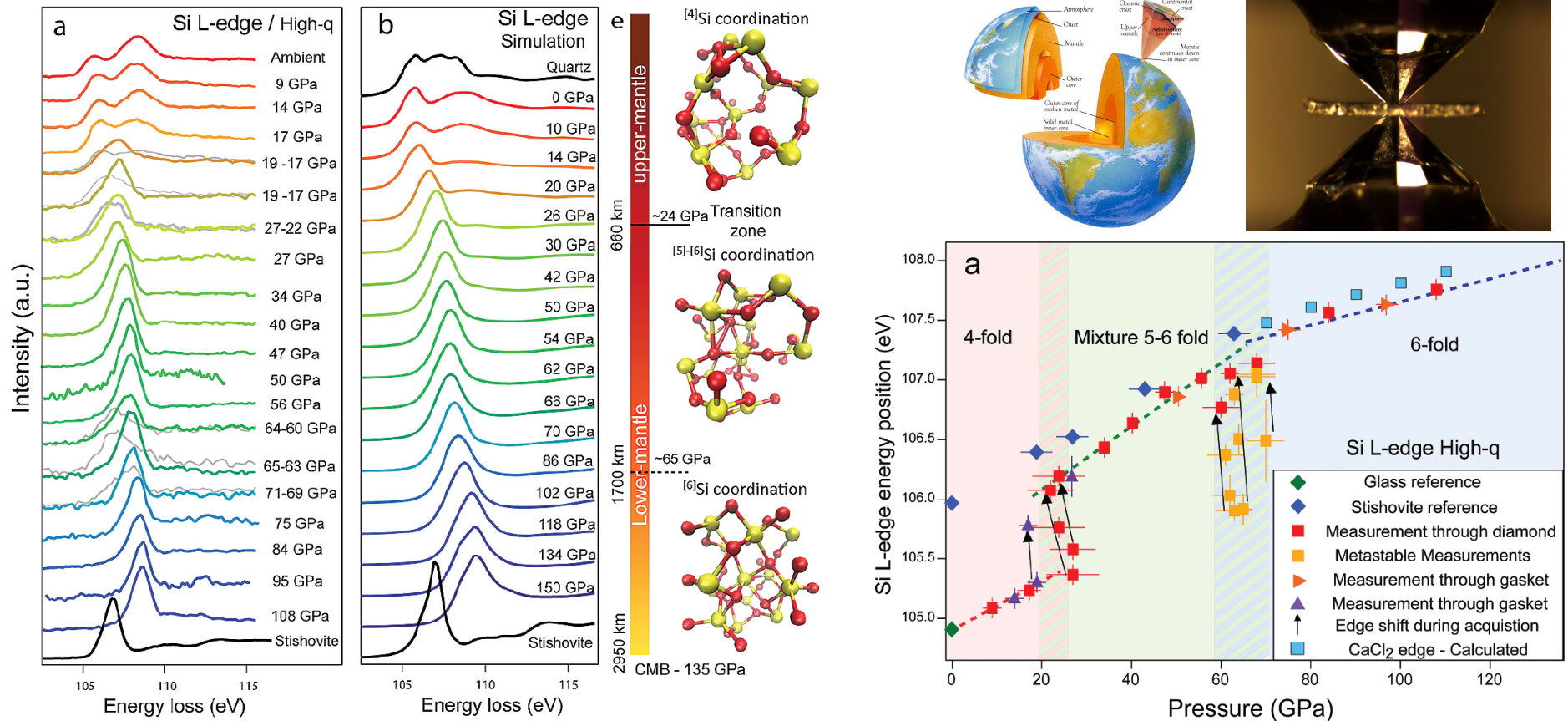
Similarity with soft XAS

XAS
$$T(\epsilon, \omega_i) = \sum_f |\langle f | \epsilon \cdot \mathbf{r}_i | g \rangle|^2 \delta(E_f - E_g - \hbar\omega_i)$$

XRS
$$S(\mathbf{q}, \omega) \approx \sum_f |\langle f | \mathbf{q} \cdot \mathbf{r}_i | g \rangle|^2 \delta(E_f - E_g - \hbar\omega)$$

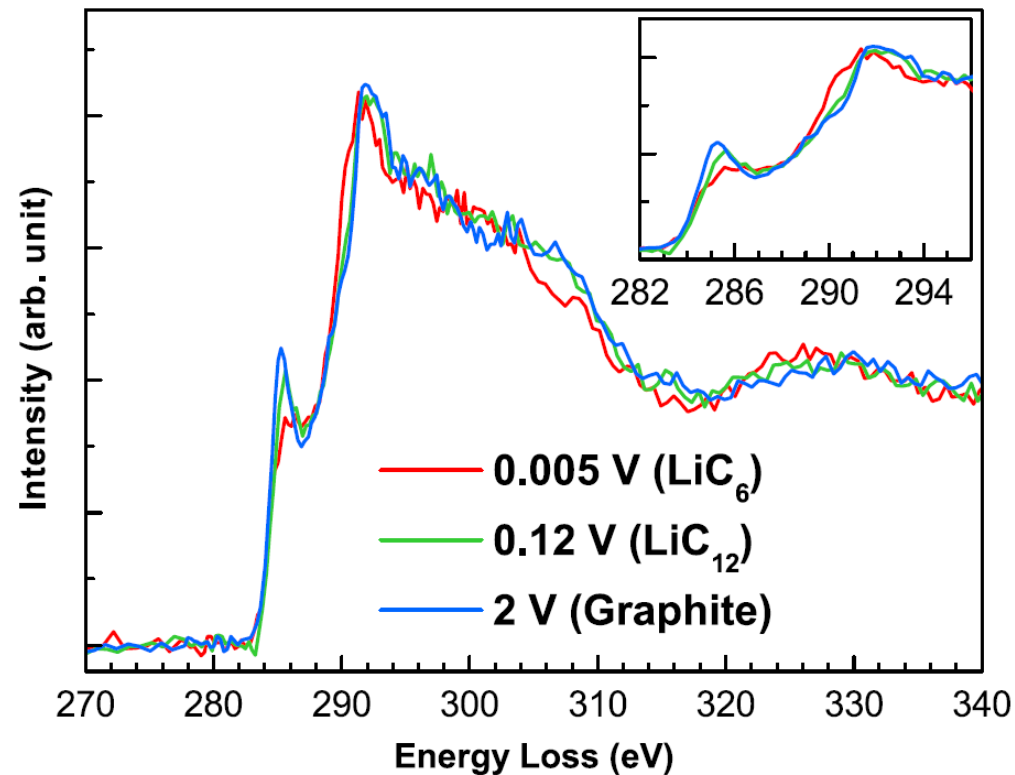
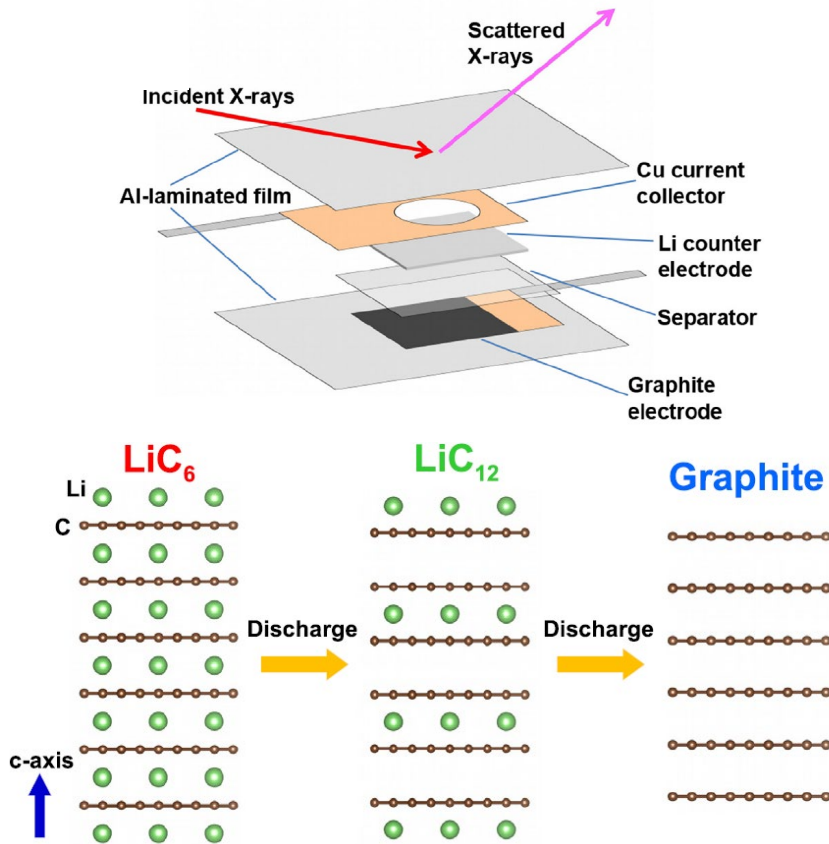
(N)IXS of core electron excitations – XRS

Silica (SiO_2) at high pressure



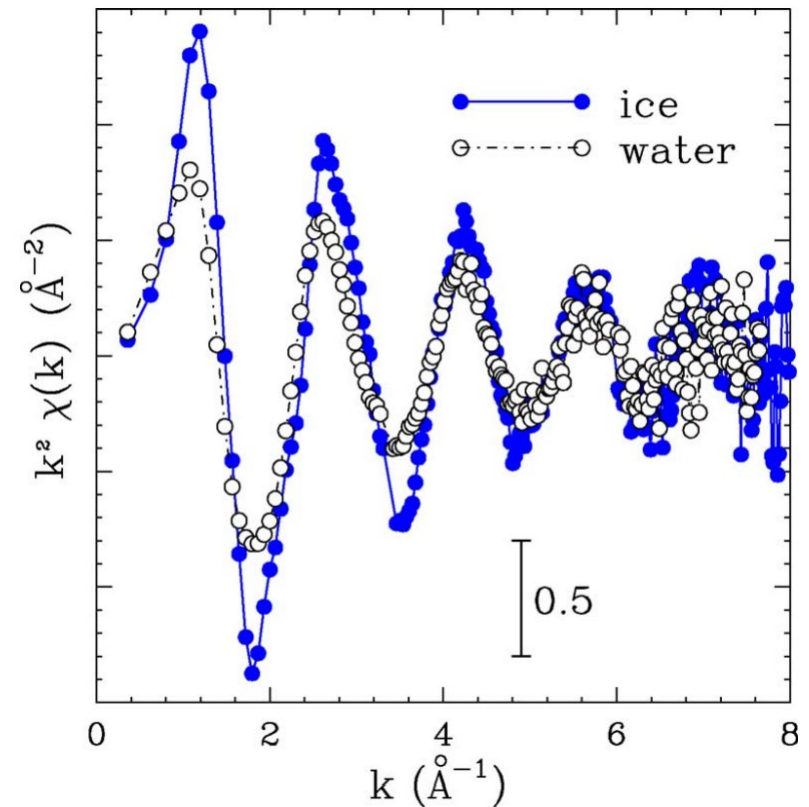
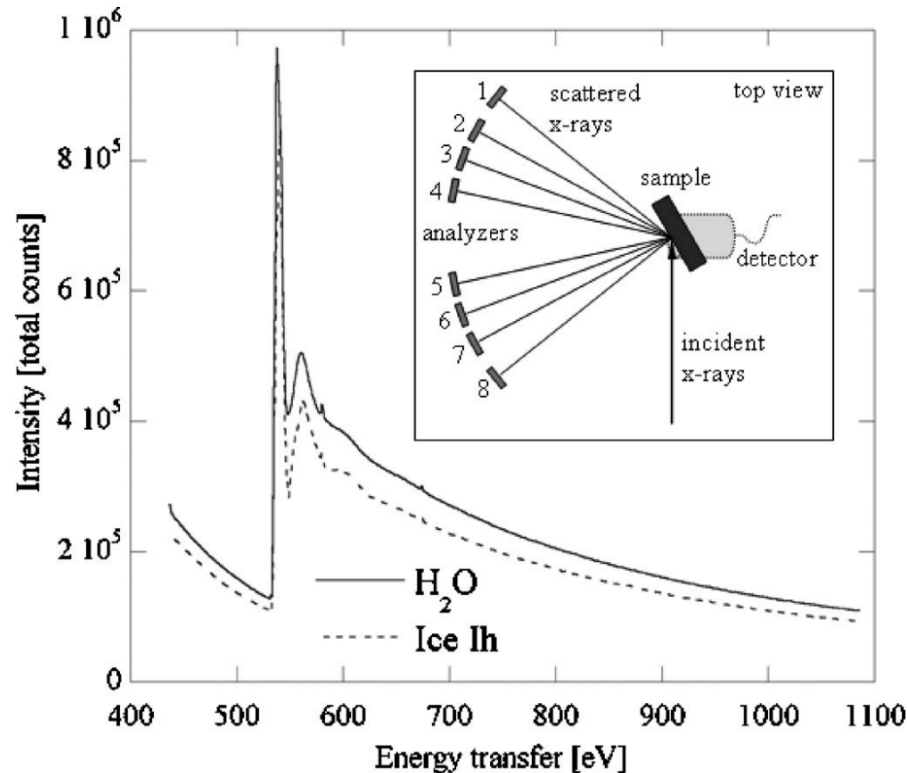
(N)IXS of core electron excitations – XRS

XRS of graphite electrode for lithium-ion batteries



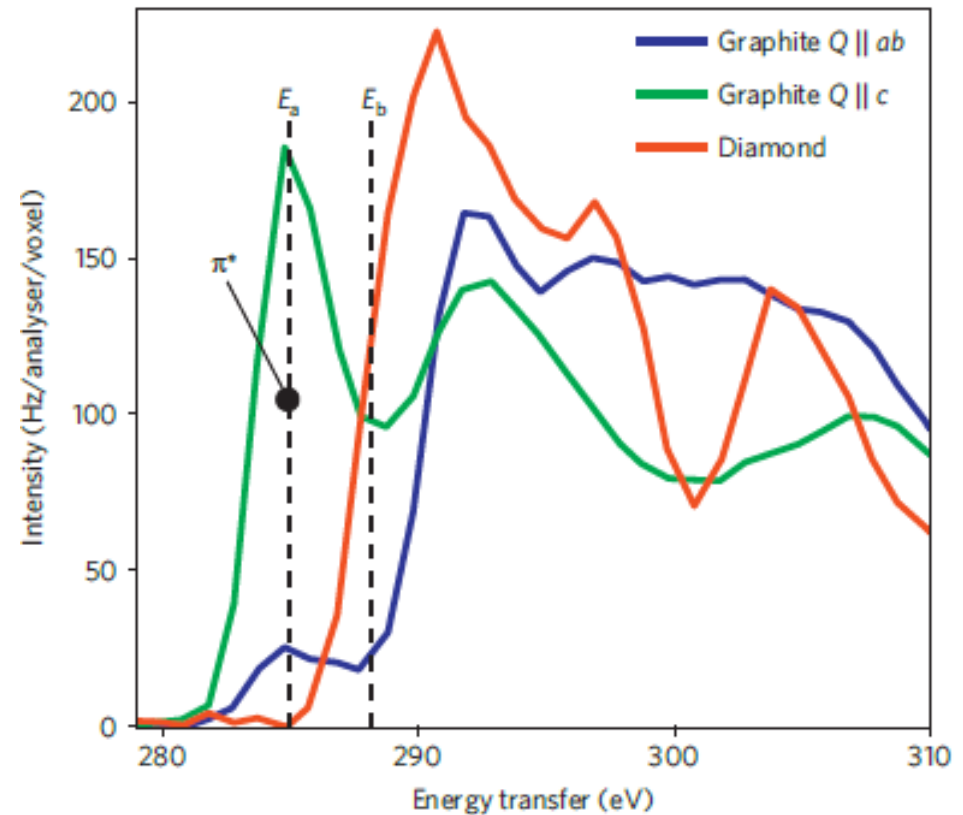
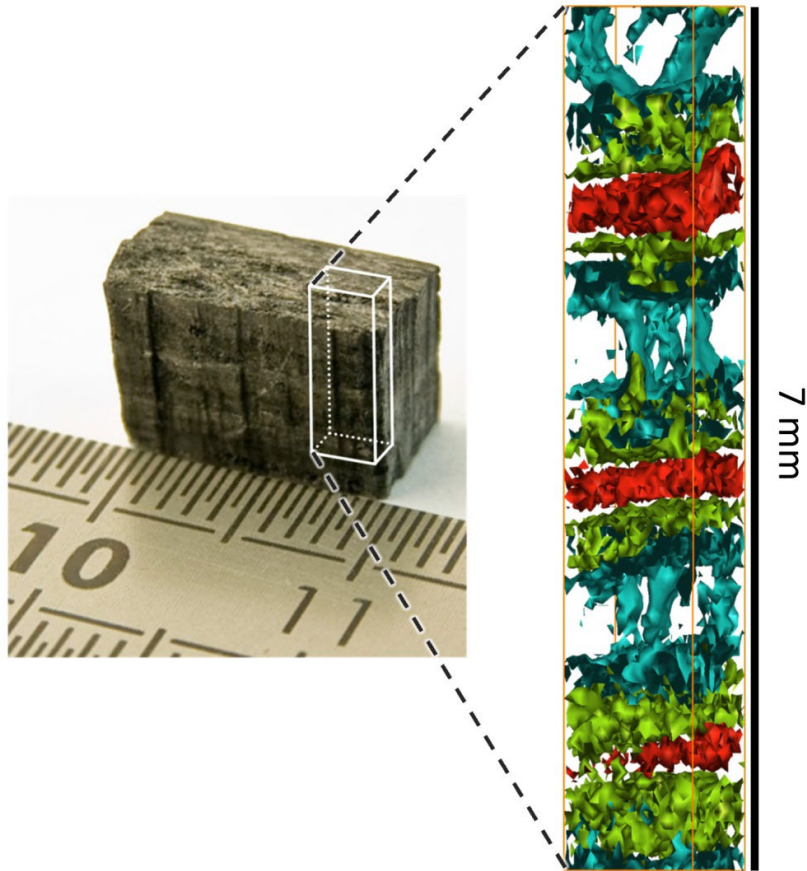
(N)IXS of core electron excitations – XRS

EXAFS in water by XRS



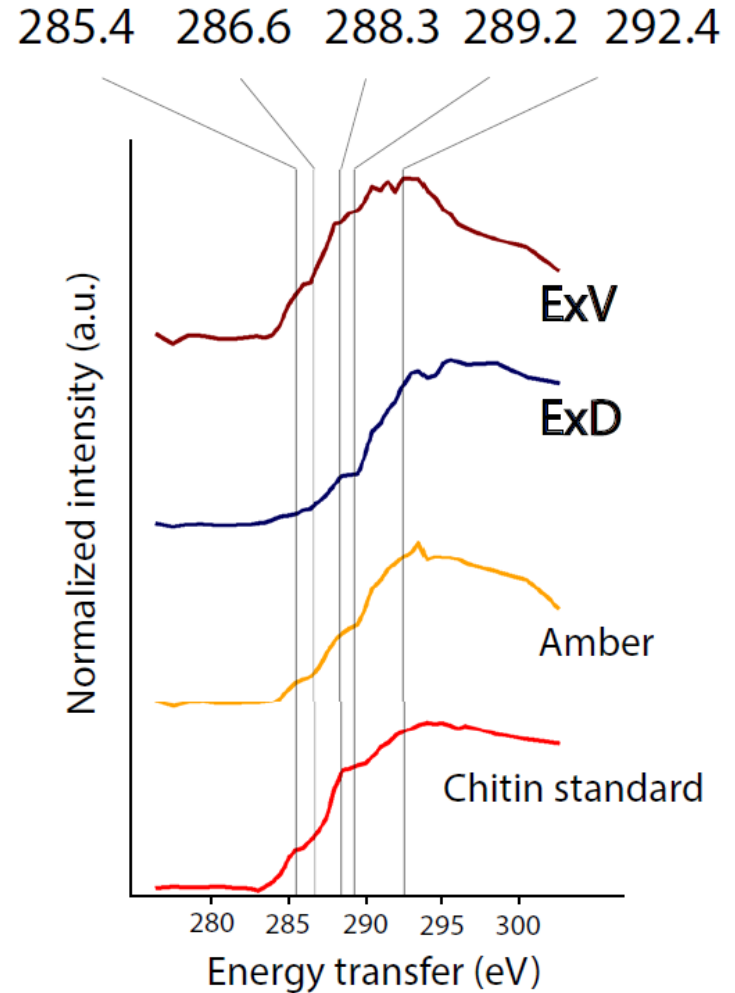
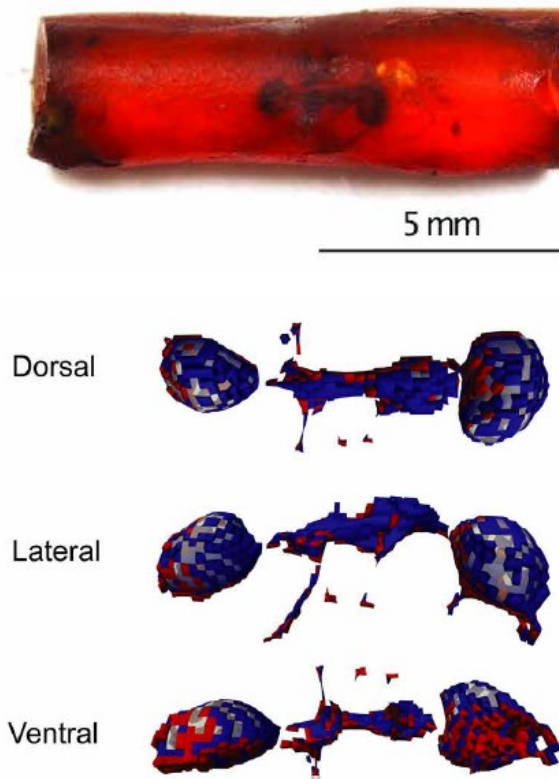
(N)IXS of core electron excitations – XRS

XRS based imaging of carbon fiber-reinforced silicon carbide



(N)IXS of core electron excitations – XRS

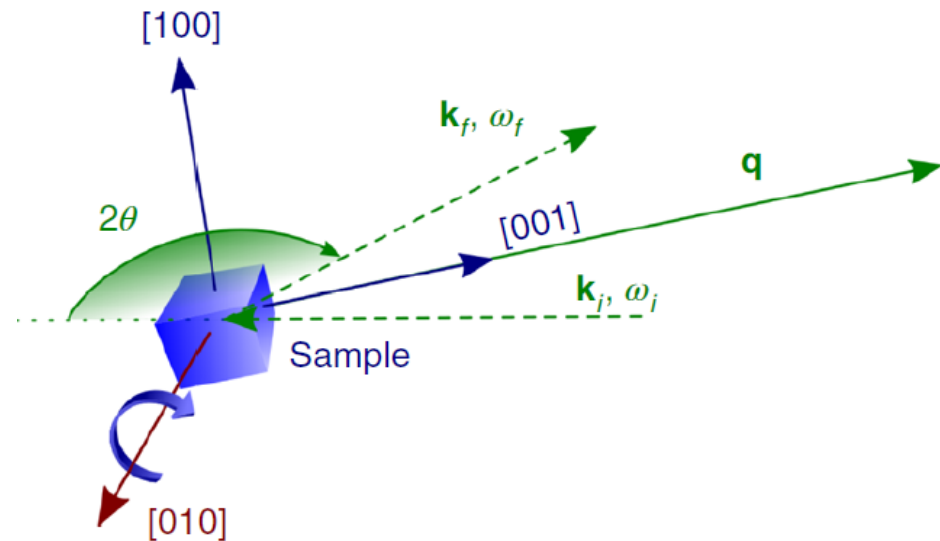
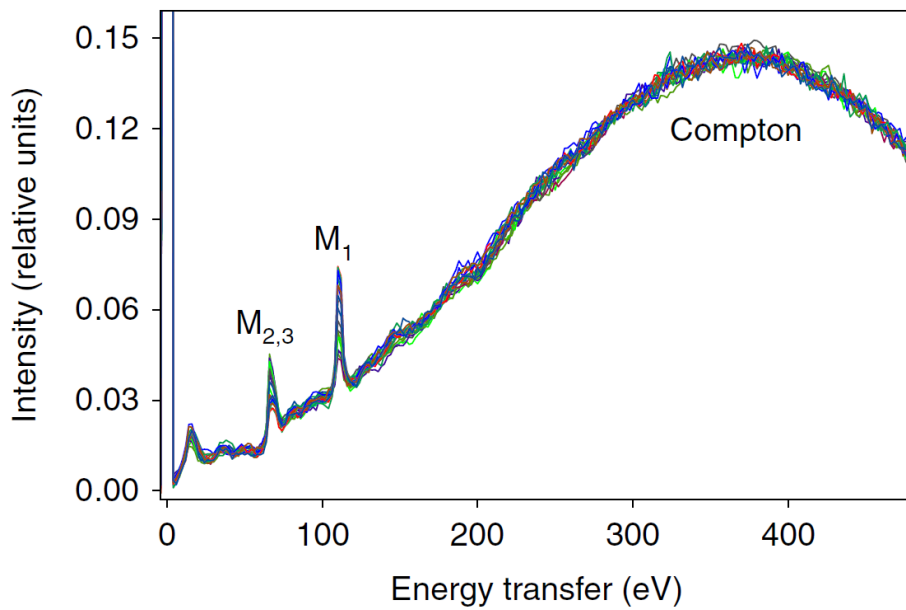
Insect in amber (ca. 53 Ma old)



(N)IXS of core electron excitations – XRS

XRS not limited to dipole transitions. The case of NiO

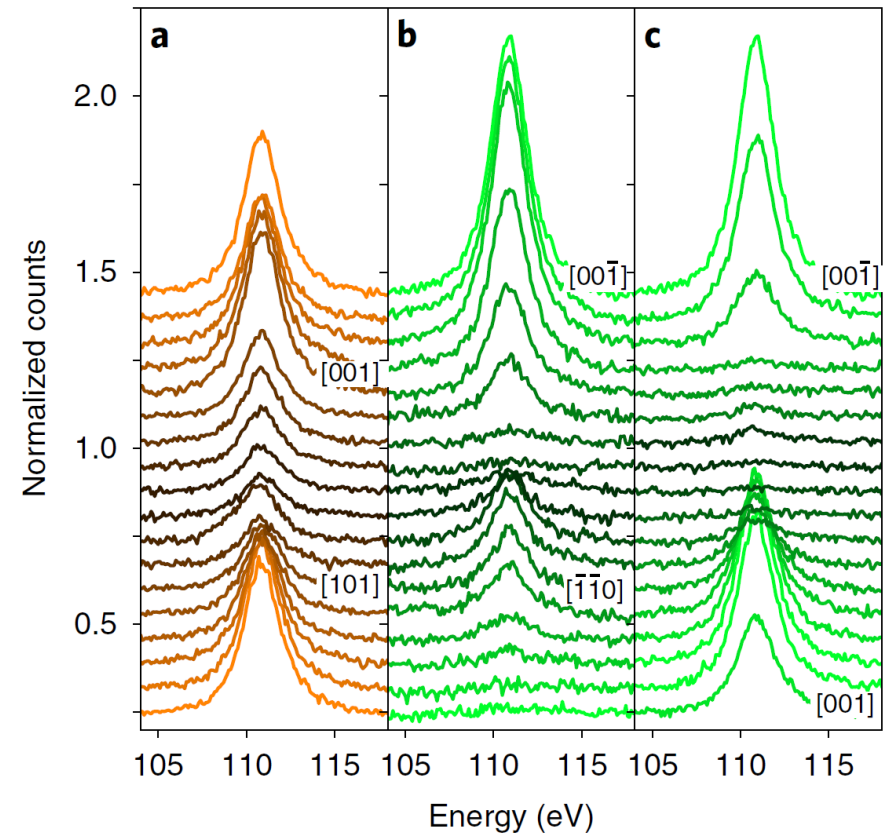
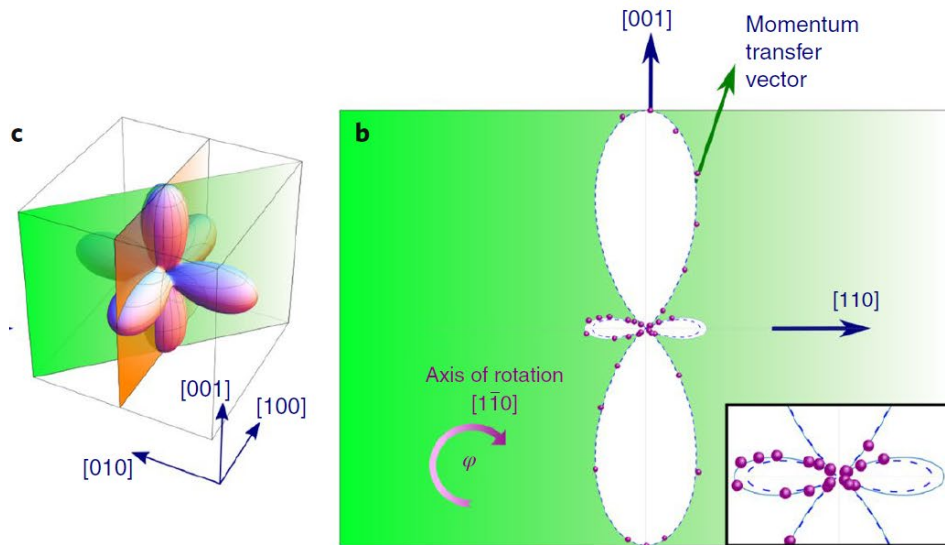
Ni M_1 ($3s \rightarrow 3d$)



(N)IXS of core electron excitations – XRS

XRS not limited to dipole transitions. The case of NiO

Ni M_1 ($3s \rightarrow 3d$)



Inelastic X-ray scattering

(R)IXS cross-section from light – matter interaction...

$$\begin{aligned}\mathcal{H} &= \sum_i^N \frac{[\mathbf{p}_i + e\mathbf{A}(\mathbf{r}_i)]^2}{2m} + \dots = \sum_i^N \frac{\mathbf{p}_i^2 + 2e\mathbf{p}_i \cdot \mathbf{A}(\mathbf{r}_i) + e^2\mathbf{A}(\mathbf{r}_i)^2}{2m} + \dots \\ &= \sum_i^N \frac{\mathbf{p}_i^2}{2m} + \mathcal{H}' + \dots = \mathcal{H}_0 + \mathcal{H}'\end{aligned}$$

...in second order perturbation theory

$$w = \frac{2\pi}{\hbar} \sum_f \left| \langle f | \mathcal{H}' | g \rangle + \sum_n \frac{\langle f | \mathcal{H}' | n \rangle \langle n | \mathcal{H}' | g \rangle}{E_g + \hbar\omega_i - E_n} \right|^2 \delta(E_f + \hbar\omega_o - E_g - \hbar\omega_i)$$

non-resonant

resonant

Resonant inelastic X-ray scattering

Resonant x-ray scattering cross-section

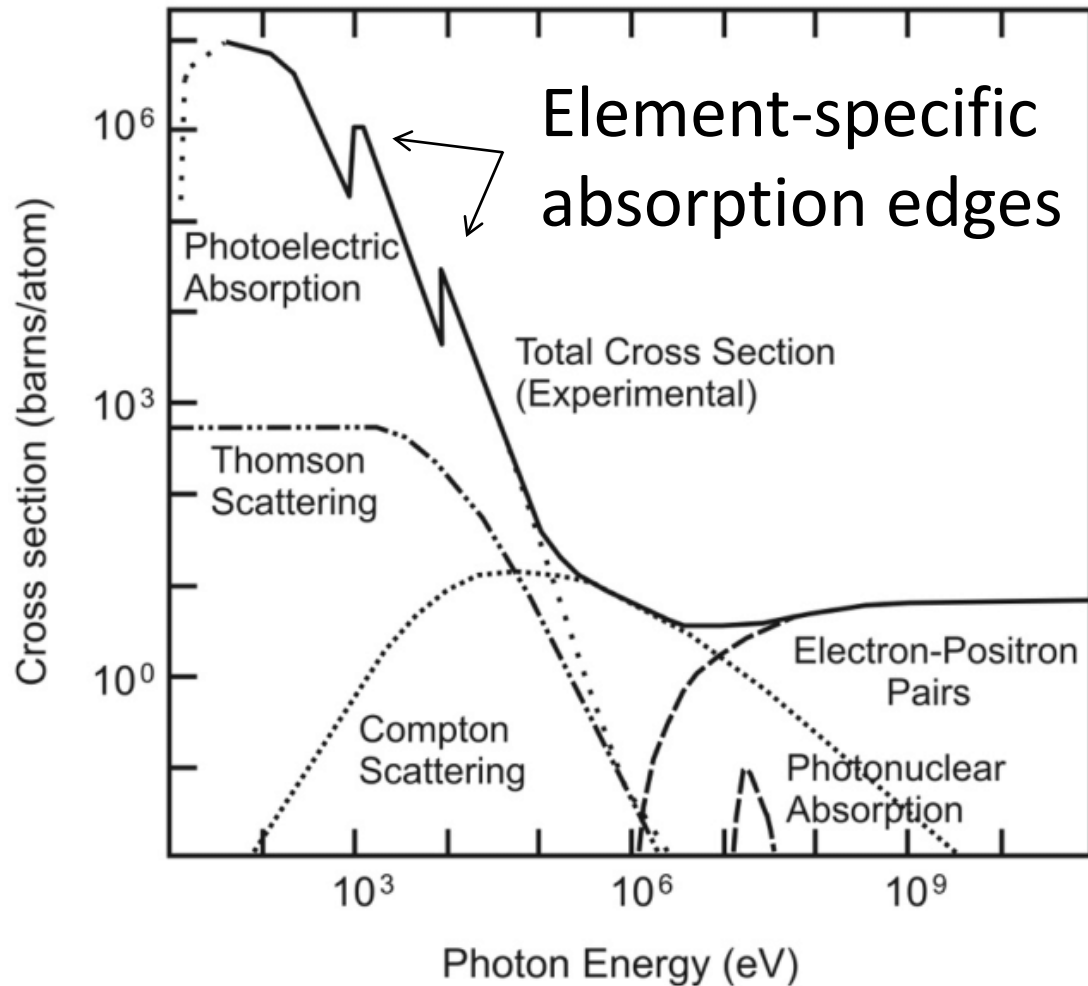
$$w \sim \sum_f \left| \sum_n \sum_{i,j}^N \frac{\langle f | \mathbf{r}_j \cdot \boldsymbol{\epsilon}_o | n \rangle \langle n | \mathbf{r}_i \cdot \boldsymbol{\epsilon}_i | g \rangle}{E_g + \hbar\omega_i - E_n} \right|^2 \delta(E_f + \hbar\omega_o - E_g - \hbar\omega_i)$$

Kramers-Heisenberg equation

XAS + **XES** + interference effects

Resonant inelastic X-ray scattering

Photoelectric absorption dominates below 10^5 eV



Resonant inelastic X-ray scattering



At the absorption edge core-electrons are promoted into the unoccupied states just above the Fermi level

Resonant inelastic X-ray scattering



Once the core-hole is created (no matter how), electrons from occupied states fill the hole, e.g., by emitting an x-ray

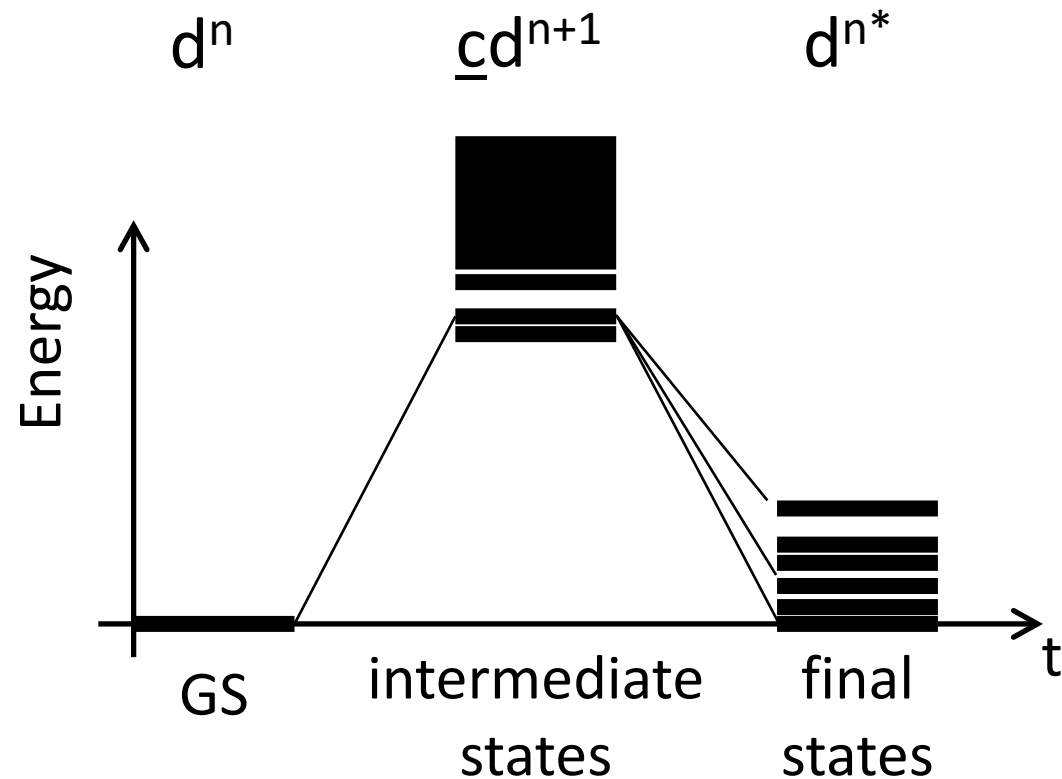
Resonant inelastic X-ray scattering



RIXS : coherent combination of XAS and XES processes

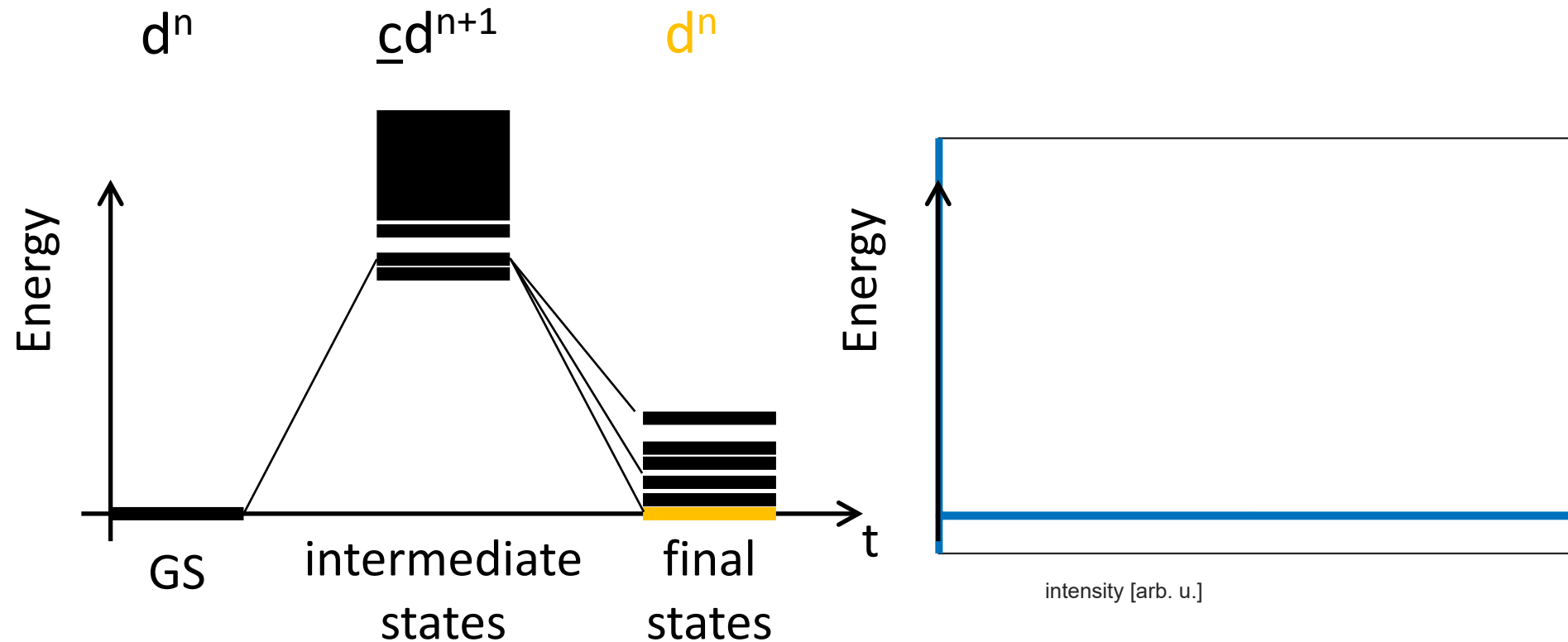
Resonant inelastic X-ray scattering

RIXS in the total energy diagram



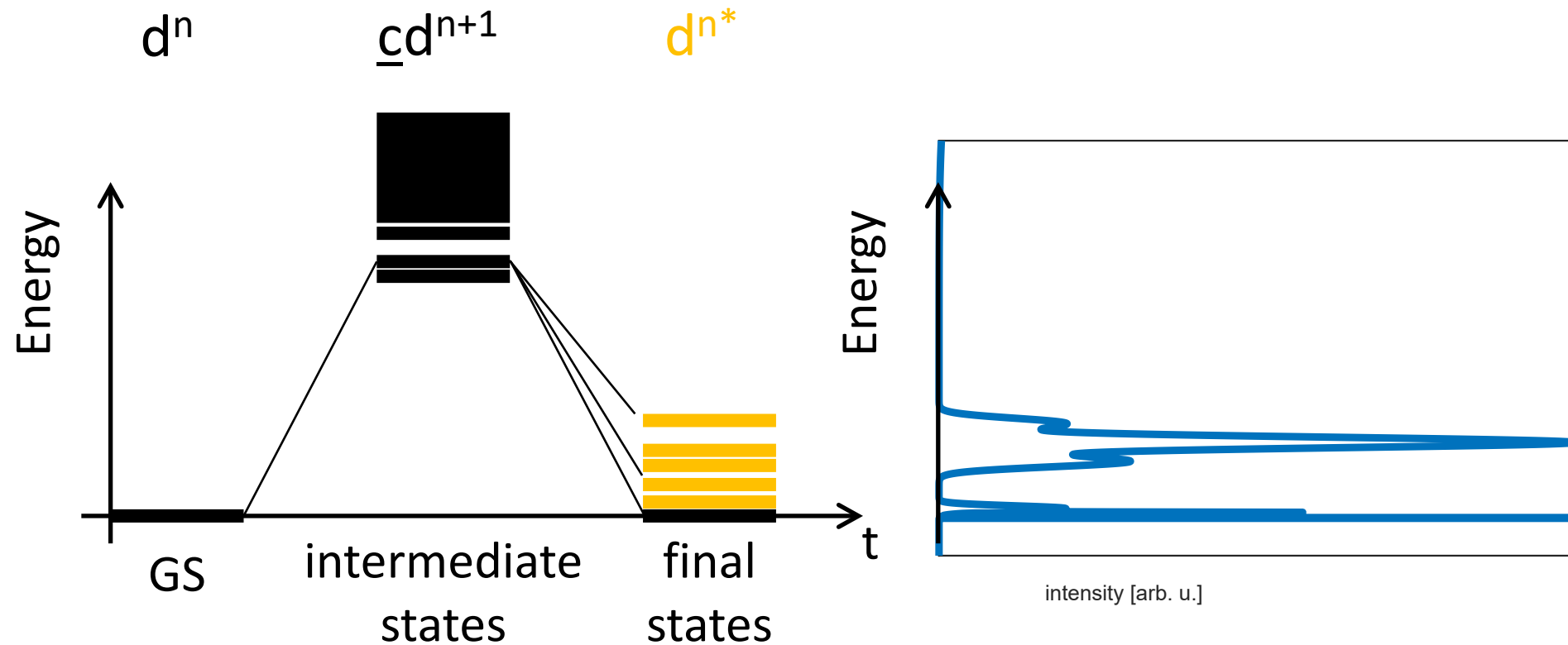
Resonant inelastic X-ray scattering

RIXS in the total energy diagram

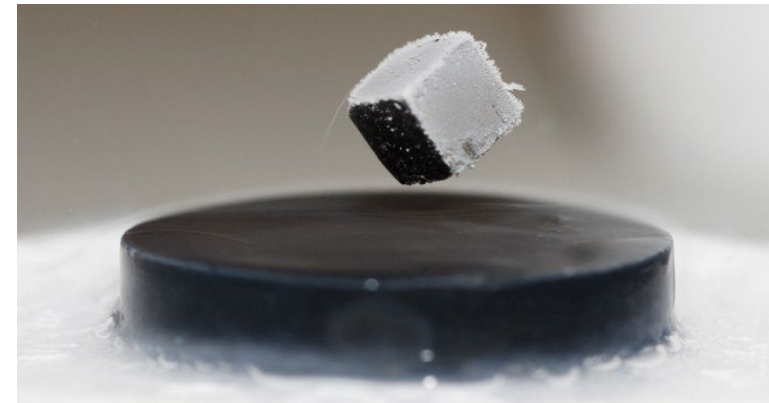
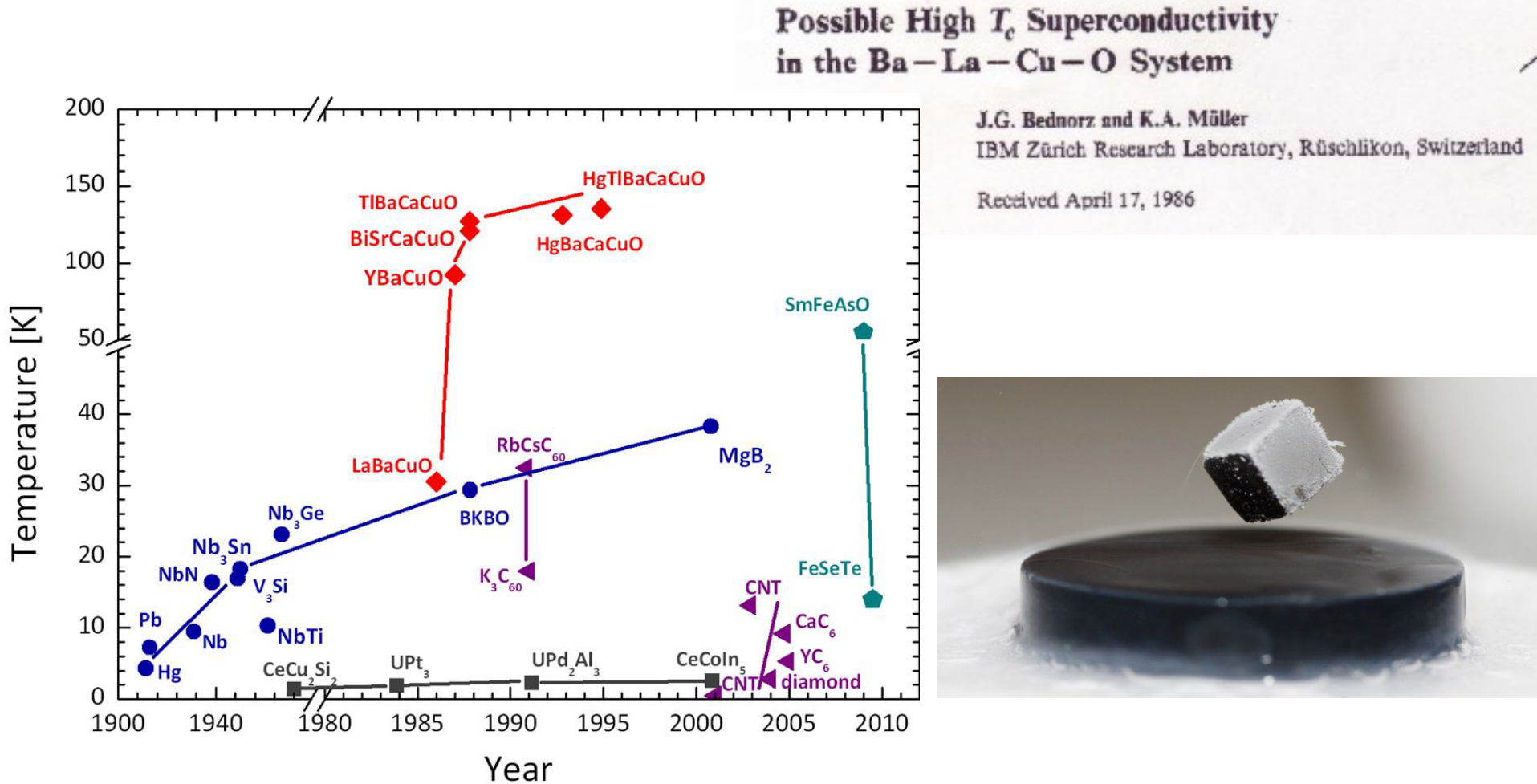


Resonant inelastic X-ray scattering

RIXS in the total energy diagram

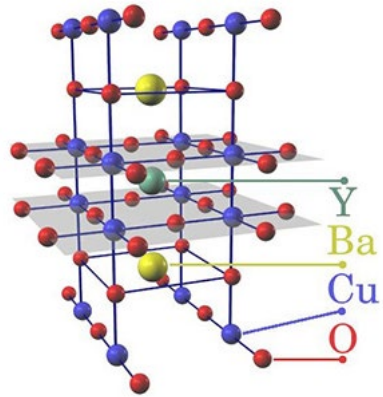


High T_c superconductors

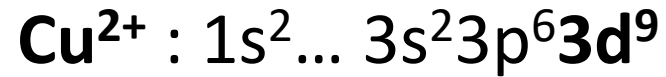


High T_c superconductors

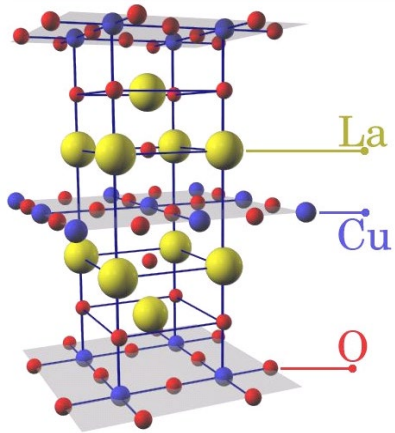
undoped : 2D $S=1/2$ Heisenberg AFM insulator



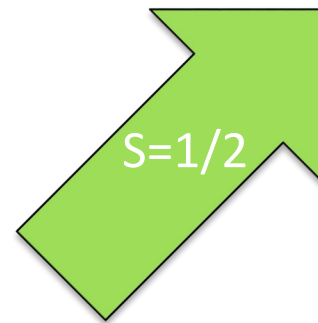
YBa₂Cu₃O₆ (YBCO)



one particle (hole) $S = 1/2$ system

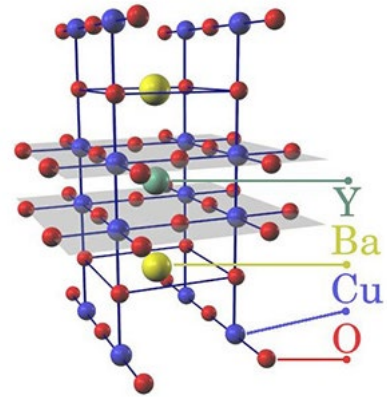


La₂CuO₄ (LCO)

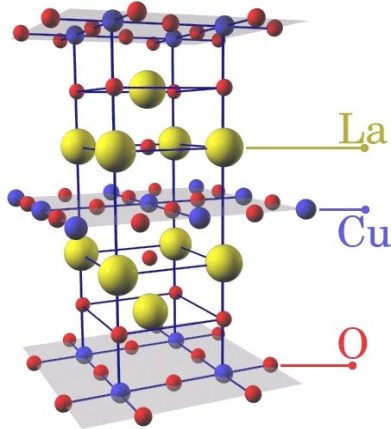
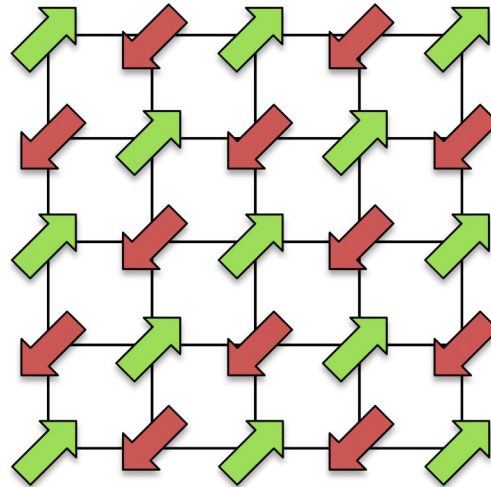


High T_c superconductors

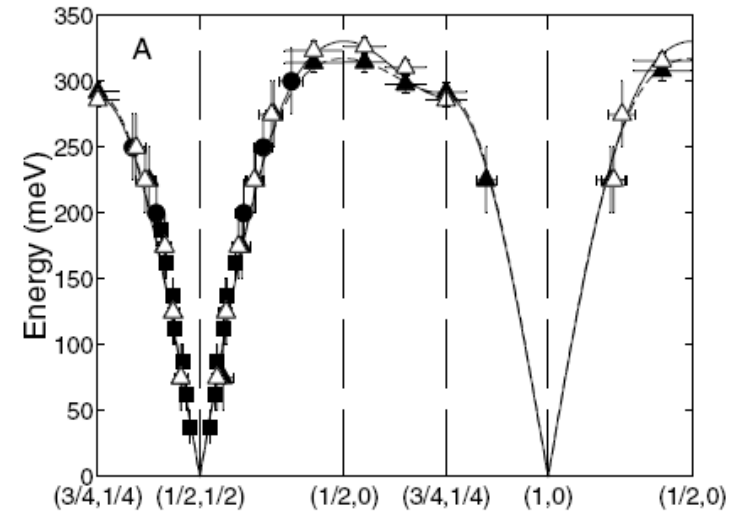
undoped : 2D $S=1/2$ Heisenberg AFM insulator



$\text{YBa}_2\text{Cu}_3\text{O}_6$ (YBCO)



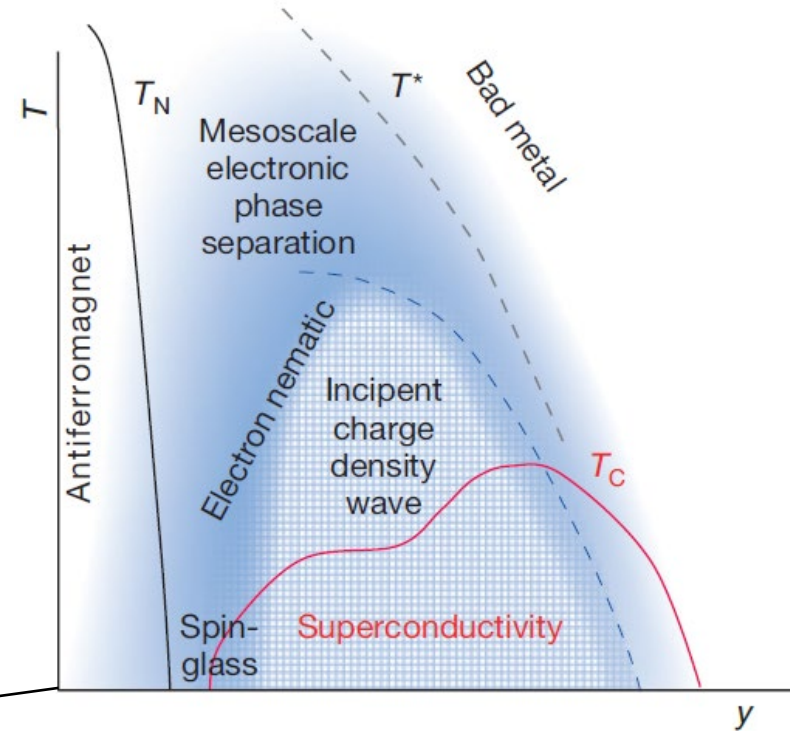
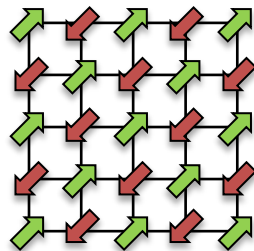
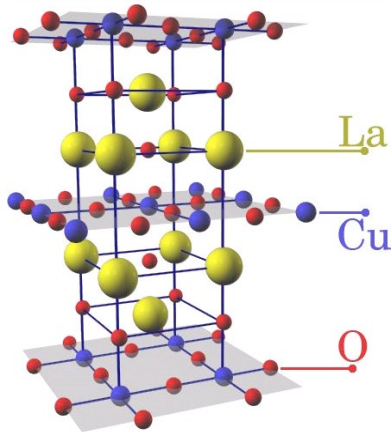
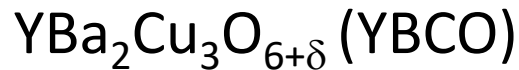
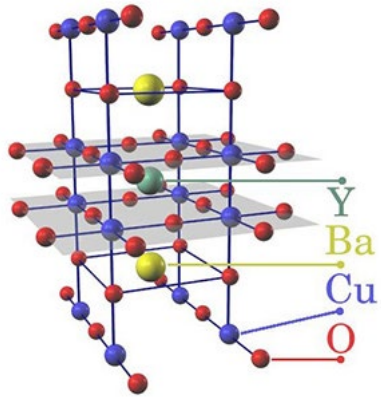
La_2CuO_4 (LCO)



$J \sim 100$ meV

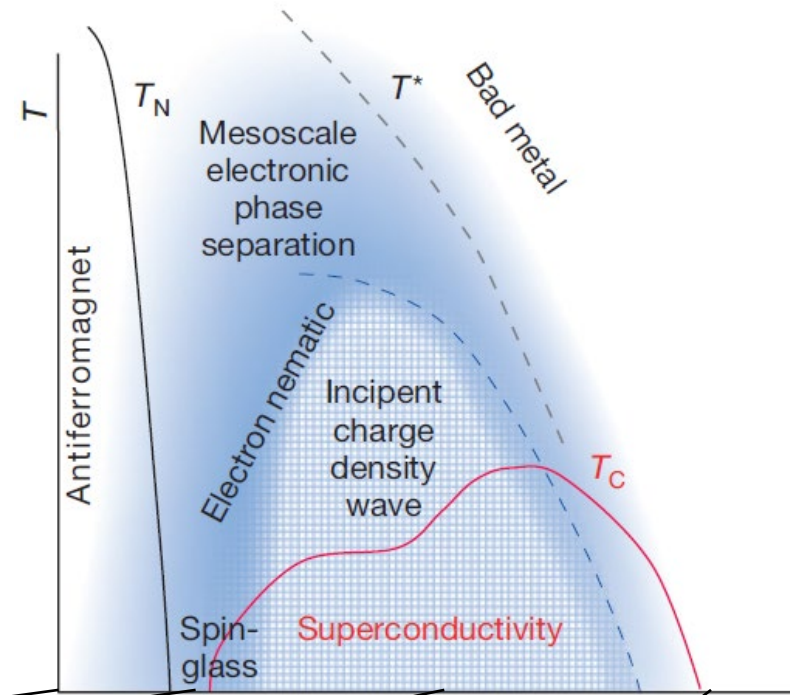
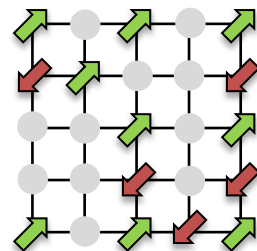
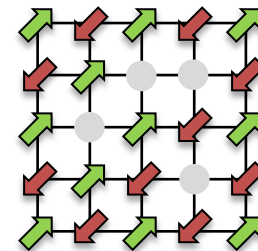
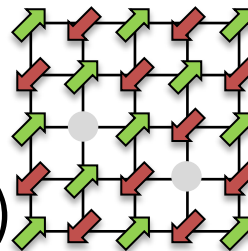
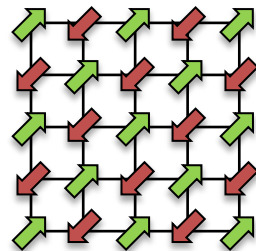
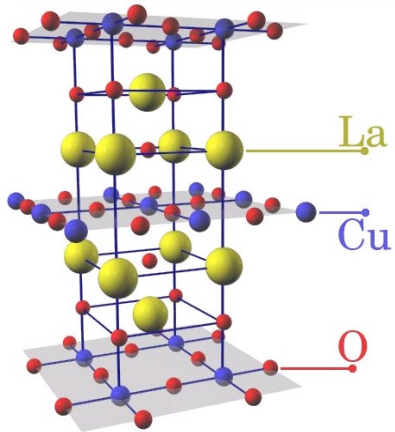
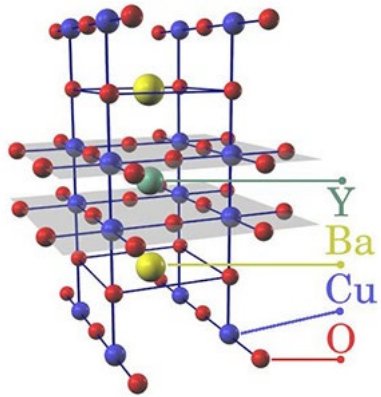
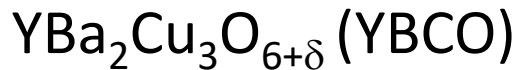
High T_c superconductors

Phase diagram : T vs. doping



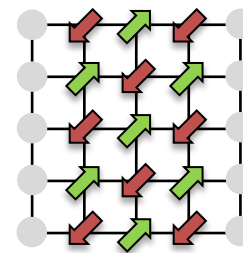
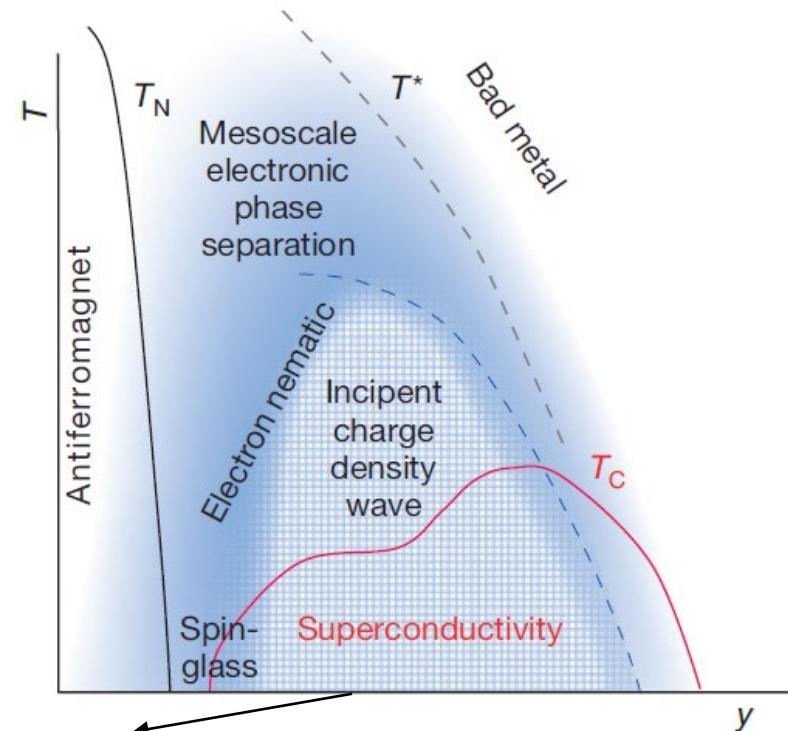
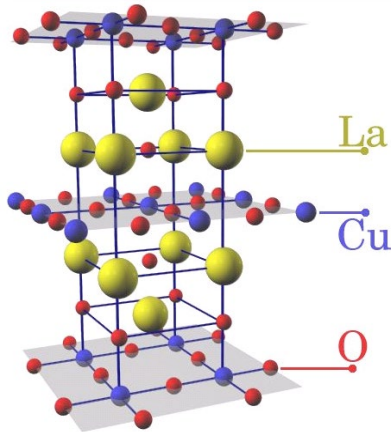
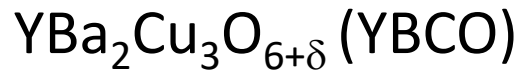
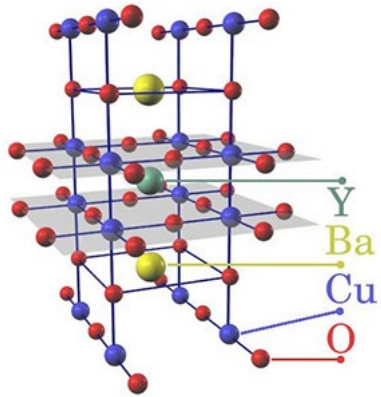
High T_c superconductors

Phase diagram : T vs. doping



High T_c superconductors

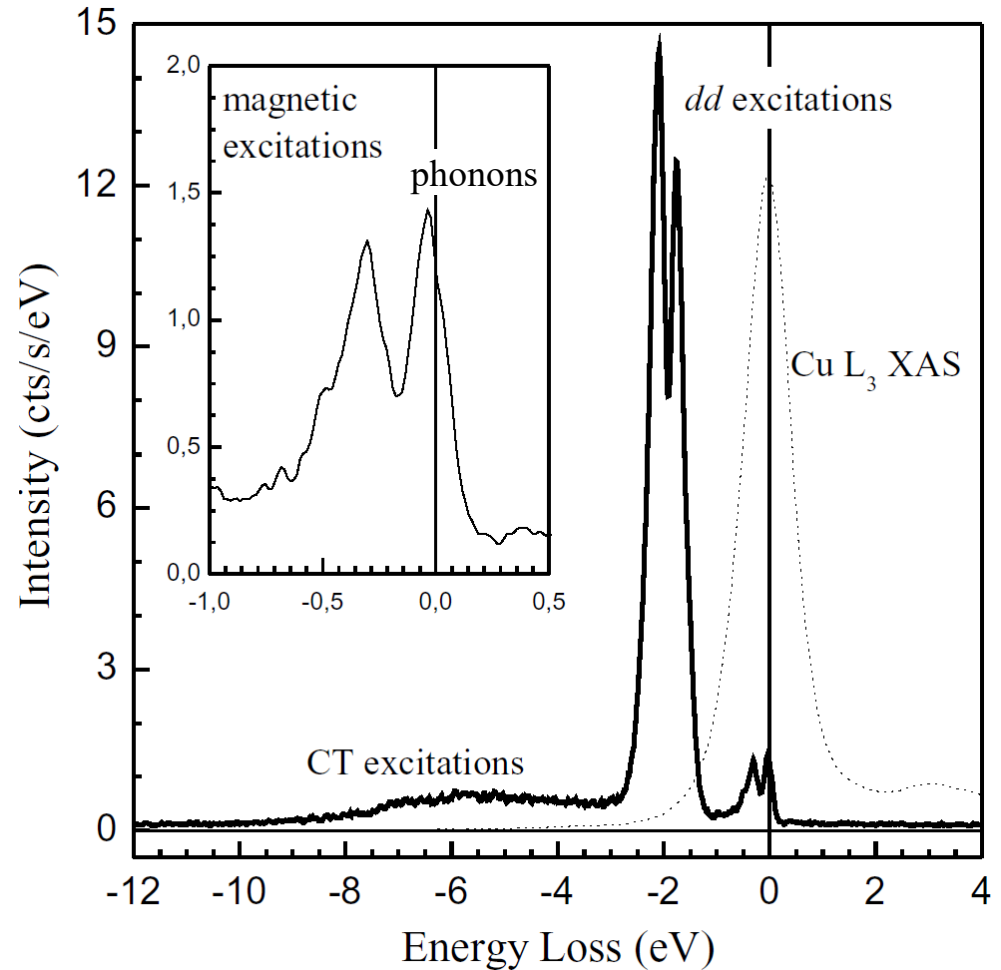
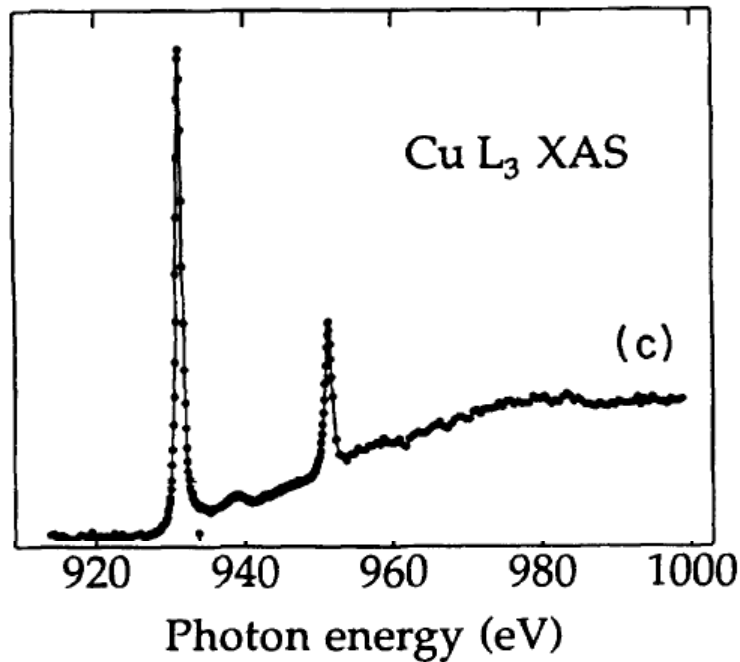
Phase diagram : T vs. doping



doped holes tend to order

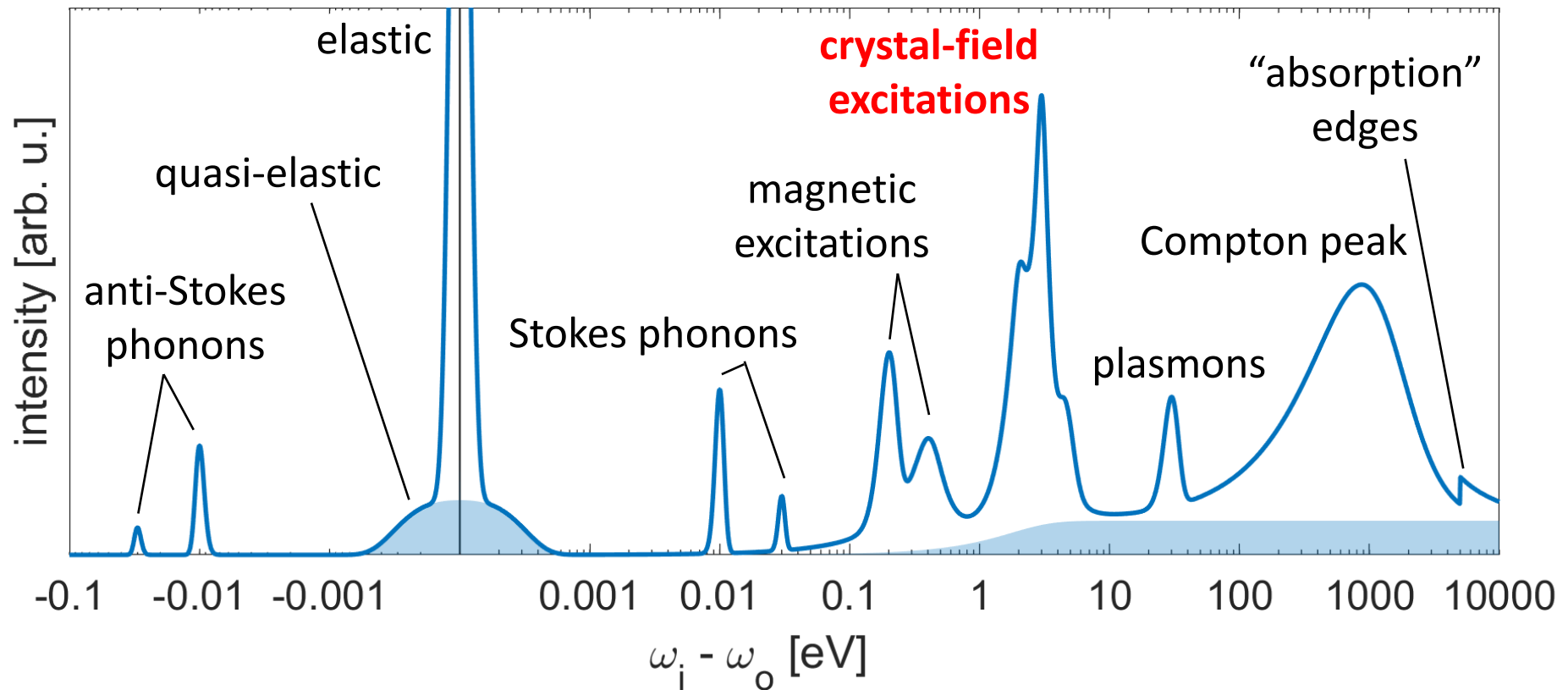
High T_c superconductors

While XAS is very simple,
RIXS of La_2CuO_4 is very rich



Resonant inelastic X-ray scattering

RIXS of crystal field excitations



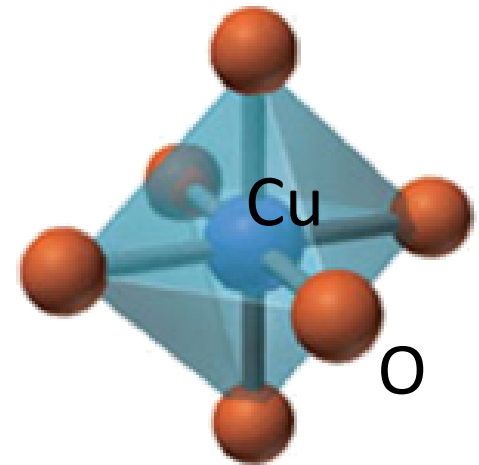
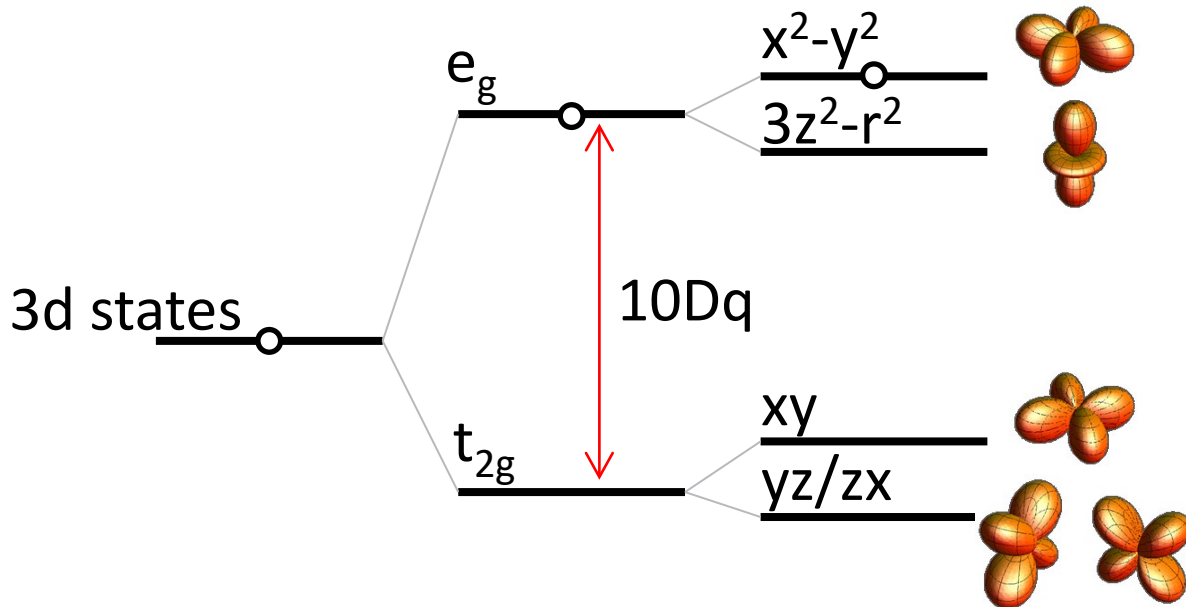
RIXS of crystal field excitations

“multiplet” structure of Cu^{2+}
no e-e, no SO, no hybrid., only CF

spherical

O_h

D_{4h}



trivial Sugano-Tanabe diagram

RIXS of crystal field excitations

“multiplet” structure of Cu^{2+}
no e-e, no SO, no hybrid., only CF

GS

Intermediate state

final state

x^2-y^2
—○—
 $3z^2-r^2$
—



—
—

—○—
—



xy
—
 yz/zx
—

—
—

—
—

$2p^6 3d^9$

$2p^5 3d^{10}$

$2p^6 3d^{9*}$

RIXS of crystal field excitations

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○
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xy

yz/zx

○



$2p^6 3d^9$

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—
—

—
—

xy
—
 yz/zx
—

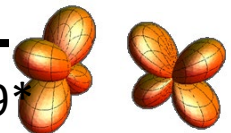
$2p^6 3d^9$

—
—

$2p^5 3d^{10}$

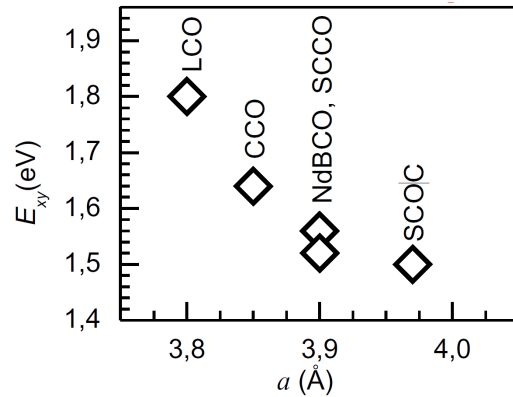
—
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$2p^6 3d^{9*}$

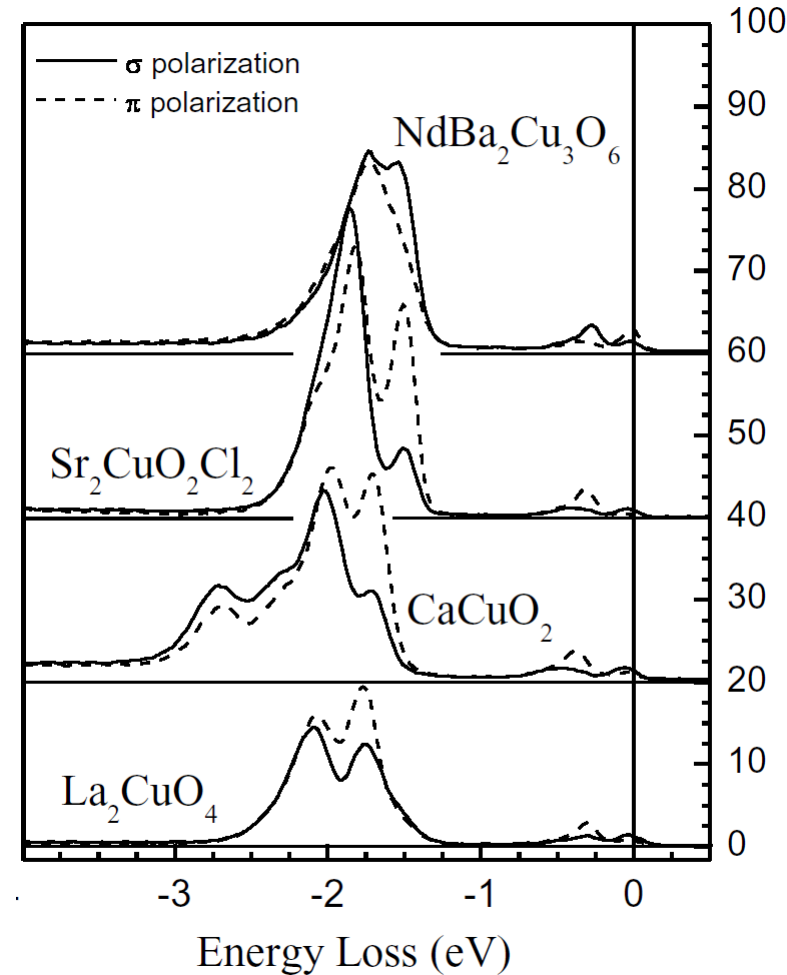


RIXS of crystal field excitations

CF (or d-d) transitions are very sensitive to Cu coordination

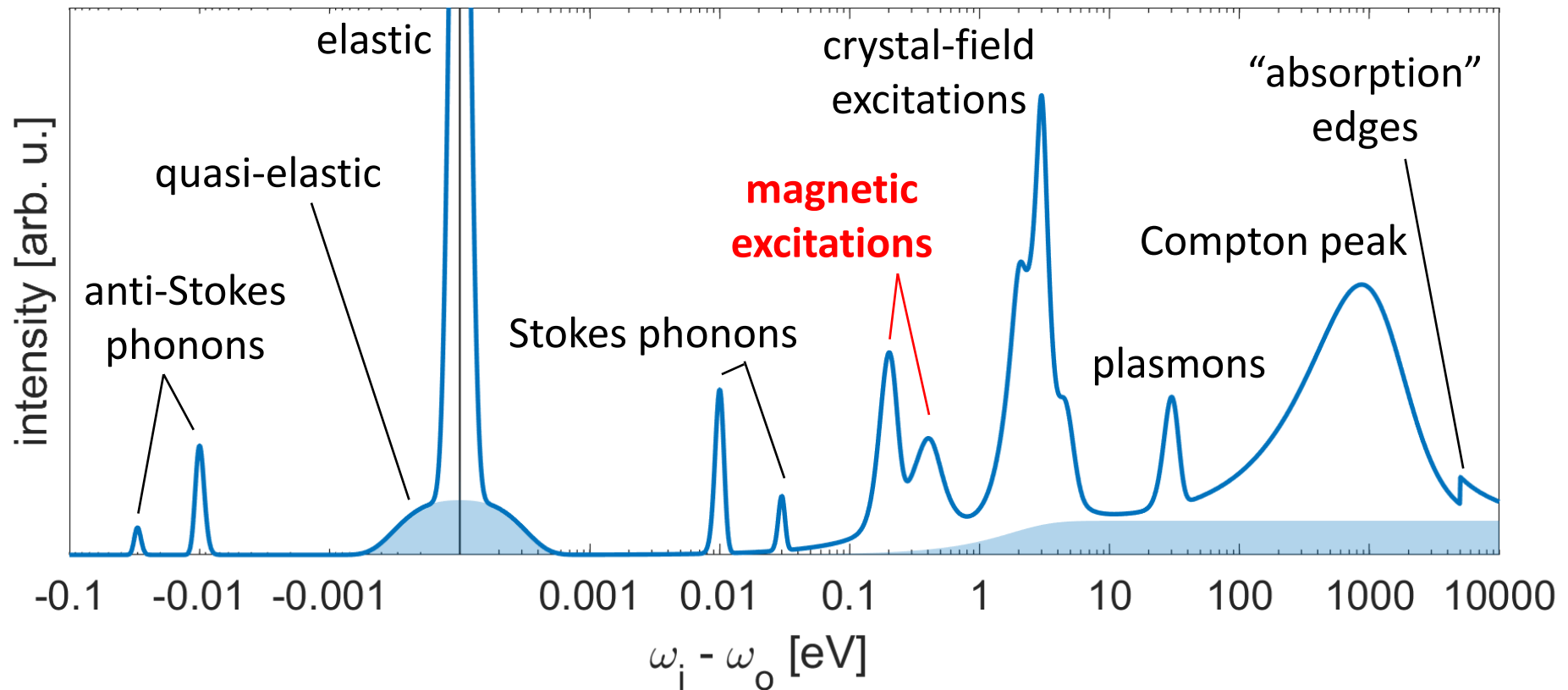


	La ₂ CuO ₄	Sr ₂ CuO ₂ Cl ₂	CaCuO ₂	Sr _{0.5} Ca _{0.5} CuO ₂	NdBa ₂ Cu ₃ O ₇
$E_{3z^2-r^2} (\Gamma_{3z^2-r^2})$ (eV)	1.70 (0.14)	1.97 (0.10)	2.65 (0.12)	2.66	1.98 (0.18)
$E_{xy} (\Gamma_{xy})$ (eV)	1.80 (0.10)	1.50 (0.08)	1.64 (0.09)	1.56	1.52 (0.10)
$E_{xz/yz} (\Gamma_{xz/yz})$ (eV)	2.12 (0.14)	1.84 (0.10)	1.95 (0.12)	1.93	1.75 (0.12)
ΔE_{e_g}	1.70	1.97	2.65	2.66	1.98
$\Delta E_{t_{2g}}$	0.32	0.33	0.31	0.36	0.23
$10Dq$ (eV)	1.80	1.50	1.64	1.56	1.52
D_s (eV)	0.29	0.33	0.42	0.43	0.32
D_t (eV)	0.11	0.13	0.19	0.19	0.14



Resonant inelastic X-ray scattering

Spin-flip and magnetic excitations



Spin-flip and magnetic excitations

“multiplet” structure of Cu^{2+}
no e-e, no SO, no hybrid., only CF

GS

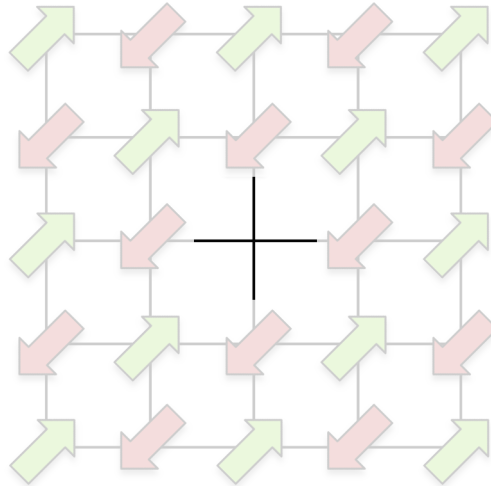
x^2-y^2

 $3z^2-r^2$



xy

 yz/zx

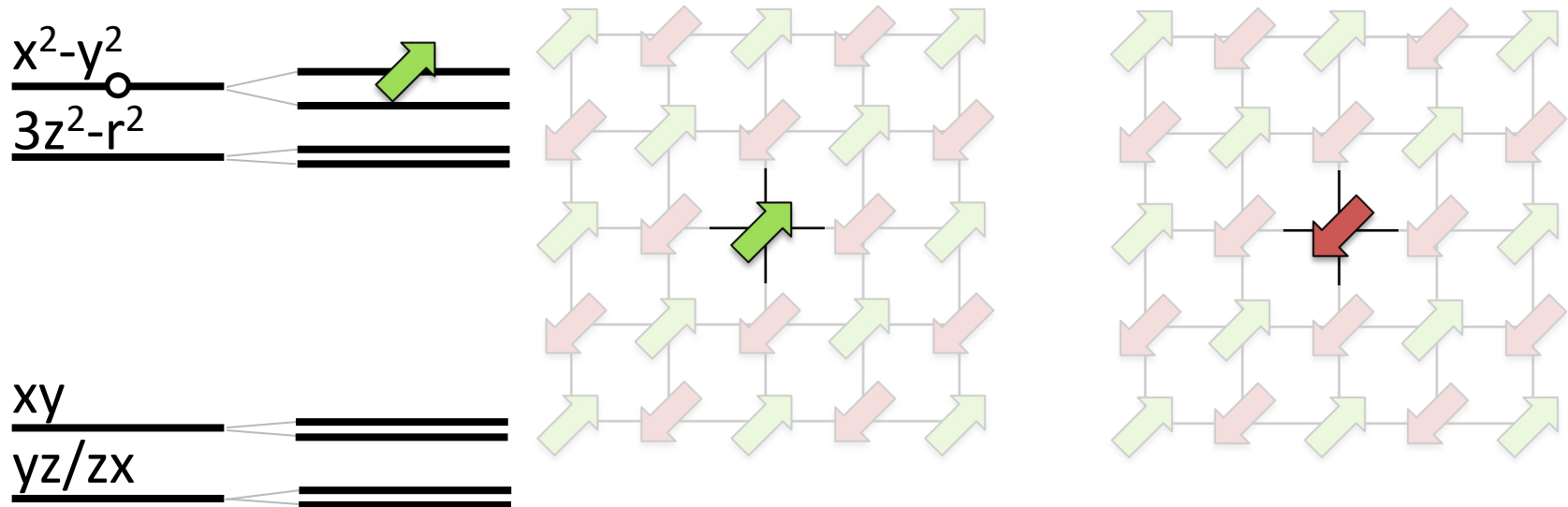


Spin-flip and magnetic excitations

“multiplet” structure of Cu^{2+}

no e-e, no SO, no hybrid., only CF and AFM

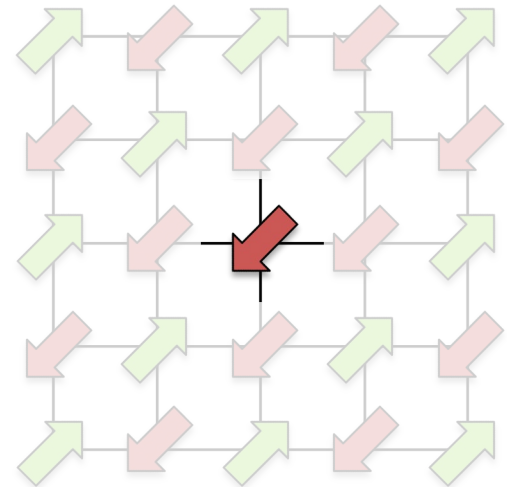
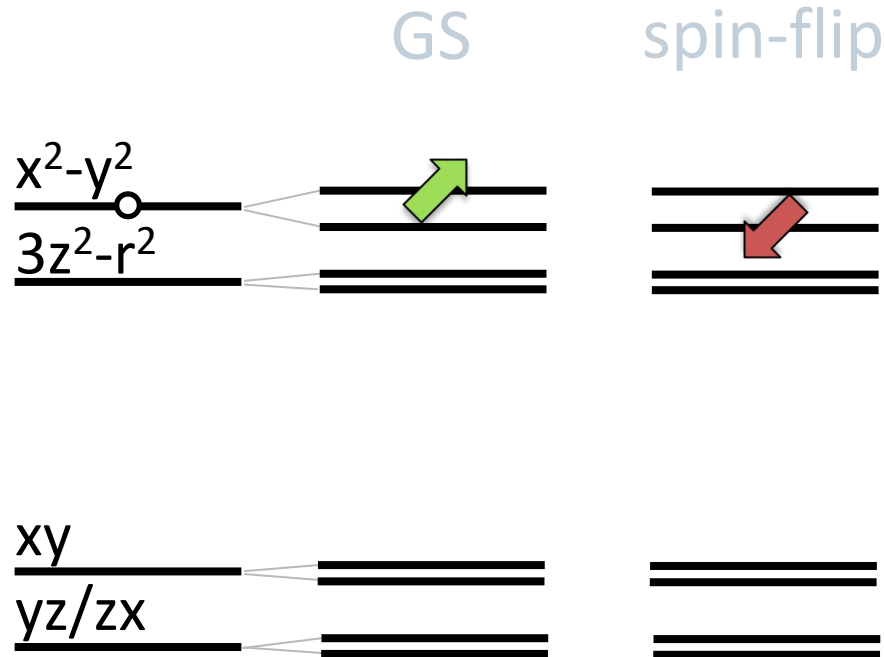
GS



Spin-flip and magnetic excitations

“multiplet” structure of Cu^{2+}

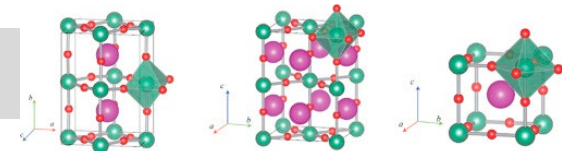
no e-e, no SO, no hybrid., only CF and AFM



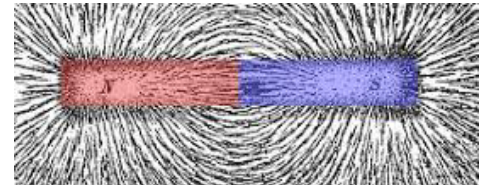
Spin-flip and magnetic excitations

Relevance of magnetic excitations

structural properties (phase transitions, ...)



magnetic properties (magnetic interactions, Curie/Neel temperatures, ...)



transport properties (conductivity, superconductivity? ...)



Spin-flip and magnetic excitations

How can dipolar (spin-conserving) transitions give rise to spin-flip excitations?

$$\mathcal{A}_{|\text{blue clover}\rangle}^{\epsilon\epsilon'} = \sum_n \frac{\langle \text{blue clover} | \mathcal{D}_{\epsilon'}^\dagger | n \rangle \langle n | \mathcal{D}_\epsilon | \text{orange clover} \rangle}{E_g - E_n + \hbar\omega + i\Gamma_n}$$

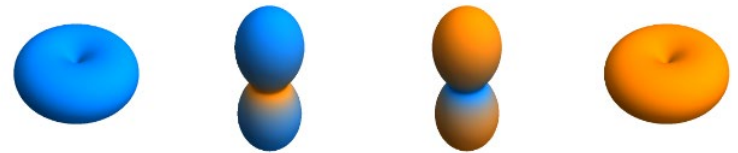
Spin-flip and magnetic excitations

How can dipolar (spin-conserving) transitions give rise to spin-flip excitations?

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Spin-orbit coupled
intermediate state

$2p_{3/2}$



Spin-flip and magnetic excitations

How can dipolar (spin-conserving) transitions give rise to spin-flip excitations?

$$\begin{aligned}
 A_{| \text{blue } \text{xy} \rangle}^{\text{xy}'} &\propto \sum_n \langle \text{blue } \text{xy} | \text{blue } \text{xy} | n \rangle \langle n | \text{orange } \text{xy} \rangle = \\
 &= \langle \text{blue } \text{xy} | \text{blue } \text{xy} | \text{blue } \text{xy} \rangle \langle \text{blue } \text{xy} | \text{orange } \text{xy} \rangle + \\
 &\quad + \langle \text{blue } \text{xy} | \text{blue } \text{xy} | \text{blue } \text{xy} \rangle \langle \text{blue } \text{xy} | \text{orange } \text{xy} \rangle + \\
 &\quad + \langle \text{blue } \text{xy} | \text{blue } \text{xy} | \text{blue } \text{xy} \rangle \langle \text{blue } \text{xy} | \text{orange } \text{xy} \rangle + \\
 &\quad + \langle \text{blue } \text{xy} | \text{blue } \text{xy} | \text{blue } \text{xy} \rangle \langle \text{blue } \text{xy} | \text{orange } \text{xy} \rangle \neq 0
 \end{aligned}$$

Spin-flip and magnetic excitations

Spin-flip requires rotation of the polarization

$$\mathcal{A}_{\text{spin-flip}}^{L_3} = \begin{pmatrix} 0 & i \sin \theta_s & 0 \\ -i \sin \theta_s & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

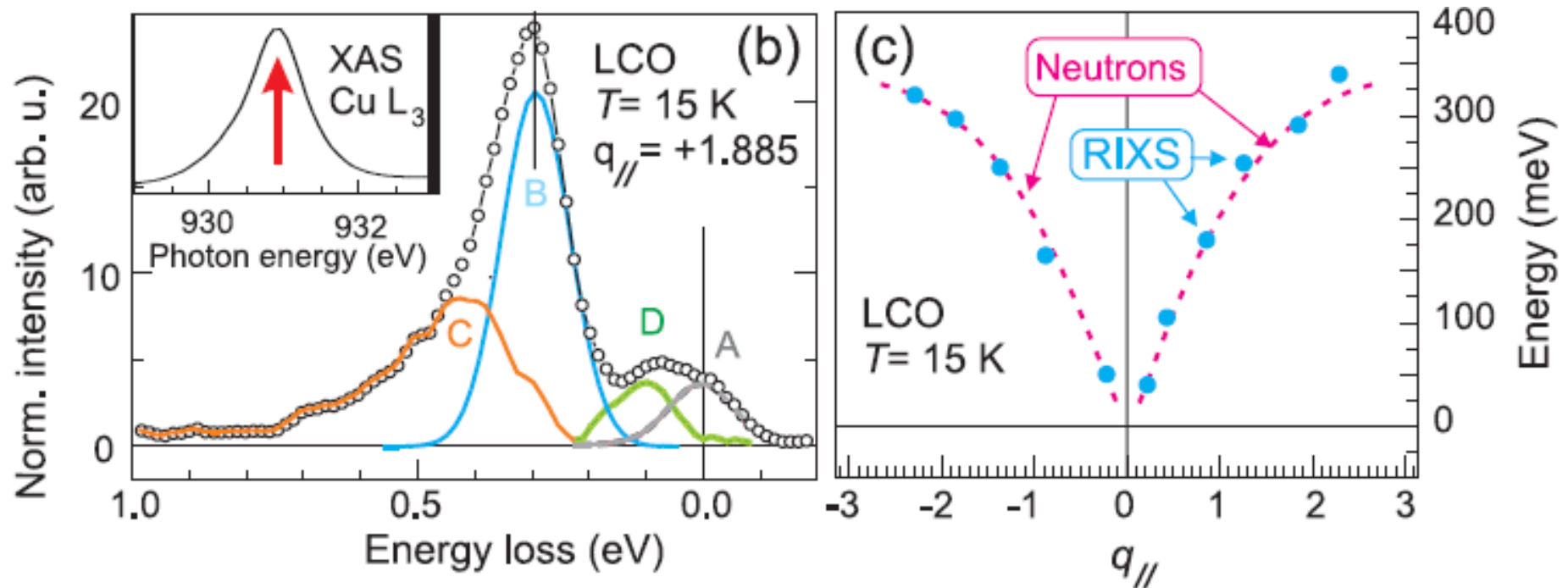
No spin-flip in the absence
of spin-orbit coupling

$1s$



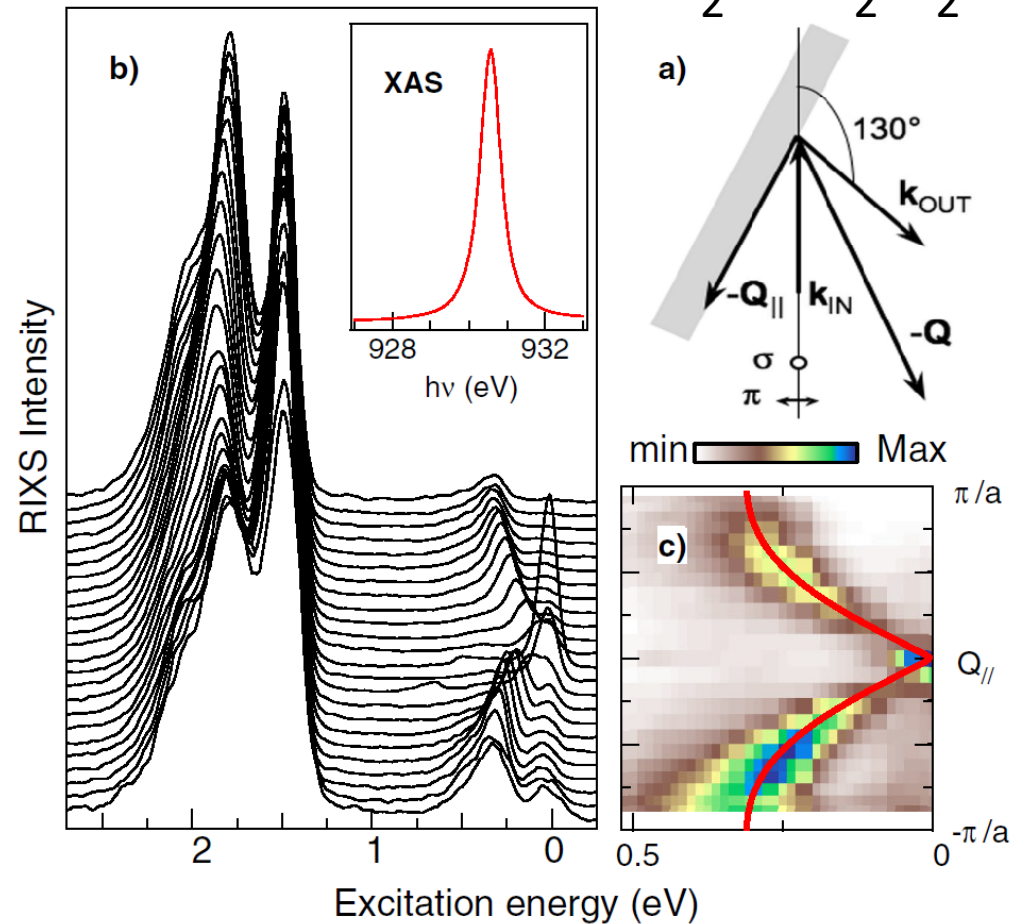
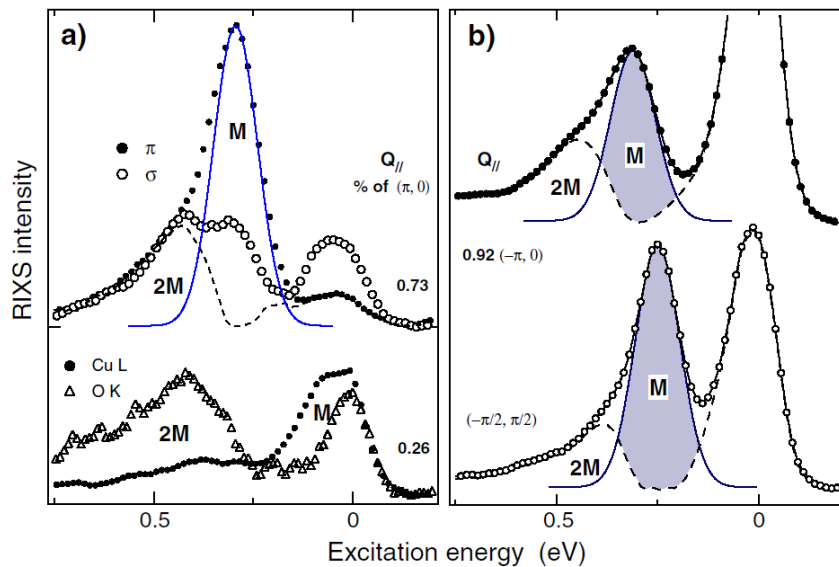
Spin-flip and magnetic excitations

First RIXS evidence of magnons



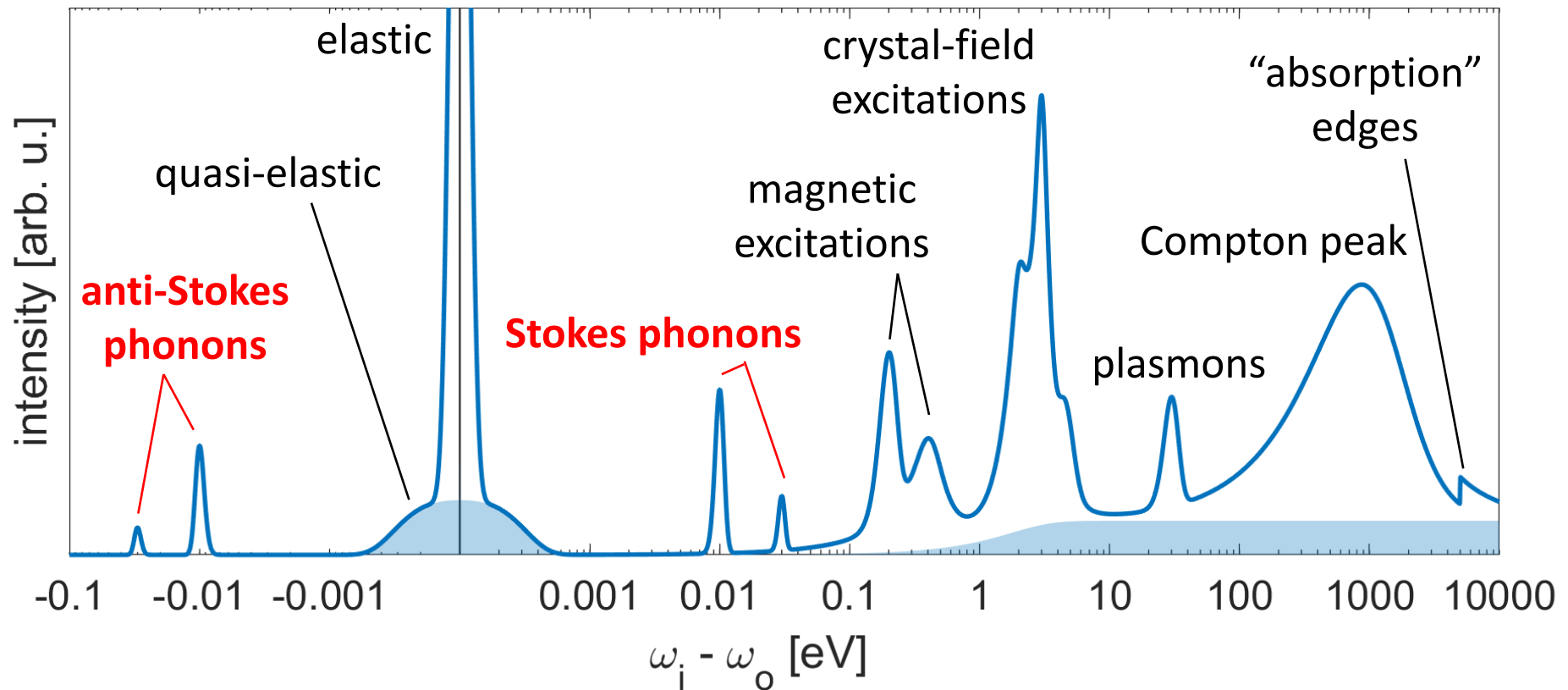
Spin-flip and magnetic excitations

Spin-flip transitions
propagate throughout the
lattice (magnons) :
pronounced $\mathbf{q}$ dependence



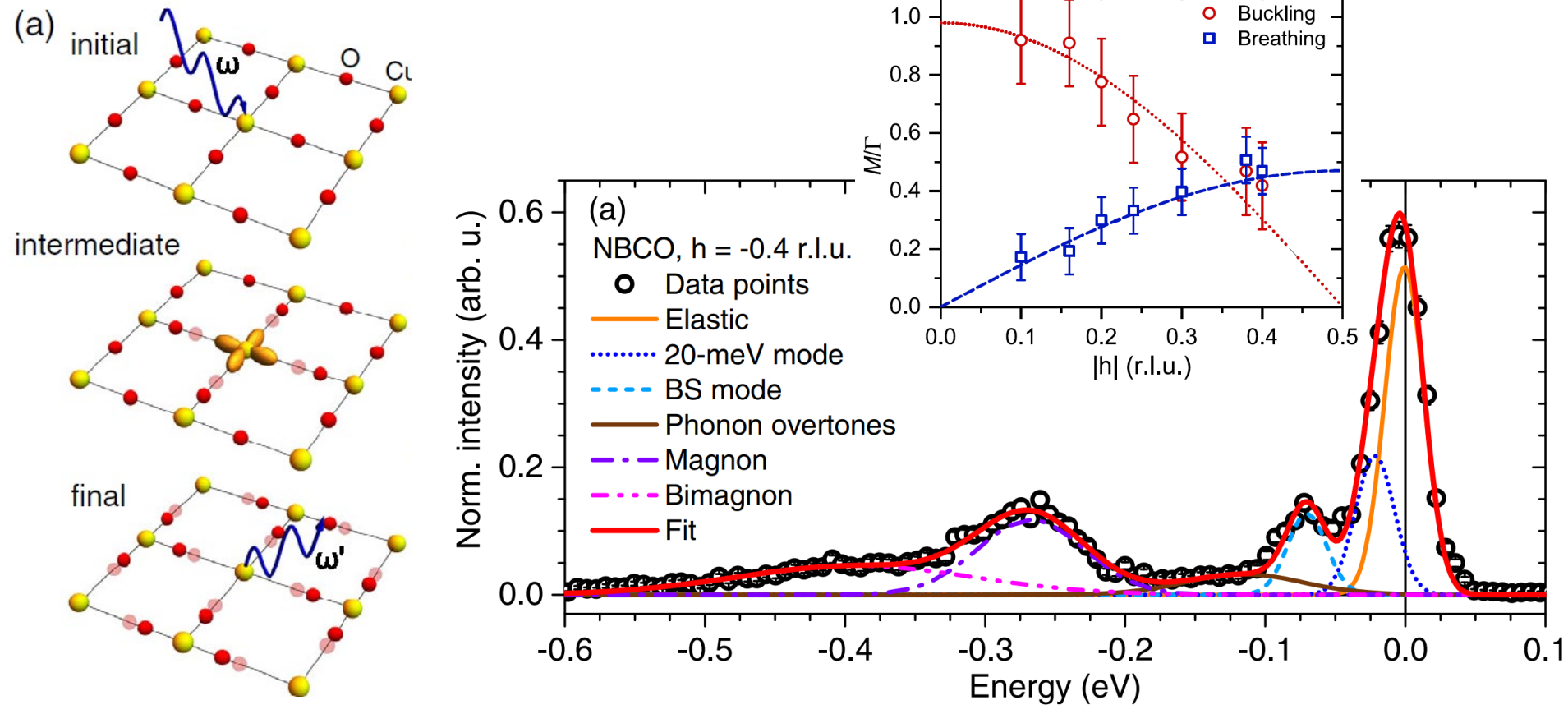
Resonant inelastic X-ray scattering

Resonant inelastic x-ray scattering of phonons



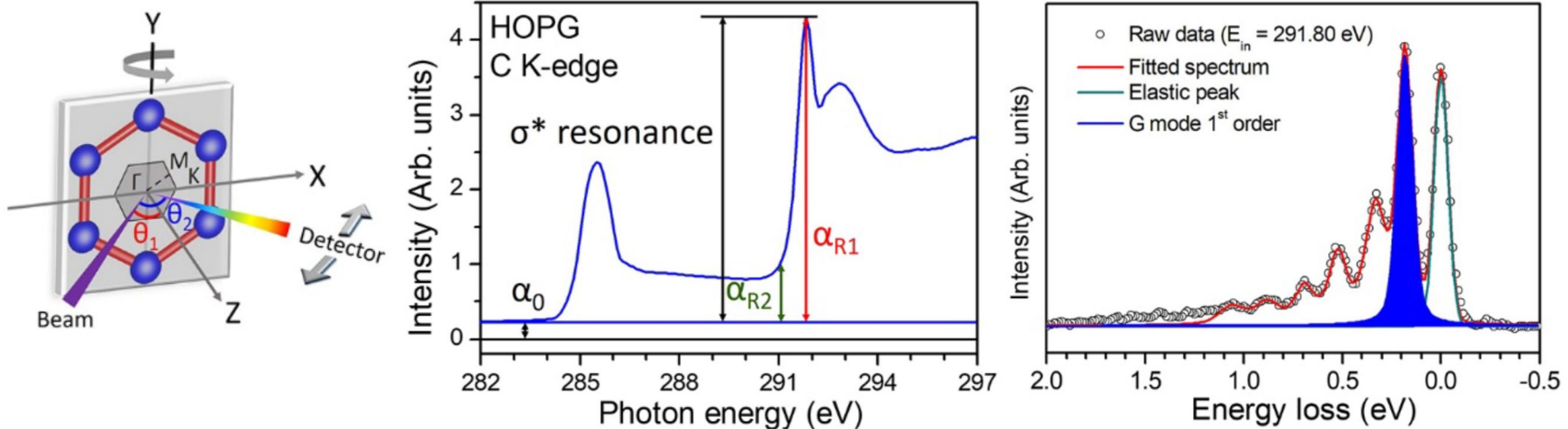
Resonant inelastic x-ray scattering of phonons

RIXS probes phonons through EPC



Resonant inelastic x-ray scattering of phonons

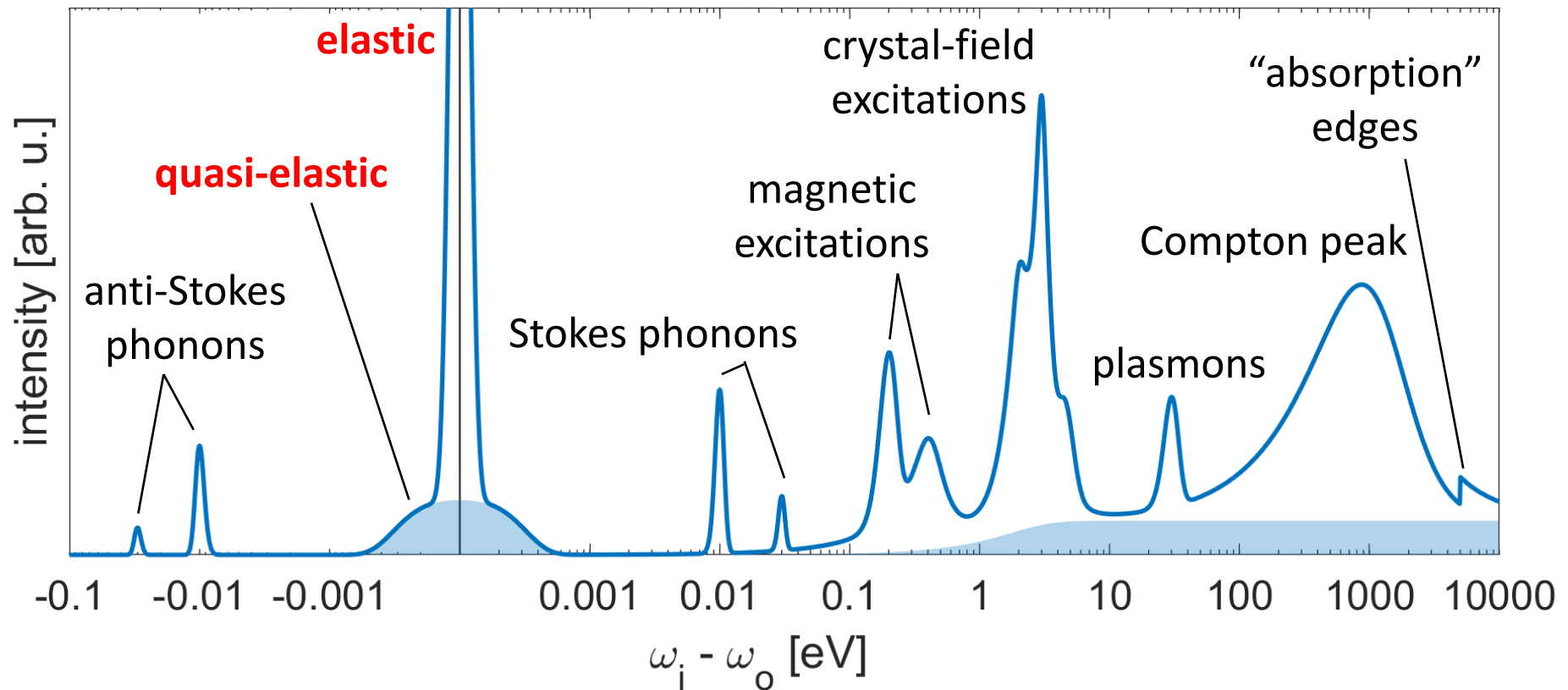
RIXS probes phonons through EPC, not only in cuprates



EPC strength $M_G = \sqrt{g\omega_0}$ of ~ 0.42 eV

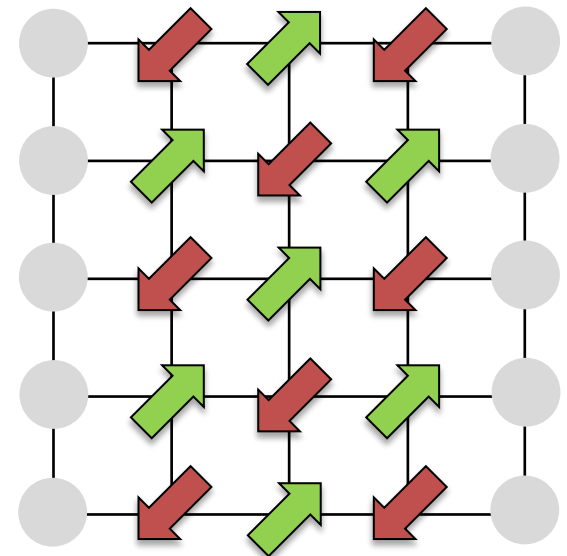
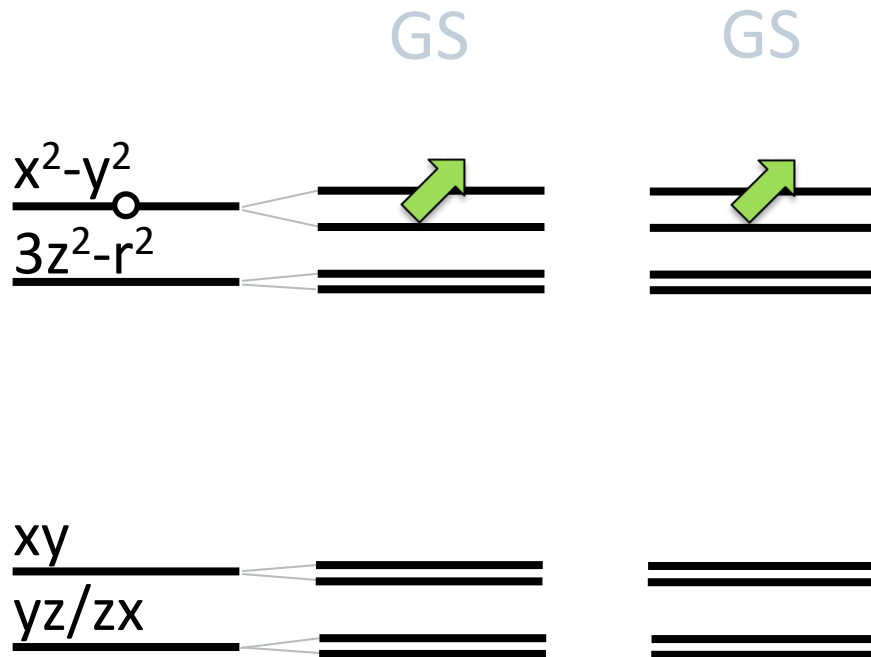
Resonant inelastic X-ray scattering

Resonant (quasi-)elastic x-ray scattering



Resonant (quasi-)elastic x-ray scattering

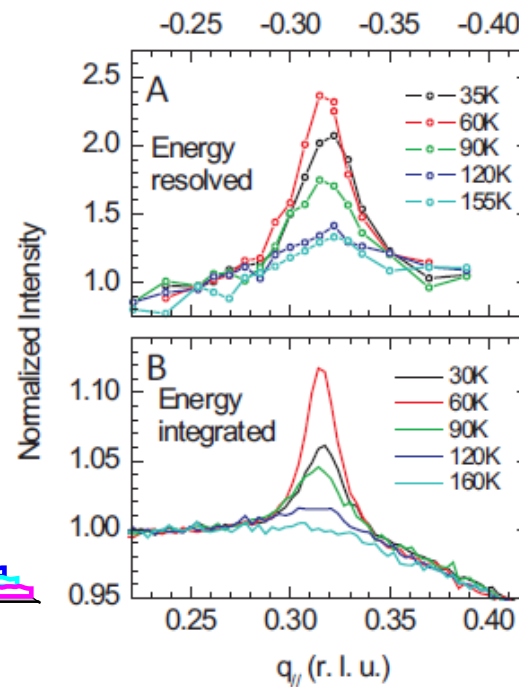
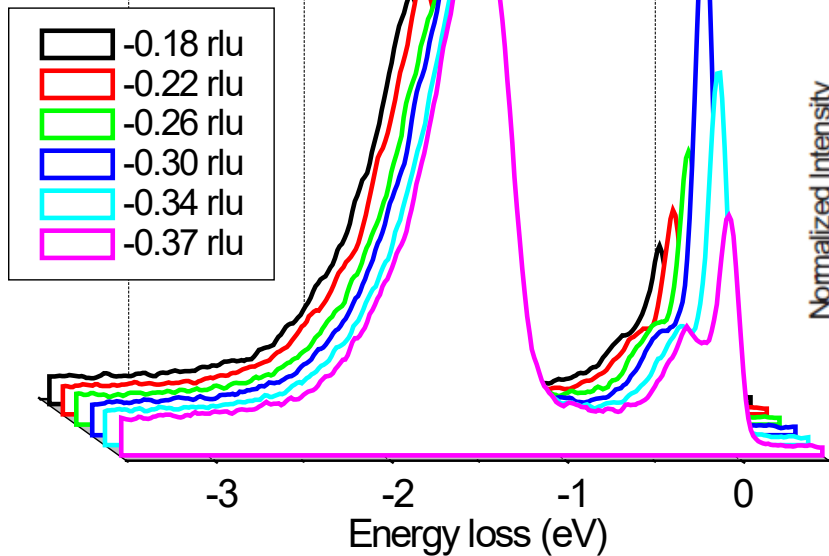
Diffraction from tiny (fraction of e) periodic modulations of charge density : mostly invisible to XRD



Resonant (quasi-)elastic x-ray scattering

Charge-order is ubiquitous in high T_c superconductors

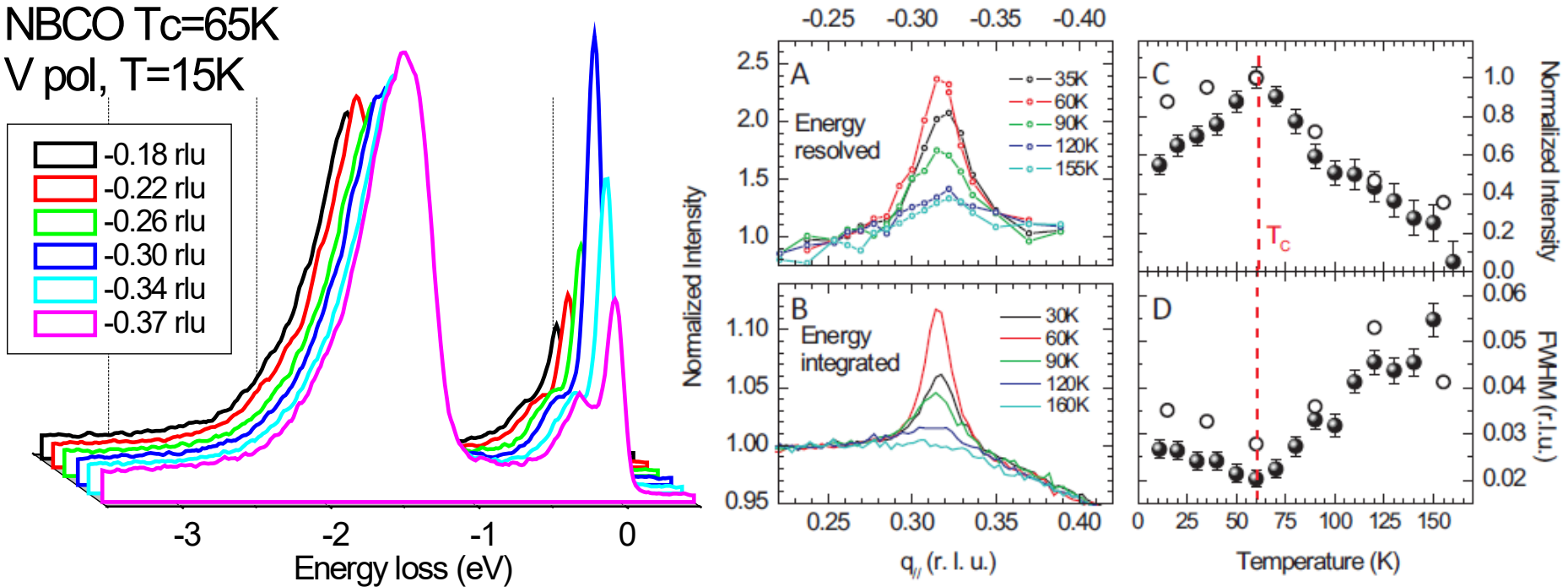
NBCO $T_c=65K$
V pol, $T=15K$



Resonant (quasi-)elastic x-ray scattering

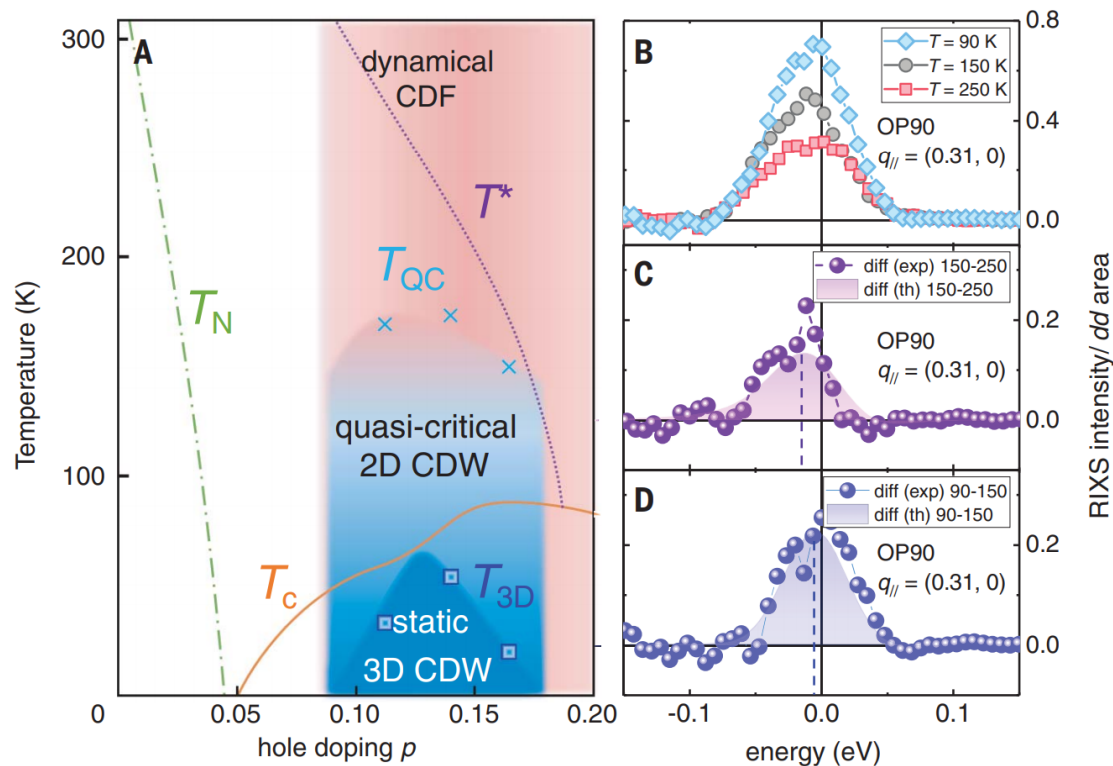
Charge-order is ubiquitous in high T_c superconductors and competes with SC

NBCO $T_c=65K$
V pol, $T=15K$



Resonant (quasi-)elastic x-ray scattering

CDF's pervade a large area of the phase diagram and are characterized by energies of a few milli-electron volts

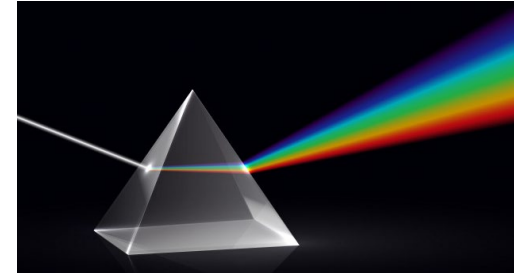


IXS instrumentation

IXS requirements

precise knowledge of ω_i and ω_o :
monochromator and spectrometer with
high resolving power

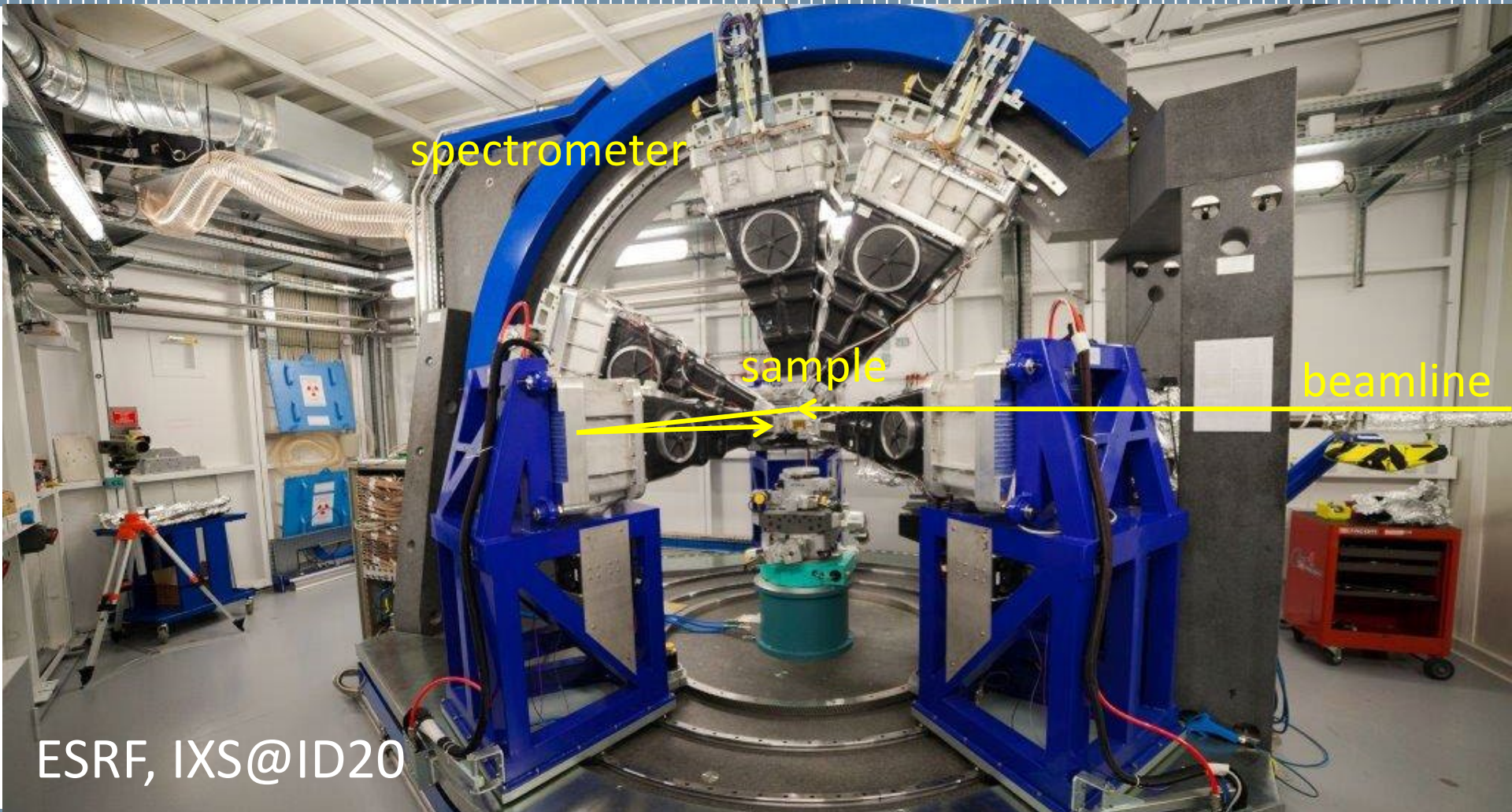
brilliant sources of polarized x-rays in a
small spot size



Soft x-rays : diffraction gratings, ultra-high vacuum

Hard x-rays : Bragg optics, better if vacuum

hard (N)IXS – XRS instrumentation



hard (N)IXS – XRS instrumentation

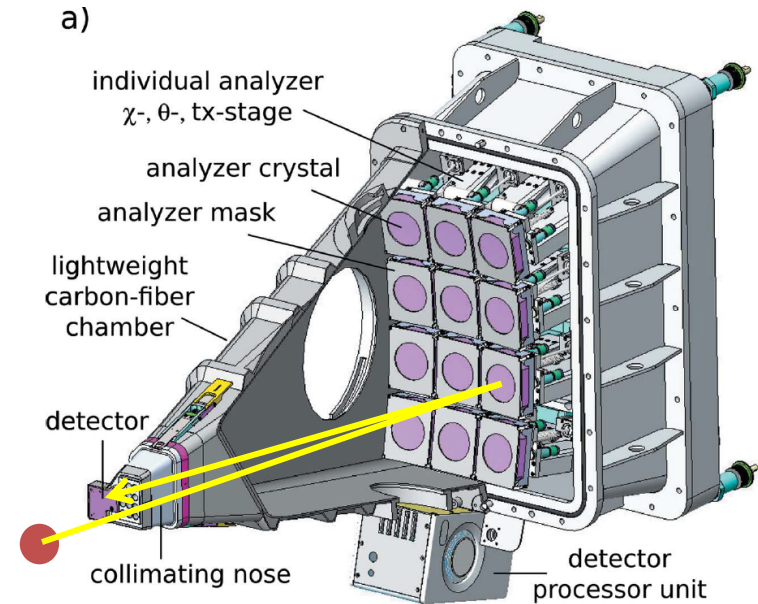


ESRF, IXS@ID20

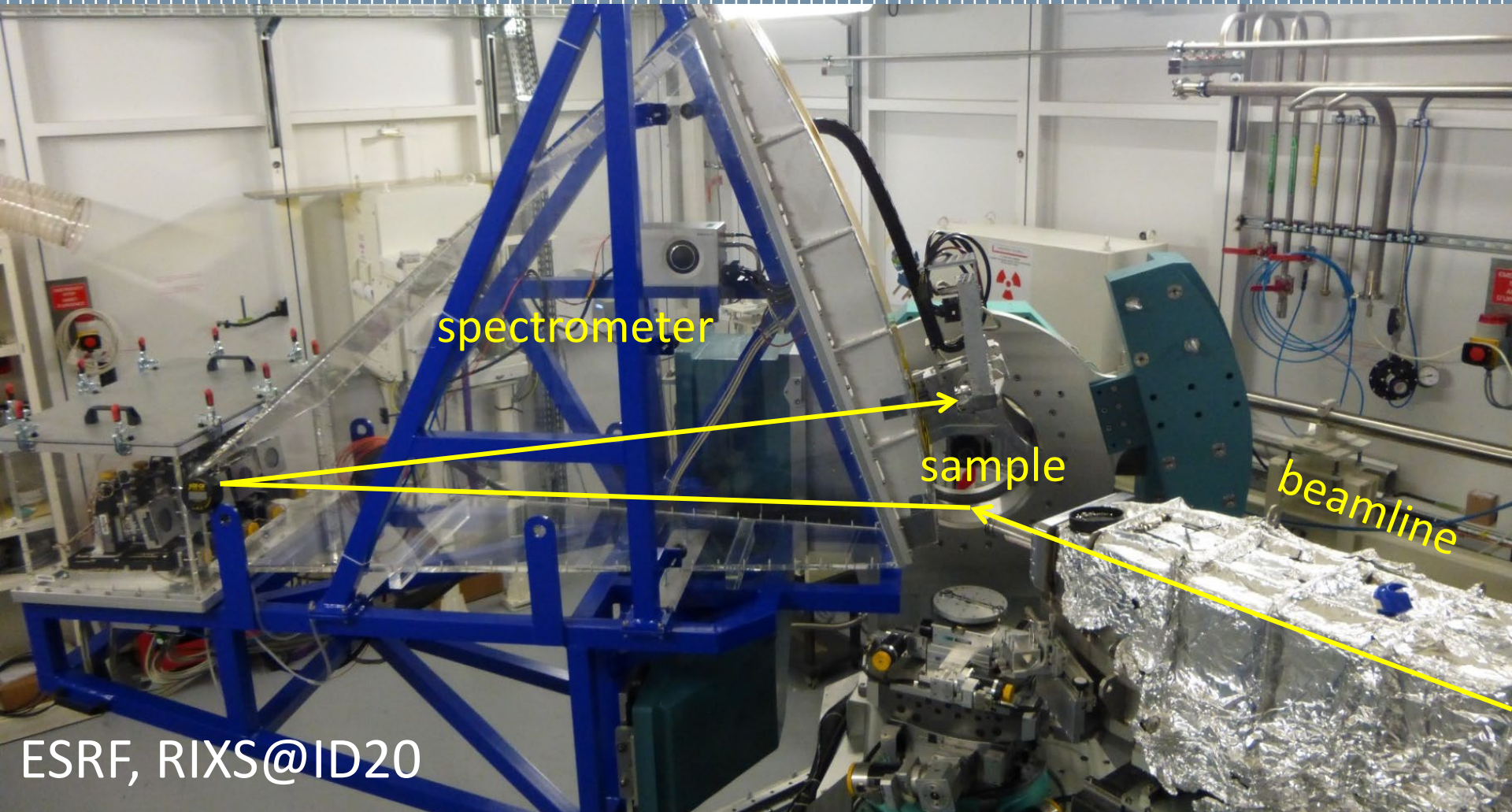
hard (N)IXS – XRS instrumentation

72 analysers at 1 m
0.4 – 1.8 eV energy resolution

Reflection	Energy (keV)	Si(111) + Si(311)	Calc.	Si(111)	Calc.
$2z = 75 \text{ mm}$					
Si(4,4,0)	6.46	0.32 ± 0.01	0.42	0.89 ± 0.01	0.79
Si(6,6,0)	9.69	0.65 ± 0.02	0.69	1.39 ± 0.02	1.21
Si(8,8,0)	12.92	1.15 ± 0.02	1.18	2.03 ± 0.01	1.77
Si(10,10,0)	16.15	1.72 ± 0.08	1.78	2.62 ± 0.02	2.43
$2z = 140 \text{ mm}$					
Si(4,4,0)	6.46	0.42 ± 0.02	0.51	0.90 ± 0.02	0.84
Si(6,6,0)	9.69	0.73 ± 0.03	0.84	1.49 ± 0.05	1.30
Si(8,8,0)	12.92	1.24 ± 0.03	1.31	2.08 ± 0.01	1.86
Si(10,10,0)	16.15	1.77 ± 0.10	1.92	2.70 ± 0.04	2.53

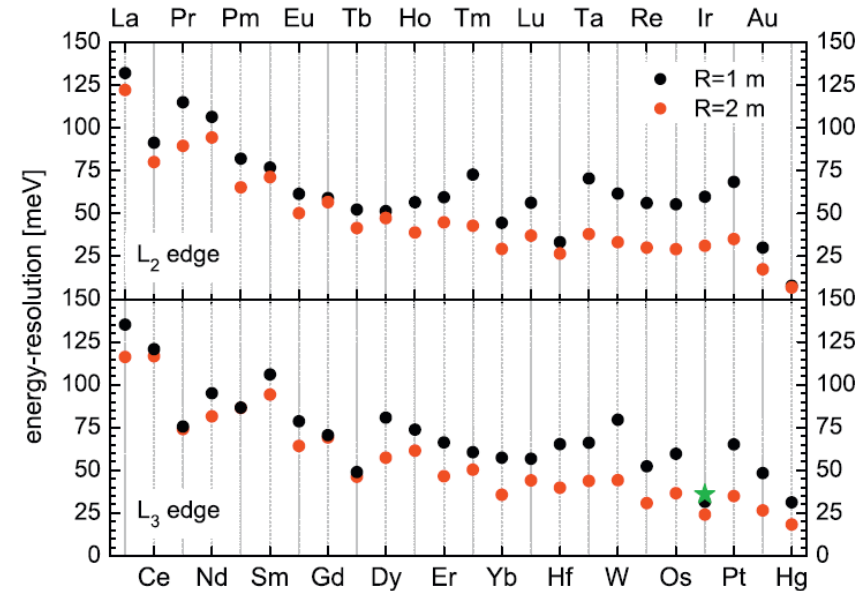
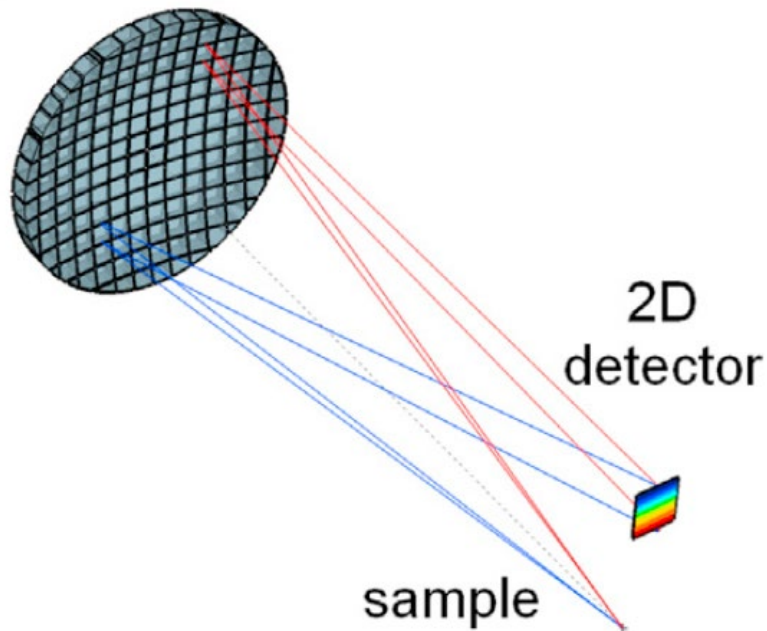


hard RIXS instrumentation



hard RIXS instrumentation

5 analysers at 1 or 2 m
20 – 100 meV energy resolution



high-resolution IXS instrumentation



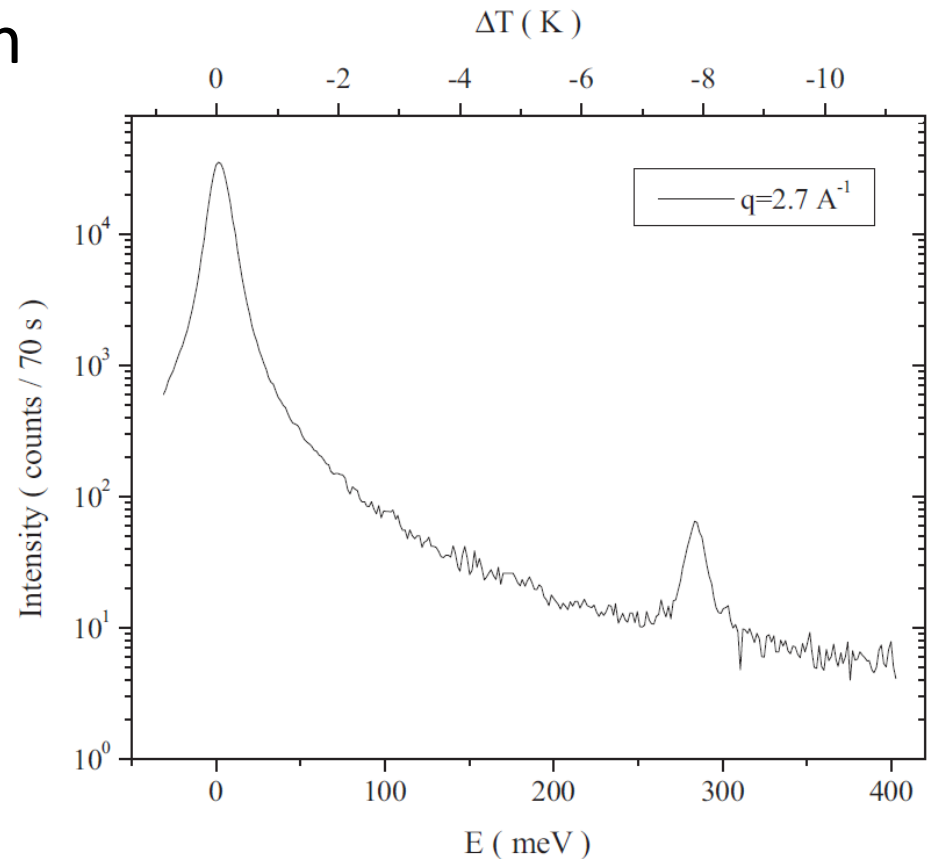
high-resolution IXS instrumentation

5 analysers at 7 or 12 m

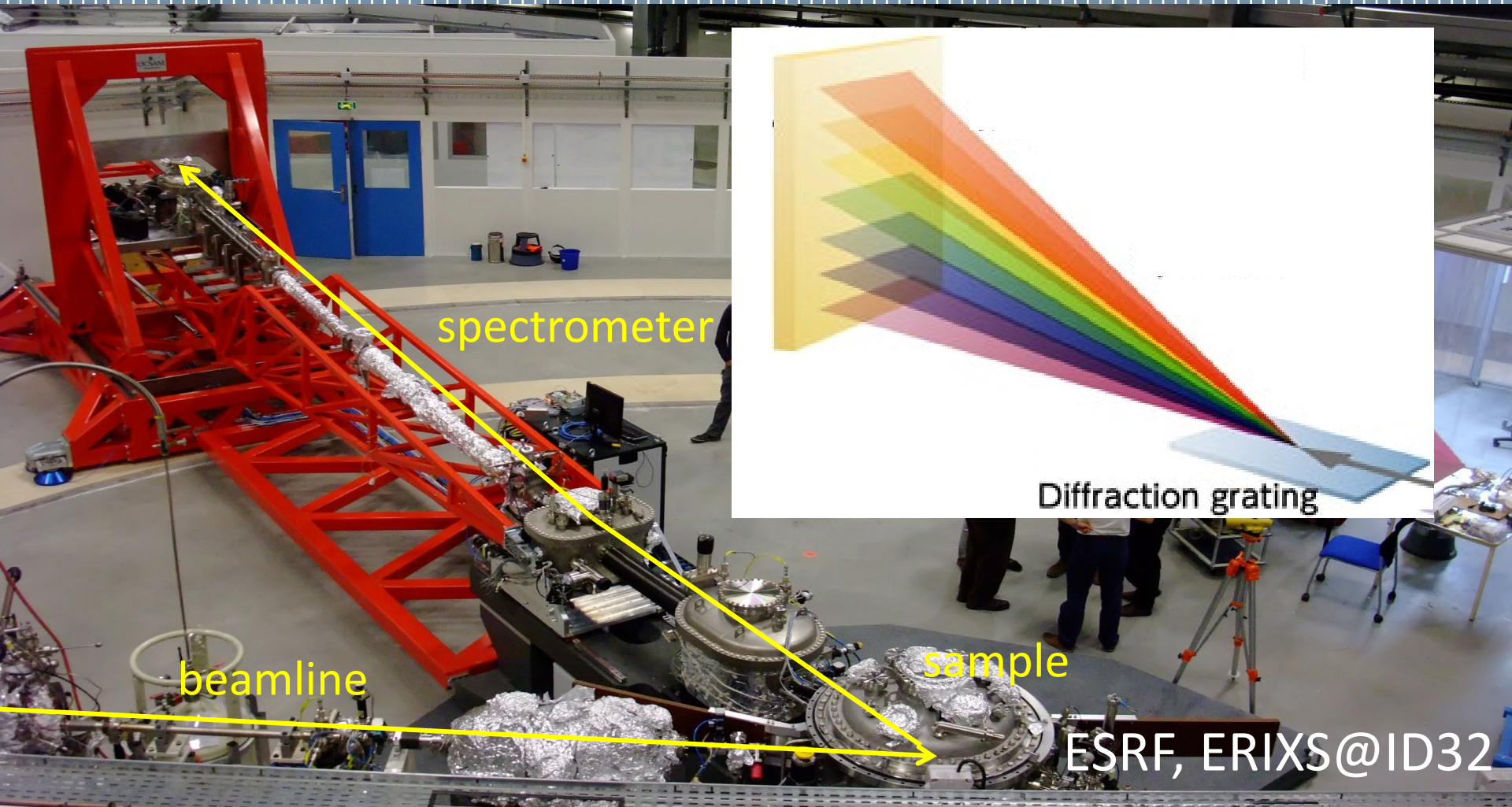
0.5 – 5 meV energy resolution

$$d(T) = d_0(1 + \alpha_0\Delta T + \beta/2\Delta T^2)$$

Reflection	Energy [keV]	δE [meV]
Si(7,7,7)	13.840	5.30
Si(8,8,8)	15.817	4.40
Si(9,9,9)	17.794	2.20
Si(11,11,11)	21.747	0.83
Si(12,12,12)	23.725	0.73
Si(13,13,13)	25.704	0.50



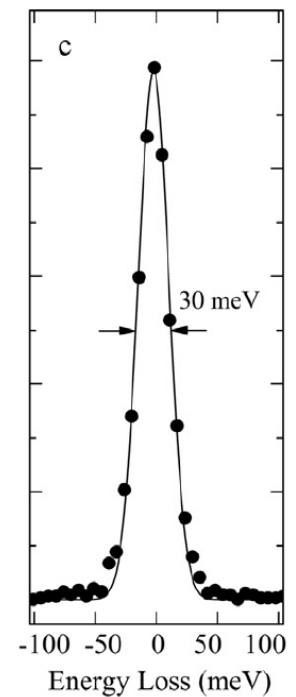
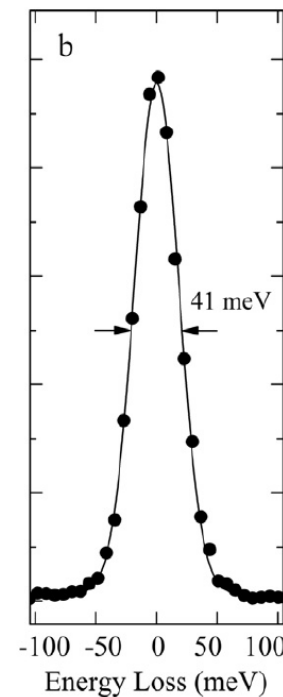
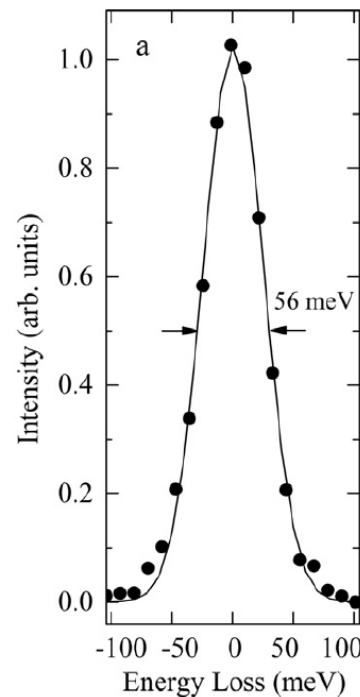
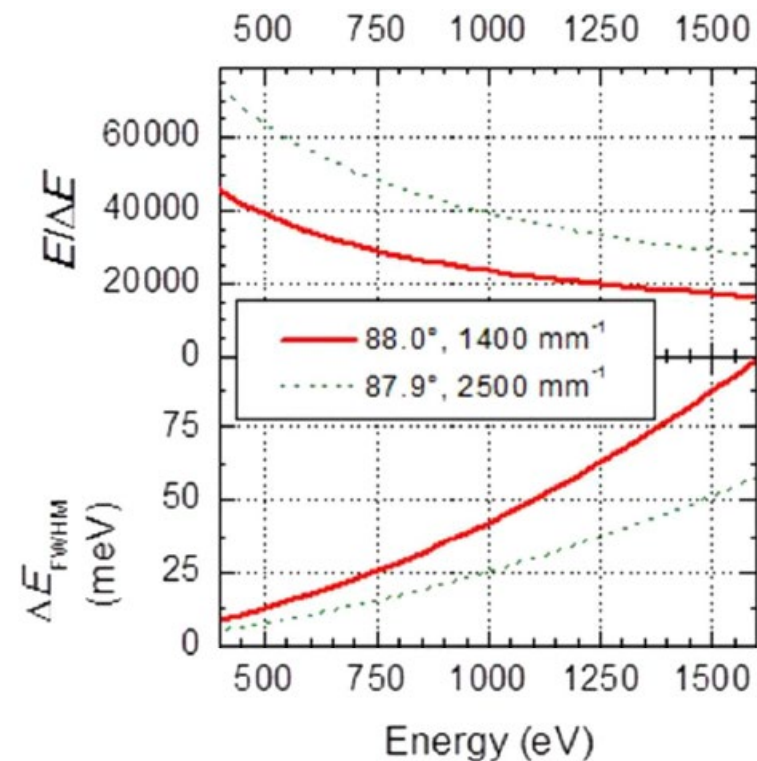
soft RIXS instrumentation



soft RIXS instrumentation

~10 m arm spectrometer

10 – 100 meV energy resolution



Why inelastic x-ray scattering?

Complex behavior of materials
due to interactions between
multiple degrees of freedom

Why inelastic x-ray scattering?

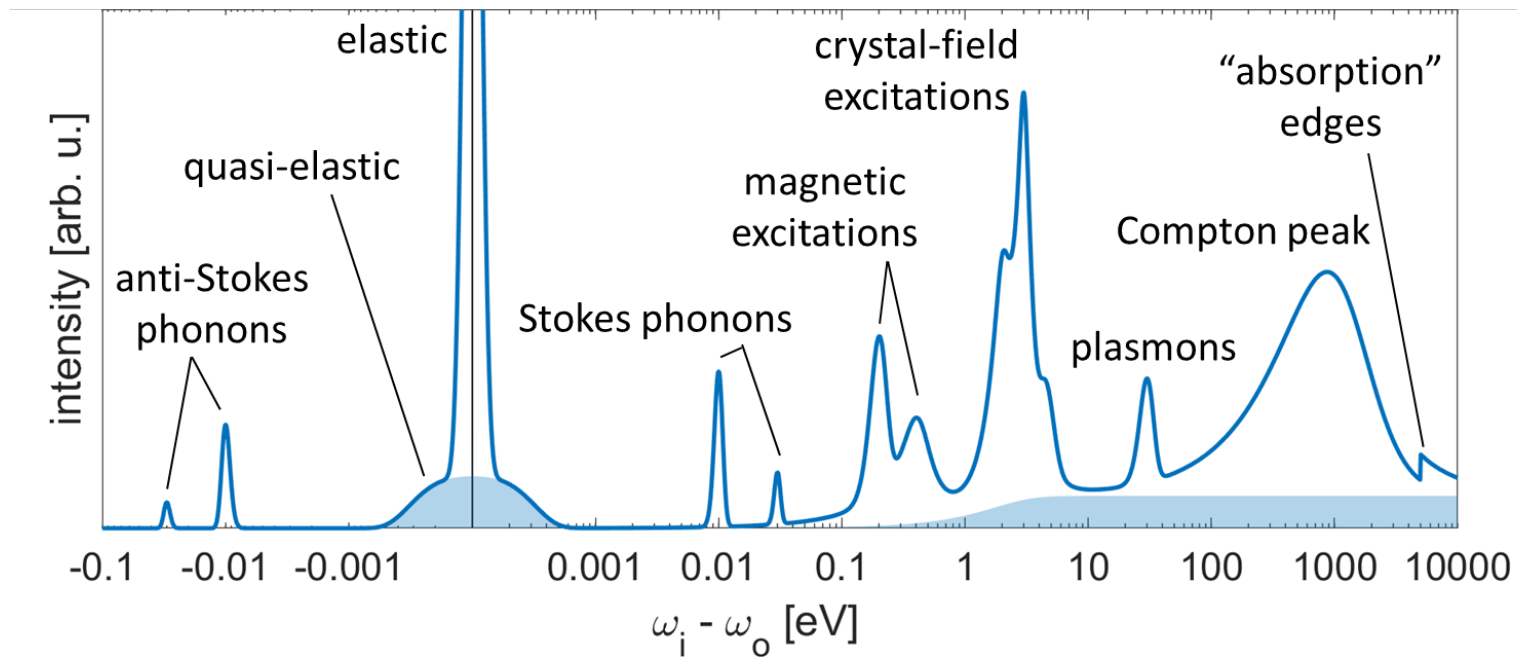
Complex behavior of materials
due to interactions between
multiple degrees of freedom

(R)IXS can probe them **all** with

- energy resolution
- linear (and angular)
momentum resolution
- (element and valence selectivity)
- bulk sensitivity

IXS in a nutshell

Excited states reflect **ground state** properties.



Inelastic x-ray scattering is an energy and momentum resolved probe of **excited states** of materials.