



**The Abdus Salam
International Centre for Theoretical Physics**



2221-7

Hands-on Tutorial on Electronic Structure Computations

17 - 21 January 2011

X-ray absorption

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XSPECTRA

A tool for X-ray absorption spectra (XAS) calculations

Matteo Calandra

/afs/ictp/public/shared/qetutorial/Matteo/References/Lectures_XAS.pdf

C. Gougoussis, M. Calandra, A. P. Seitsonen, and F. Mauri
Phys. Rev. B **80**, 075102 (2009)

P. Giannozzi et al., J. Phys. Condens. Matter **21**, 395502 (2009).



XSPECTRA (General questions)

What is it ?

XSPECTRA calculate K and L₁ X-ray absorption dipolar and quadrupolar cross sections in the pre-edge to near-edge region.

Where can I find XSPECTRA ?

XSPECTRA is distributed in the QUANTUM-ESPRESSO package.

Can I use it ?

XSPECTRA is distributed under the GNU licence, so you can use it for free. Please remember to cite the following papers to acknowledge people building the software:

P. Giannozzi et al., J. Phys. Condens. Matter **21**, 395502 (2009).

C. Gougoussis, M. Calandra, A. P. Seitsonen, and F. Mauri, Phys. Rev. B **80**, 075102 (2009)

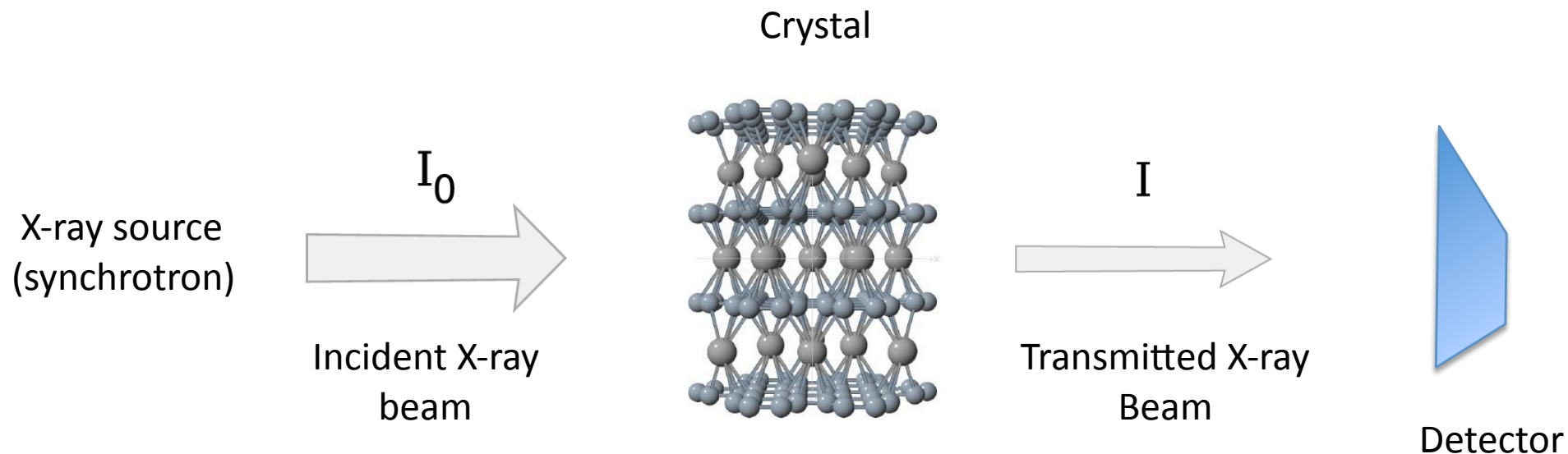
How does it work ?

This is what we will learn today...

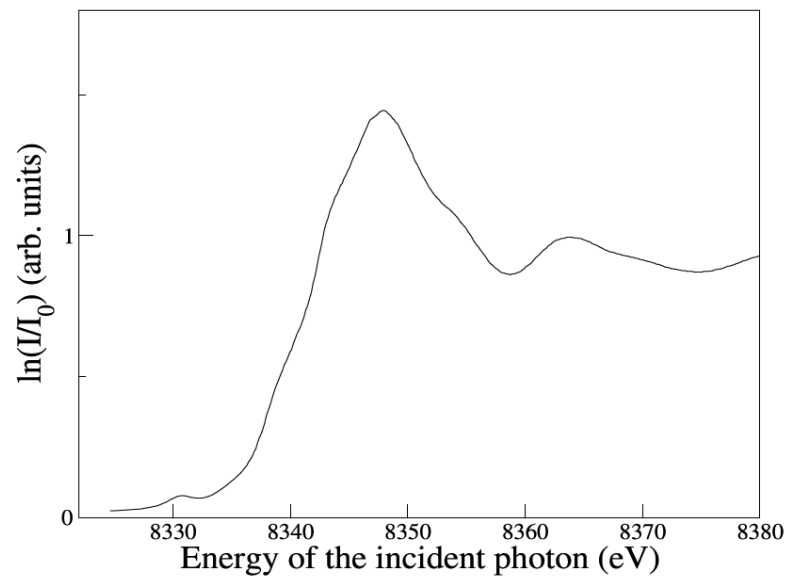
Outline

- XAS in a nutshell.
- XSPECTRA
 - ➔ Theory (PAW)
 - ➔ The Lanczos Method
 - ➔ Running XSPECTRA
- Tutorials
 - ➔ Diamond
 - ➔ SiO₂
- Conclusion

What is XAS ?



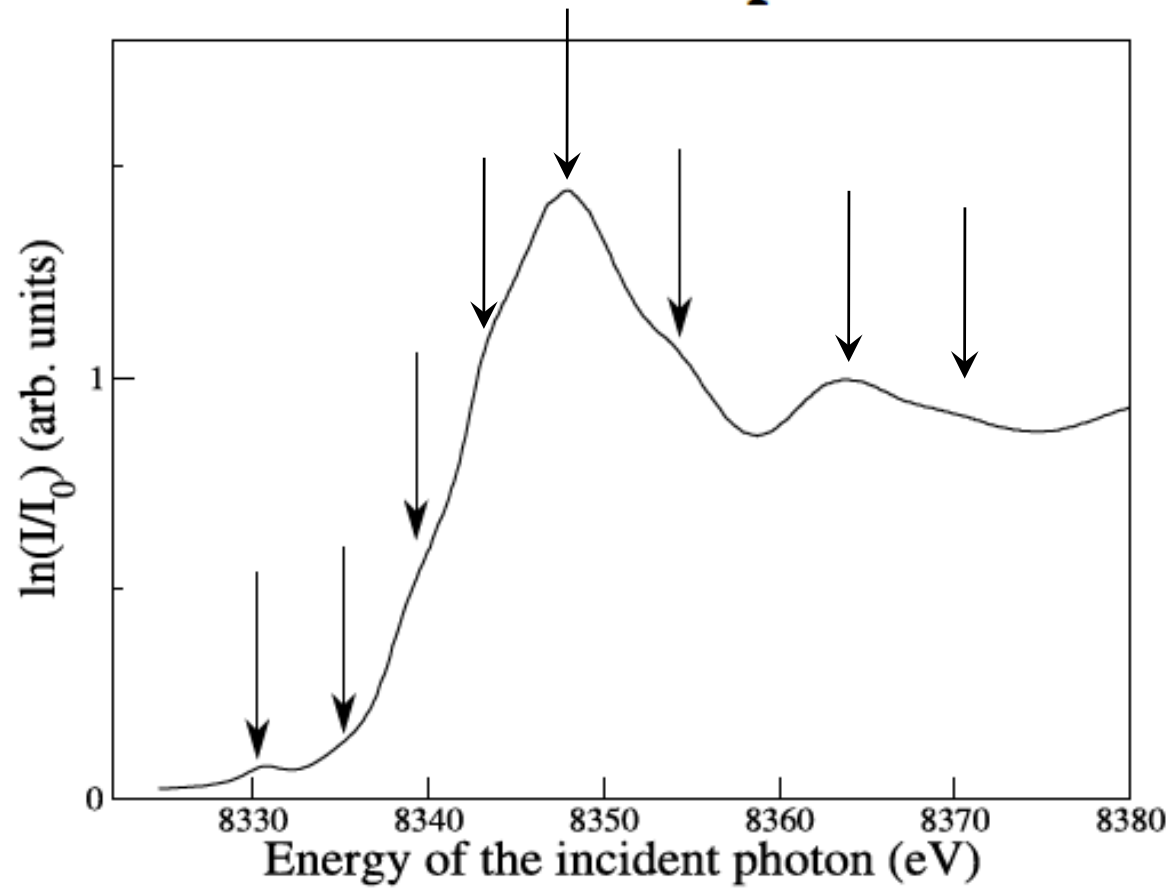
Result :



Ni K-edge XAS of NiO

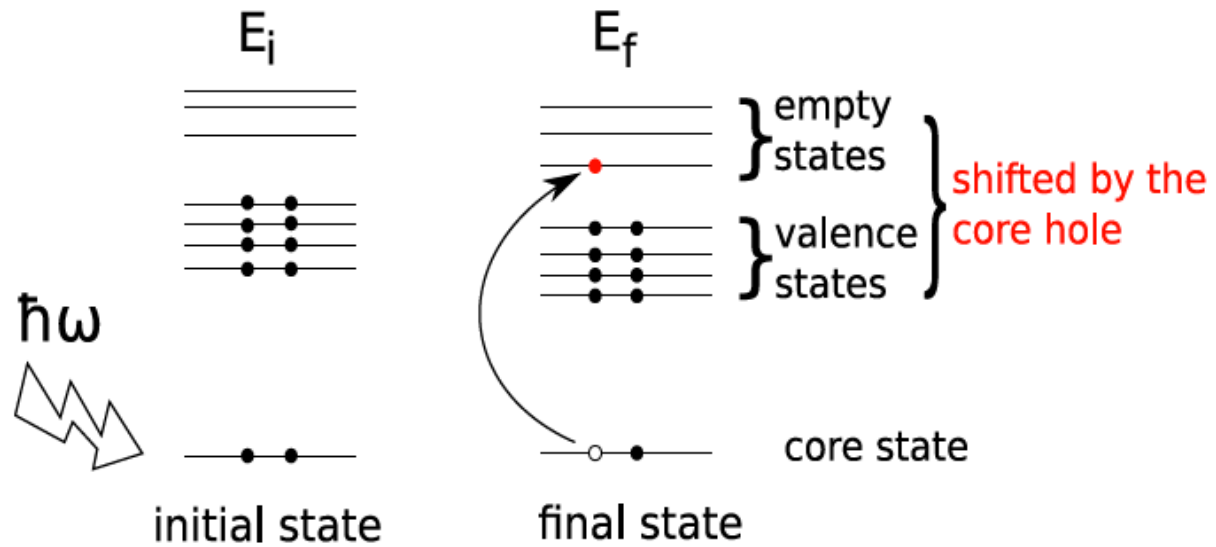
What is XAS ?

What are those peaks ?



XSPECTRA was built to answer this question.

XAS Physical process



Challenge: describe core-hole attraction from first principles.

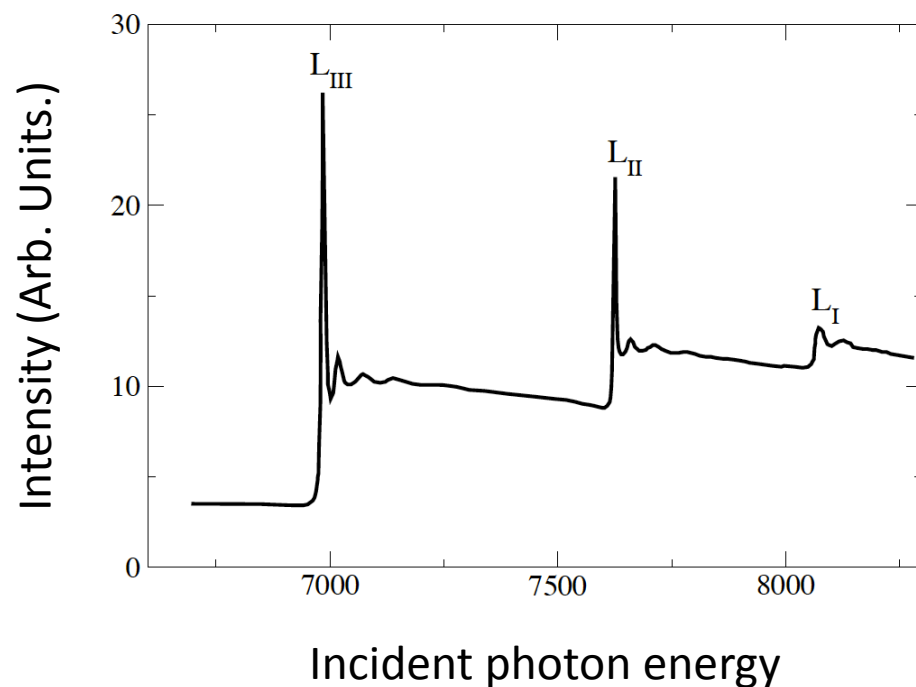
Chemical and Orbital selectivity

The choice of the incident photon energy selects the core electron excited.

It permits to choose

- (i) the atom from which the electron is excited (**absorbing atom**).
- (ii) the atomic level from which the electron is excited.

Example: Eu L_1 , L_2 , L_3 edges



Core state

Edge name

1s	K
2s	L_1
$2p_{1/2}$	L_2
$2p_{3/2}$	L_3
3s	M_1

Chemical and Orbital selectivity

The choice of the incident photon energy selects which core electron is excited.

Experimentalists are then free to choose:

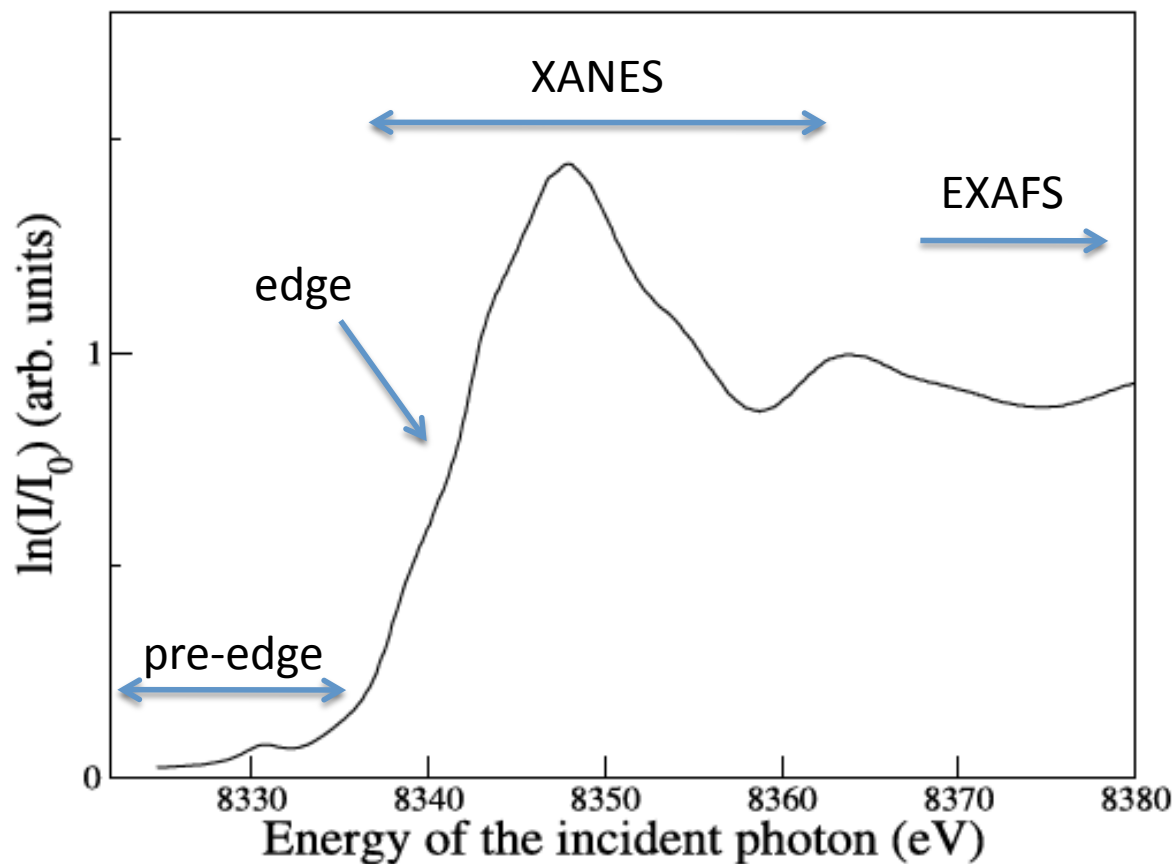
- (i) the atom from which the electron is excited (**absorbing atom**).
- (ii) the atomic level from which the electron is excited.

Note that core-state binding energies of atoms are very different:

Element	K 1s	L ₁ 2s	L ₂ 2p _{1/2}	L ₃ 2p _{3/2}	M ₁ 3s	M ₂ 3p _{1/2}	M ₃ 3p _{3/2}
1 H	13.6						
2 He	24.6*						
3 Li	54.7*						
4 Be	111.5*						
5 B	188*						
6 C	284.2*						
7 N	409.9*	37.3*					
8 O	543.1*	41.6*					
9 F	696.7*						
10 Ne	870.2*	48.5*	21.7*	21.6*			
11 Na	1070.8†	63.5†	30.65	30.81			
12 Mg	1303.0†	88.7	49.78	49.50			
13 Al	1559.6	117.8	72.95	72.55			
14 Si	1839	149.7*b	99.82	99.42			
15 P	2145.5	189*	136*	135*			
16 S	2472	230.9	163.6*	162.5*			
17 Cl	2822.4	270*	202*	200*			
18 Ar	3205.9*	326.3*	250.6†	248.4*	29.3*	15.9*	15.7*
19 K	3608.4*	378.6*	297.3*	294.6*	34.8*	18.3*	18.3*
20 Ca	4038.5*	438.4†	349.7†	346.2†	44.3 †	25.4†	25.4†
21 Sc	4492	498.0*	403.6*	398.7*	51.1*	28.3*	28.3*
22 Ti	4966	560.9†	460.2†	453.8†	58.7†	32.6†	32.6†

For more see <http://xdb.lbl.gov/>

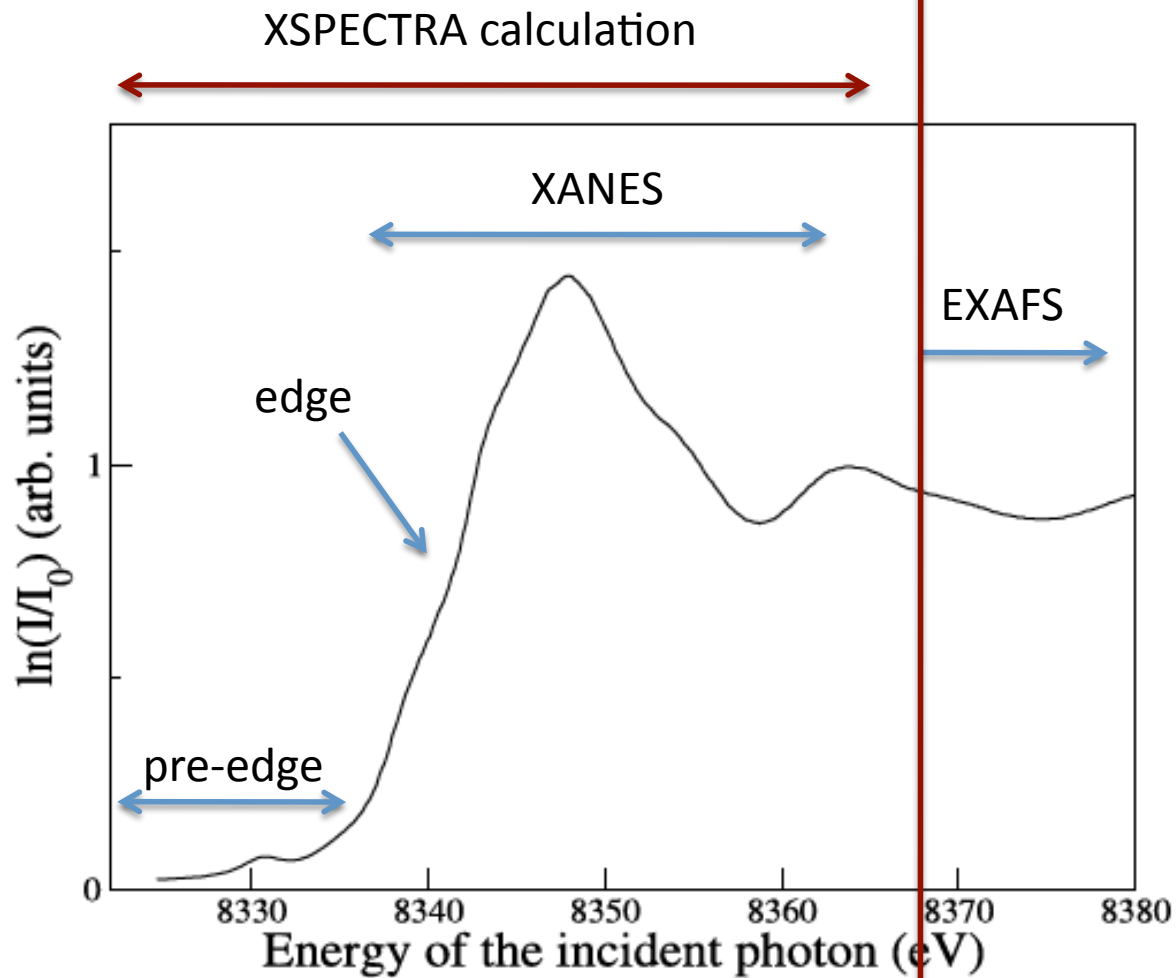
Name of XAS structures



XANES=X-ray near edge structures.

EXAFS=Extended X-Ray Absorption Fine Structure.

Name of XAS structures



XANES=X-ray near edge structures.

EXAFS=Extended X-Ray Absorption Fine Structure.

XAS cross section

From Fermi golden-rule:

$$\sigma(\hbar\omega) = 4\pi^2 \alpha \hbar\omega \sum_f |\langle f | \mathcal{O} | i \rangle|^2 \delta(E_f - E_i - \hbar\omega)$$

Final state with a core-hole Initial state: no core-hole Incident-photon energy

The matrix element is:

$$\mathcal{O} = \underbrace{\boldsymbol{\epsilon} \cdot \boldsymbol{r}}_{\text{electric dipole}} + \frac{i}{2} (\boldsymbol{k} \cdot \boldsymbol{r}) \underbrace{(\boldsymbol{\epsilon} \cdot \boldsymbol{r})}_{\text{electric quadrupole}}$$

1s \rightarrow p states 1s \rightarrow d states

See Ch. Brouder, J. Phys. Cond. Matt. **2**, 701 (1990) for more details.

XAS cross section

In the absence of a magnetic field the cross section can be separated in dipolar and quadrupolar terms (cross terms are zero in this case):

$$\sigma = \sigma_D + \sigma_Q$$

with:

$$\sigma_D = 4\pi^2\alpha\hbar\omega \sum_f \left| \langle f | \sum_j \boldsymbol{\epsilon} \cdot \mathbf{r}_j | i \rangle \right|^2 \delta(E_f - E_i - \hbar\omega)$$

$$\sigma_Q = 4\pi^2\alpha\hbar\omega \sum_f \left| \langle f | \frac{1}{2} \sum_j (\boldsymbol{\epsilon} \cdot \mathbf{r}_j)(\mathbf{k} \cdot \mathbf{r}_j) | i \rangle \right|^2 \delta(E_f - E_i - \hbar\omega)$$

and the two terms can be calculated separately.

The quadrupolar part is in the pre-edge region.

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XAS cross section needs all-electron states

$$\sigma(\hbar\omega) = 4\pi^2 \alpha \hbar\omega \sum_f |\langle f | \mathcal{O} | i \rangle|^2 \delta(E_f - E_i - \hbar\omega)$$

Final state with a core-hole Initial state: no core-hole Incident-photon energy

ALL ELECTRON STATES

However we have pseudopotentials and we do not have all-electron states!

How to solve this problem ?

Use the projected augmented wave (PAW) method!

P. E. Blöchl, Phys. Rev. B **50**, 17953 (1994)

PAW for XAS – short explanation

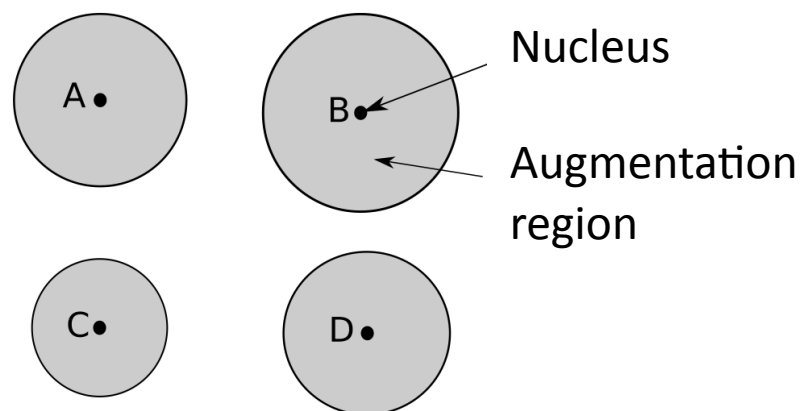
As we use pseudopotentials, the electron wavefunction that we obtain in our simulation is different from the all-electron wavefunction:



Assume that a linear mapping exists between the two wavefunctions:

$$|\psi\rangle = \mathcal{T}|\tilde{\psi}\rangle$$

As the pseudowavefunction differs from the AE one only in the augmentation region (core region) then the mapping operator is different from the identity only in the augmentation region.



PAW for XAS – short explanation

The mapping is written as:

$$\mathcal{T} = 1 + \sum_{\mathbf{R}} \mathcal{T}_{\mathbf{R}}$$

\mathbf{R} = coordinates of the nuclei

with

$$\mathcal{T} = \mathbf{1} + \sum_{\mathbf{R},n} \left(|\phi_{\mathbf{R},n}\rangle - |\tilde{\phi}_{\mathbf{R},n}\rangle \right) \langle \tilde{p}_{\mathbf{R},n}|$$

AE PARTIAL WAVES
(e.g. AE atomic wavefunctions)

PSEUDO PARTIAL WAVES
(e.g. atomic pseudo Wavefunctions)

PAW Projectors
identified by the condition
 $\langle \tilde{p}_{\mathbf{R},n} | \tilde{\phi}_{\mathbf{R}',n'} \rangle = \delta_{\mathbf{R}\mathbf{R}'} \delta_{nn'}$
The projectors are non-zero only in the augmentation region.

PAW for XAS – short explanation

Replacing $|\psi_f\rangle = \tau|\tilde{\psi}_f\rangle$ in the XAS cross section and using the localization of the core state we obtain

$$\sigma(\omega) = 4\pi^2\alpha_0\hbar\omega \sum_f \left| \langle \tilde{\psi}_f | \tilde{\phi}_{\mathbf{R}_0} \rangle \right|^2 \delta(E_f - E_i - \hbar\omega)$$

where

$$|\tilde{\phi}_{\mathbf{R}_0}\rangle = \sum_n |\tilde{p}_{\mathbf{R}_0,n}\rangle \langle \phi_{\mathbf{R}_0,n} | O | \psi_i \rangle \quad \text{and} \quad O = \boldsymbol{\epsilon} \cdot \mathbf{r} + \frac{i}{2}(\mathbf{k} \cdot \mathbf{r})(\boldsymbol{\epsilon} \cdot \mathbf{r})$$

and \mathbf{R}_0 is the position of the absorbing atom.

Thus in order to calculate the matrix-element one needs:

- .1. ψ_i = The core wavefunction of the absorbing atom (e. g. 1s state for K-edge)
WITHOUT A CORE-HOLE.
- .2. ϕ = The AE partial waves centered on the absorbing atom (e.g. AE atomic states)
- .3. PAW projectors.

PAW for XAS – short explanation

WARNING: The sum

$$|\tilde{\phi}_{\mathbf{R}_0}\rangle = \sum_n |\tilde{p}_{\mathbf{R}_0,n}\rangle \langle \phi_{\mathbf{R}_0,n} | O | \psi_i \rangle$$

is actually over a complete set (infinite number) of projector (unfeasible).

In practice we have to reduce the number of projectors to a finite number.

You need two projectors per channel (i.e. per angular momentum l) in order to have correct XAS intensity up to ~ 50 eV from the Fermi level.

Use of a single projector gives incorrect dipole/quadrupole ration and in most of the case gives wrong intensities.

Projectors have to be linearly independent, namely they must really span a dimension 2 subspace.

XSPECTRA (The lanczos method)

In the XAS cross-section you need to perform a sum over all empty states

$$\sigma(\omega) = 4\pi^2 \alpha_0 \hbar \omega \sum_f \left| \langle \tilde{\psi}_f | \tilde{\varphi}_{\mathbf{R}_0} \rangle \right|^2 \delta(E_f - E_i - \hbar\omega)$$

This is of course very demanding if done in a brute-force way.

XSPECTRA use the lanczos method. Rewriting:

$$\sigma(\omega) = 4\pi^2 \alpha_0 \hbar \omega \operatorname{Im} \langle \tilde{\varphi}_{\mathbf{R}_0} | (E_i + \hbar\omega - H + i\gamma)^{-1} | \tilde{\varphi}_{\mathbf{R}_0} \rangle$$

And this can be computed using the Lanczos method and the continuous fraction.

Thus in the XSPECTRA input we will have to specify:

xniter=Maximal number of iteration to be used in the lanczos method.

xerror=Convergence threshold for the Lanczos method (On the integral of the XAS cross section).

xcheck_conv=Number of iteration between two convergence checks.

xgamma=Lorentzian broadening (core-hole linewidth)

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Before going on...

1. Login
2. `cd /scratch/`
3. Create a directory with your name: `mkdir yourname`
4. `cp /afs/ictp/public/shared/qetutorial/Matteo/ /scratch/yourname/`

Directory structure

Subdirectory ./Binaries/

Here all the Binaries needed to run xspectra are included.
PLEASE USE THESE BINARIES.

Subdirectory ./Gipaw_Pseudo_Generation/

Here all the input files necessary to generate GIPAW pseudopotentials with and without a core-hole are included.

Subdirectory ./Diamond/ /Diamond_nohole/ /SiO2/

Examples and exercises.

Subdirectory ./References/

Relevant papers with fully converged results and these lectures.

Running XSPECTRA

1

Prepare GIPAW pseudo
and supercell scf input file

2

`./pw.x < prefix.scf.in > prefix.scf.out`

3

Generate core state of the
absorbing atom (`upf2plotcore.sh`)

4

`./xspectra.x < prefix.xspectra.in > prefix.xspectra.out`

(GI)PAW – what do we need ?

- .1. ψ_i = The core wavefunction of the absorbing atom (e. g. 1s state for K-edge)
WITHOUT A CORE-HOLE
- .2. ϕ = The AE partial waves centered on the absorbing atom (e.g. AE atomic states)
- .3. Blochl projectors.

All these quantities can be calculated from the atomic code as they involve only the solution for an isolated atom.

These informations are contained in (GI)PAW pseudopotentials.

A GIPAW pseudopotential is needed only for the absorbing atom,
for the other atomic species use any other pseudopotential available

Now we see how to generate them in the case of Carbon.

Generation of (GI)PAW pseudopotentials

We generate a pseudopotential to study dipolar K-edge XAS transition in diamond,

$$1s \rightarrow p \text{ empty states}$$

so we need to generate a pseudopotential with two p projectors. As an exercise (even if not needed) we also include two s projectors.

We choose to generate the projectors as follows:

Projector channel	Energy first projector	Energy second projector
s	2s state	3s state
p	2p state	3p state

Generation of (GI)PAW pseudopotentials

[C]=1s² 2s² 2p²

File ./Gipaw_Pseudo_Generation/C/C.ld1.in

NO CORE-HOLE

```
&input  
  title='Ch',  
  prefix='Ch',  
  zed=6.0,
```

Carbon nuclear charge is of course unchanged.

```
  config='1s2 2s2 2p1.5 3s0 3p0 ',  
  iswitch=3,  
  dft='PBE',  
  rel=1,  
/  
....
```

As we want to generate projectors at the energies of 2s,3s,2p and 3p states we need to put these states here.
To bind these states we have to ionize a bit, namely 1s² 2s² 2p^{1.5}

iswitch=3, means: generation of a pseudopotential

Generation of (GI)PAW pseudopotentials

[C]=1s2 2s2 2p2

File ./Gipaw_Pseudo_Generation/C_Hole/Ch.Id1.in

WITH CORE-HOLE

```
&input  
  title='Ch',  
  prefix='Ch',  
  zed=6.0,
```

Carbon nuclear charge is
of course unchanged.

```
  config='1s1 2s2 2p1.5 3s0 3p0 ',  
  iswitch=3,  
  dft='PBE',  
  rel=1,
```

Core-hole

As we want to generate projectors
at the energies of 2s,3s,2p and 3p
states we need to put these states
here.

```
/  
....
```

iswitch=3, means: generation of a pseudopotential

Generation of (GI)PAW pseudopotentials

File ./Gipaw_Pseudo_Generation/C_Hole/Ch.Id1.in

```
&inputp
  pseudotype=2,
  lloc=1,
  file_pseudopw=' C.star1s-pbe-mt_gipaw.UPF',
  tm=.true.,
  lgipaw_reconstruction=.true.,
```

This flag is needed to insert (GI)PAW reconstruction information.

```
/
2
```

```
2S 1 0 2.00 0.00 1.5 1.5
2P 2 1 1.50 0.00 1.5 1.5
```

Standard valence states configuration for Carbon pseudopotential generation

```
&test
```

```
/
```

```
4
```

Total number of PAW projectors

```
2S 1 0 2.00 0.00 1.5 1.5
3S 2 0 0.00 0.00 1.5 1.5
2P 2 1 1.50 0.00 1.5 1.5
3P 3 1 0.00 0.00 1.5 1.5
```

Projectors

Generation of (GI)PAW pseudopotentials

Then performing

```
./ld1.x < Ch.ld1.in > Ch.ld1.out
```

generate the pseudopotential

C.star1s-pbe-mt_gipaw.UPF

of the QE-XSPECTRA distribution.

Inside the pseudo all the informations needed to perform an XSPECTRA calculation are contained.

Pseudopotential name notation

Pseudopotentials including (GI)PAW informations are already available in the QUANTUM-ESPRESSO pseudopotential table, for example:

Ni.star1s-pbe-sp-mt_gipaw.UPF

starNs means a core-hole in the s state with principal quantum number N.

PBE is the exchange-correlation functional used

gipaw means that gipaw informations are included in the absorbing atom.

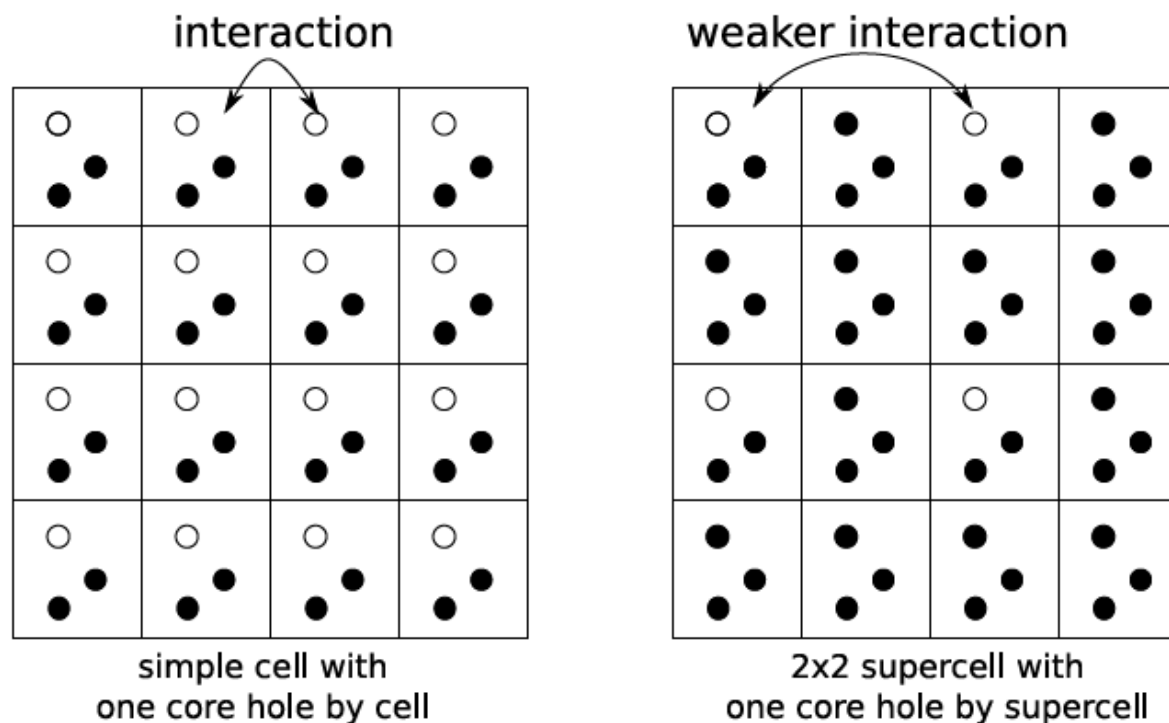
XSPECTRA (Modeling the core hole)

After generation of the core-hole pseudopotential, build your structure with your pseudopotential starNs gipaw in the absorbing atom position.

As we work with pbc we also need to build a supercell to minimize the interaction between the core-hole and its periodic image

Supercell calculations

○ atom with a core hole
● atom without core hole



XSPECTRA (Modeling the core hole)

After generation of the core-hole pseudopotential, build your structure with your pseudopotential starNs gipaw in the absorbing atom position.

As we work with pbc we also need to build a supercell to minimize the interaction between the core-hole and its periodic image

How big must the supercell be ?

Perform different calculations for different supercells and see when the result converges.

Rule of thumb: usually you need at least 6-7 Angstrom distance between the core-hole and its periodic image.

Running XSPECTRA

1

Prepare GIPAW pseudo
and supercell scf input file



2

```
./pw.x < prefix.scf.in > prefix.scf.out
```

3

Generate core state of the
absorbing atom (`upf2plotcore.sh`)

4

```
./xspectra.x < prefix.xspectra.in > prefix.xspectra.out
```

Step 2 – electronic density generation

Dir: ./Diamond/
file: diamond.scf.in

```
&control  
  calculation='scf',  
  pseudo_dir = '$PSEUDO_DIR/',  
  outdir='$TMP_DIR/',  
  prefix='diamondh',  
/
```

SCF calculation to obtain the
electronic charge density

```
&system  
 ibrav = 1,  
 celldm(1) = 6.740256,  
 nat=8,  
 ntyp=2,  
 nbnd=16,  
 tot_charge=+1.0,  
 ecutwfc=40.0,  
/
```

8 atoms supercell. Note ntyp=2
as the absorbing atom **MUST**
be considered different from the
other atomic types.

```
&electrons  
/  
ATOMIC_SPECIES
```

Needs to be specified when a
core-hole is present to compensate
for the additional electron in
empty states.

....

Step 2 – electronic density generation

```
Dir: ./Diamond/  
file: diamond.scf.in
```

```
...  
&electrons  
/  
ATOMIC_SPECIES  
Ch 12.0 Ch_PBE_TM_2pj.UPF  
C 12.0 C_PBE_TM_2pj.UPF  
ATOMIC_POSITIONS crystal  
Ch 0.0 0.0 0.0  
C 0.0 0.5 0.5  
C 0.5 0.0 0.5  
C 0.5 0.5 0.0  
C 0.75 0.75 0.25  
C 0.75 0.25 0.75  
C 0.25 0.75 0.75  
C 0.25 0.25 0.25  
K_POINTS automatic  
4 4 4 0 0 0
```

Pseudopotential for all atom types.
Ch = Carbon with core-hole.

Atomic positions of the
too small supercell.

Running XSPECTRA (more details)

1

Prepare GIPAW pseudo
and supercell scf input file



2

`./pw.x < prefix.scf.in > prefix.scf.out`



3

Generate core state of the
absorbing atom (`upf2plotcore.sh`)

4

`./xspectra.x < prefix.xspectra.in > prefix.xspectra.out`

Extracting the core-wavefunction

$$\sigma(\hbar\omega) = 4\pi^2 \alpha \hbar\omega \sum_f |\langle f | \mathcal{O} | i \rangle|^2 \delta(E_f - E_i - \hbar\omega)$$

Final state with
a core-hole

Initial state:
no core-hole

The core wavefunction ψ_i IN THE ABSENCE OF A CORE-HOLE can be obtained using the `ld1.x` code and performing an all-electron calculation on the isolated atom.

Alternatively, if you have a (GI)PAW pseudopotential without core-hole you can use the script `upf2plotcore.sh`

```
XSpectra/upf2plotcore.sh C.pbe-mt_gipaw.UPF > C.wfc
```

C.wfc is needed by the XSPECTRA program.

A copy of `upf2plotcore.sh` is saved in the directory with the C pseudopotential without core-hole.

Running XSPECTRA (more details)

1

Prepare GIPAW pseudo
and supercell scf input file



2

`./pw.x < prefix.scf.in > prefix.scf.out`



3

Generate core state of the
absorbing atom (`upf2plotcore.sh`)



4

`./xspectra.x < prefix.xspectra.in > prefix.xspectra.out`

Step 4 – XSPECTRA input file

&input_xspectra namelist, here we specify the main information to control the job:

```
&input_xspectra
```

```
  calculation='xanes_dipole',
```

```
  prefix='diamondh',
```

```
  outdir='$TMP_DIR/',
```

```
  xonly_plot=.false.,
```

```
  xniter=1000,
```

```
  xcheck_conv=50,
```

```
  xerror=0.001,
```

→ xanes_dipole/xanes_quadrupole

→ Perform a full continuous fraction calculation

→ These parameters control the Lanczos.

```
  x_save_file='diamondh.xspectra.sav',
```

→ File where the a and b coefficients of the Lanczos method are saved.

```
  ef_r=${FERMI_LEVEL},
```

→ **In Rydberg:** sets the energy zero in the final spectra. Read this from step 1 output.

```
  xiabs=1,
```

→ Type of the absorbing atom.

```
  xepsilon(1)=1.0,
```

```
  xepsilon(2)=0.0,
```

```
  xepsilon(3)=0.0,
```

→ Polarization vector of the incident beam

```
/
```


Step 4 – XSPECTRA input file

&plot namelist, is used to specify the plot of the cross-section


&plot

xgamma=0.8,  Core-hole linewidth (atomic data)

xnepoint=1000,  Number of ω points to be used for $\sigma(\omega)$

xemin=-10.0,
xemax=30.0,  Range of ω for $\sigma(\omega)$

terminator=.true.,  Use a terminator for the Lanczos (faster)

cut_occ_states=.true.,  Eliminate the occupied states from the
/
cross section. The states are eliminated below
the Fermi level specified in the previous slide.

Step 4 – XSPECTRA input file

&pseudos namelist, is used to specify the initial state wavefunction and the paw radius

```
&pseudos
```

```
filecore='C.wfc',
```



Name of the file with the core-state wavefunction generated at step 3

```
r_paw(1)=3.2,
```

```
/
```



Radius defining the augmentation region.
This is useful when your projectors are almost linearly dependent.

Do not use it if you do not know what to do.

Generally a good choice for r_paw is $r_{paw} = 3 r_{cut}/2$ or greater, and r_cut is the radius used in a norm conserving generation of the pseudo.

Step 4 – XSPECTRA input file

&cut_occ namelist specifies how to cut smoothly occupied states

```
&cut_occ  
  cut_desmooth=0.1,  
  cut_step1=0.01,  
  /
```

This is done using following ref.

Ch. Brouder, M. Alouani, K. H. Bennemann, Phys. Rev. B **54** (1996) p.7334-49.

Most of the times these parameters works. However they do not necessary represent the most efficient choice in term of CPU time.

These and other parameters control the smooth cut of occupied states. It is suggested that before modifying them you read the reference above.

Running XSPECTRA (more details)

1

Prepare GIPAW pseudo
and supercell scf input file



2

`./pw.x < prefix.scf.in > prefix.scf.out`



3

Generate core state of the
absorbing atom (`upf2plotcore.sh`)



4

`./xspectra.x < prefix.xspectra.in > prefix.xspectra.out`



Output files

Besides prefix.xspectra.out two other files are produced:

prefix.xspectra.dat

Contains the XANES cross section. It is a file of the kind:

```
# final state angular momentum: 1
# broadening parameter (in eV): 0.800000000000
# absorbing atom type: 1
# Energy (eV)  sigma
-10.00000000  0.02722740
-9.86622074   0.02766810
-9.73244147   0.02789281
-9.59866221   0.02791267
```

The file can be visualized with xmgrace / gnuplot or similar.

prefix.xspectra.sav

Contains all the informations of the Lanczos process (a and b vectors) and can be used to replot the cross section (different broadening/energy range) or to continue the Lanczos.

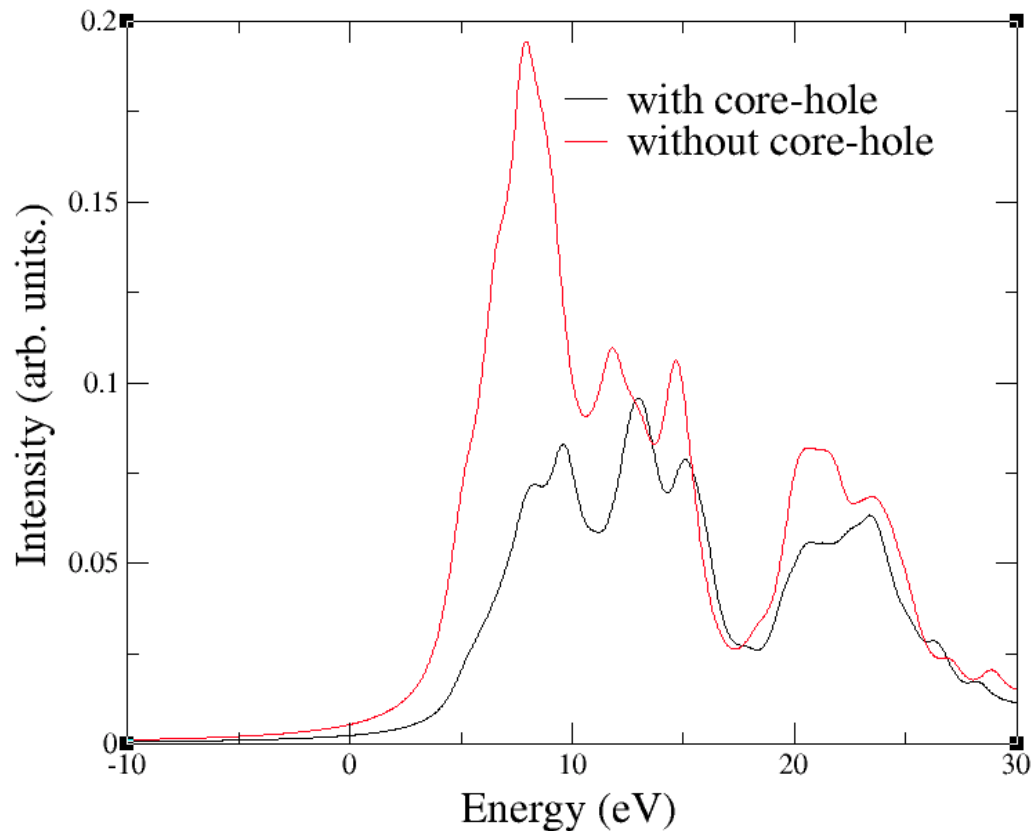
Always keep this file for replotting.

Outline

- XAS in a nutshell.
- XSPECTRA
 - ➔ Theory (PAW)
 - ➔ The Lanczos Method
 - ➔ Running XSPECTRA
- Tutorials
 - ➔ Diamond
 - ➔ SiO₂
- Conclusion

Diamond with and without core-hole

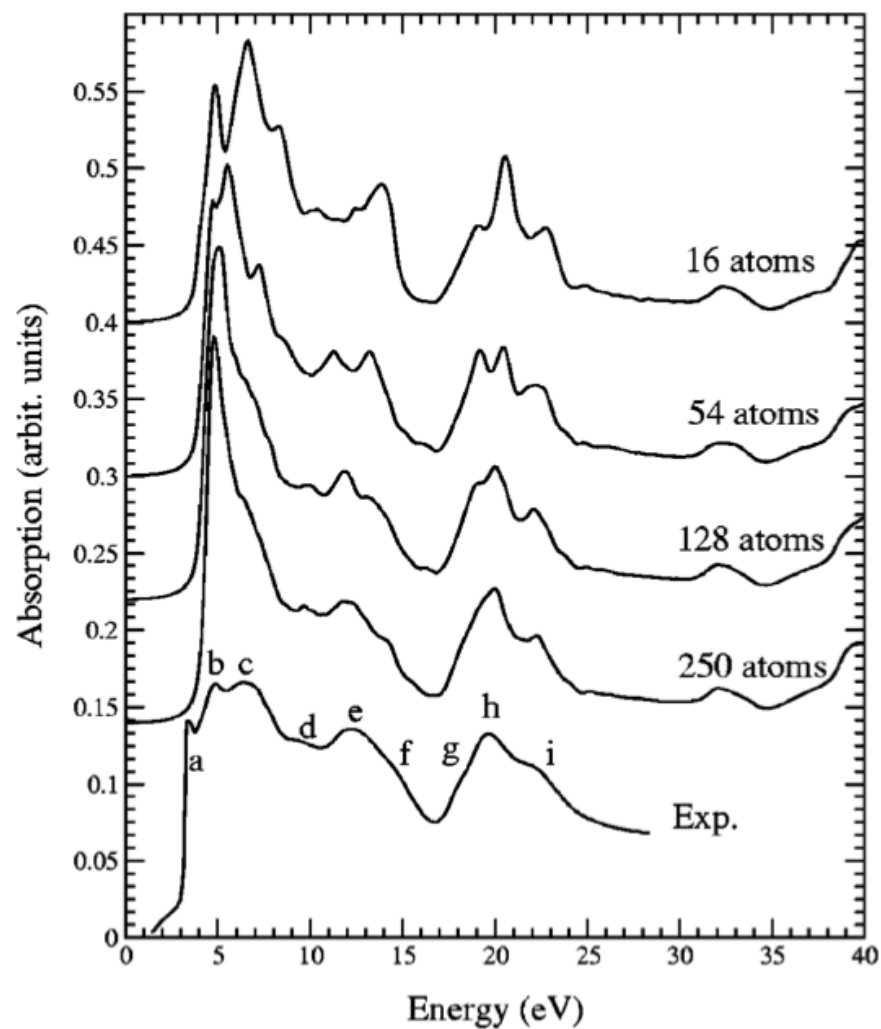
Repeat steps 2,3,4 to obtain the XANES spectrum of Diamond without a core-hole in the final state (see directory `./Diamond_nohole/`).



Note the huge core-hole effect!!!!

What happens increasing the supercell size ?

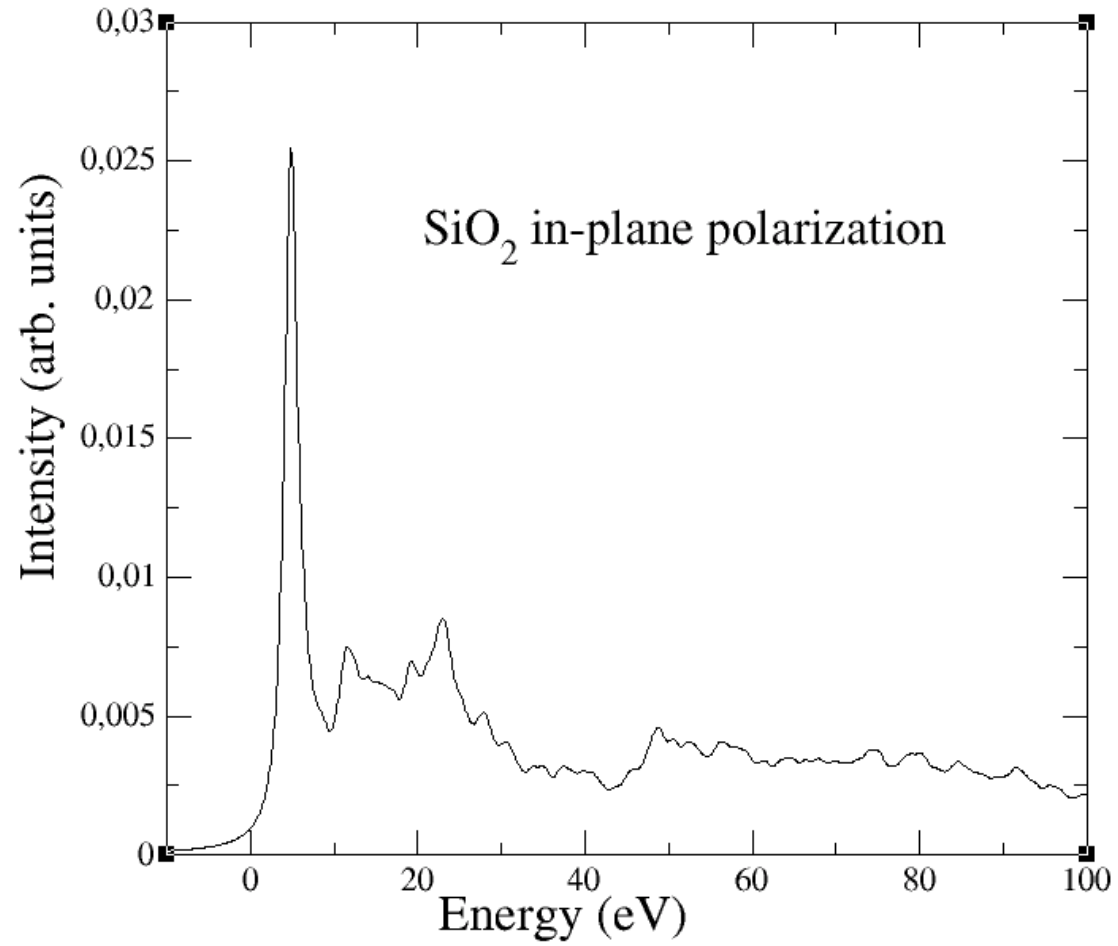
Increasing supercell size



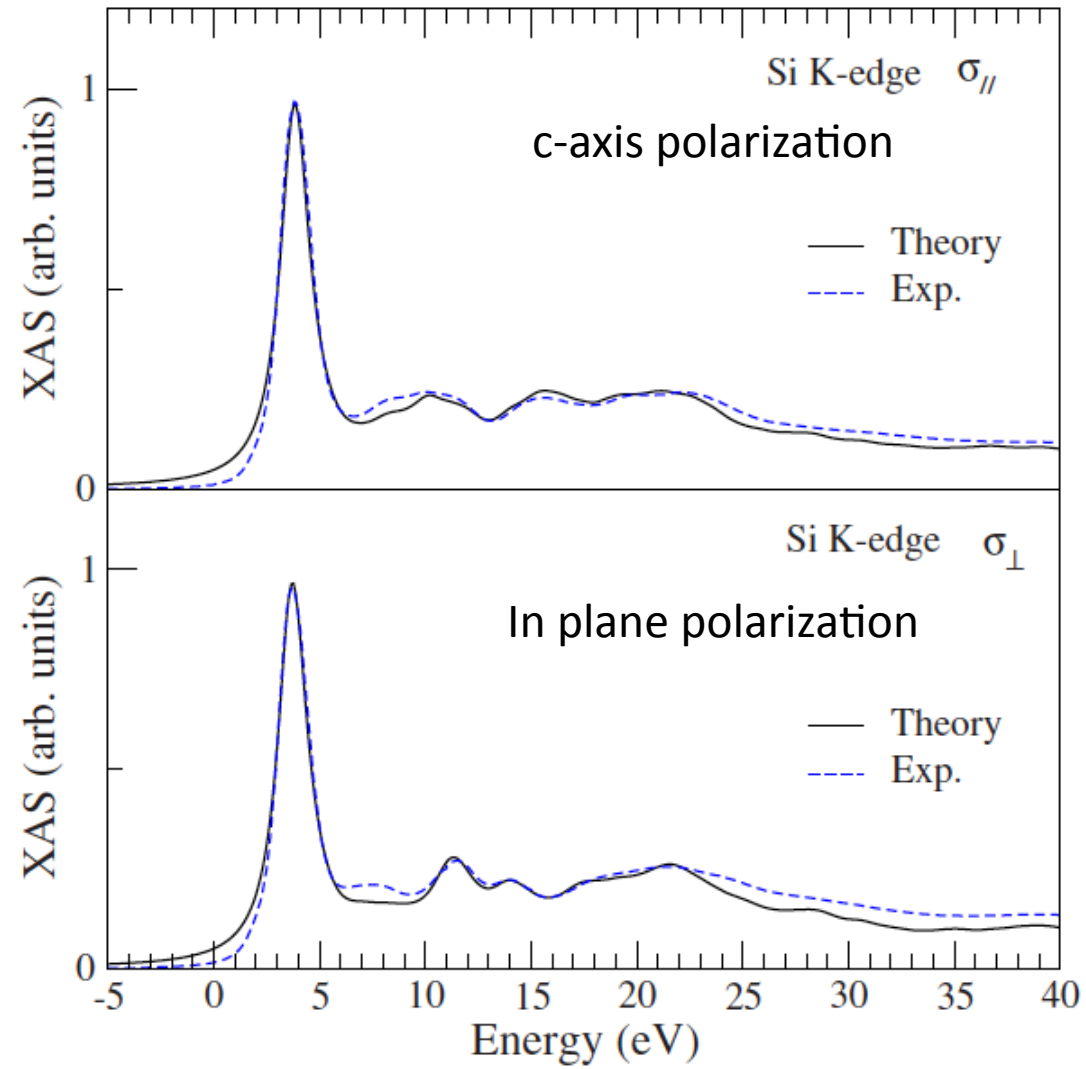
Very big size-effects, the simulation converges with 250 atoms. Note that peak A is not well described in DFT. The is well known in literature.

α quartz (SiO_2)

Hexagonal cell – in-plane polarization.



α quartz (SiO_2) – Converged results



XSPECTRA (Features)

- ➔ XSPECTRA supports all standard DFT functionals available in QUANTUM-ESPRESSO, (PZ,PBE, DFT+U,...) however not yet exact-exchange, HSE0, HSE1 or similar.
- ➔ Ultrasoft and norm-conserving pseudopotentials are supported.
- ➔ The pseudopotential of the absorbing atom **MUST** contain core-states information (GIPAW pseudopotential)
- ➔ All-electron reconstruction is performed using the **GIPAW** method.
- ➔ Empty electronic states are calculated using the Lanczos method and the continuous fraction approach.
- ➔ Dipolar and Quadrupolar XAS cross section at the K and L_1 edges.
- ➔ Core-hole is modeled in a supercell approach

Conclusions and history

The first version of XSPECTRA was written by M. Taillefumier *et al.* PRB 66, 195107 (2002)
It was calculating the dipolar cross section in the norm conserving case.

XSPECTRA was ported to QUANTUM-ESPRESSO and generalized to the quadrupolar cross-section and the DFT+U approximation by

C. Gougoussis, M. Calandra, A. Seitsonen, Ch. Broder, A. Shukla, and F. Mauri,
Phys. Rev. B **79**, 045118 (2009)

Lanczos@XSPECTRA with ultrasoft pseudopotentials was developed in

C. Gougoussis, M. Calandra, A. P. Seitsonen, and F. Mauri , Phys. Rev. B **80**, 075102 (2009)

Please cite these papers if you use XSPECTRA in your work!

and of course....



P. Giannozzi et al., J. Phys. Condens. Matter **21**, 395502 (2009).

XSPECTRA

A tool for X-ray absorption spectra (XAS) calculations

Matteo Calandra

C. Gougoussis, M. Calandra, A. P. Seitsonen, and F. Mauri
Phys. Rev. B **80**, 075102 (2009)

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