



Simulating X-ray Emission/Absorption Spectroscopy with WIEN2k

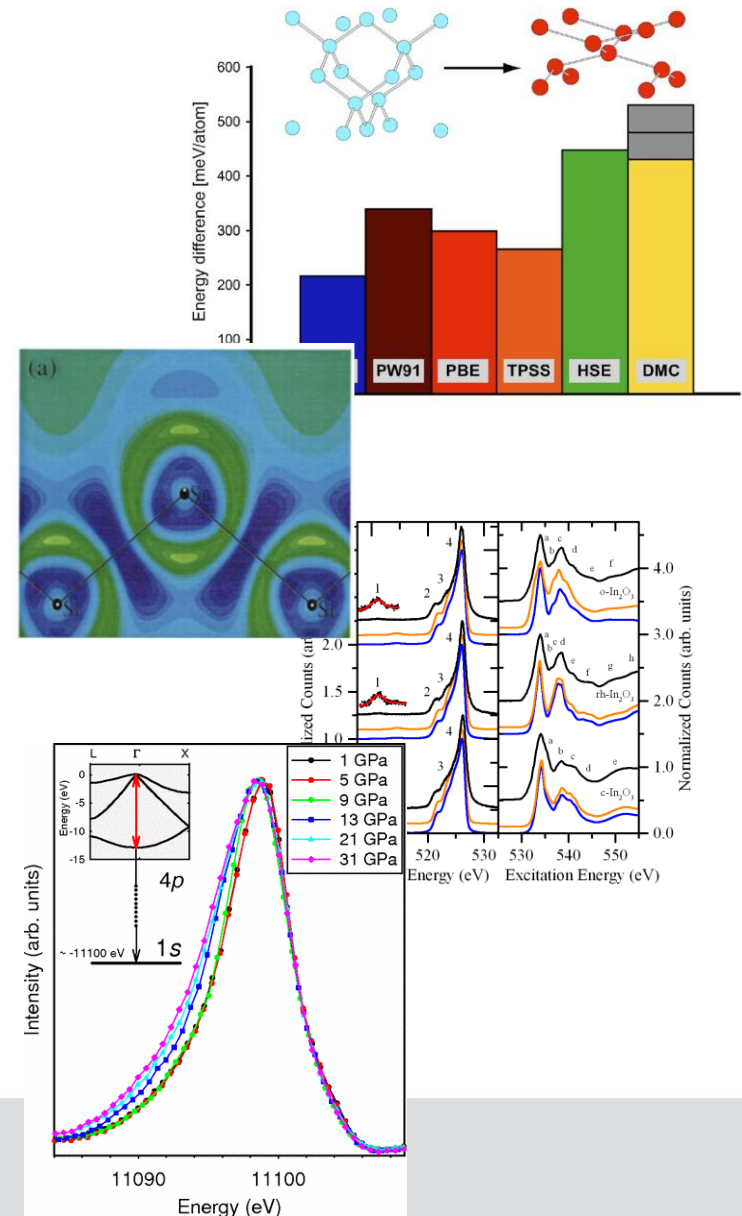
REIXS Soft X-ray Spectroscopy Workshop

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June 20, 2023

Outline

- Introduction to Density Functional Theory
- Case Studies
- Compiling WIEN2k
- Example DFT Calculations



Many-Body Problem

For a system composed of atomic nuclei and electrons, the many-body Hamiltonian is given by:

$$\begin{aligned}
 \hat{H} = & \underbrace{-\frac{\hbar^2}{2} \sum_I \frac{\nabla_I^2}{M_I}}_{T_n} + \underbrace{\frac{-\hbar^2}{2} \sum_i \frac{\nabla_i^2}{m_e}}_{T_e} + \underbrace{\frac{1}{8\pi\epsilon_0} \sum_{i \neq j} \frac{e^2}{|\vec{r}_i - \vec{r}_j|}}_{V_{ee}} \\
 & + \underbrace{\frac{-1}{4\pi\epsilon_0} \sum_{i,I} \frac{e^2 Z_I}{|\vec{R}_I - \vec{r}_i|}}_{V_{en}} + \underbrace{\frac{1}{8\pi\epsilon_0} \sum_{I \neq J} \frac{e^2 Z_I Z_J}{|\vec{R}_I - \vec{R}_J|}}_{V_{nn}}
 \end{aligned}$$

For non-trivial systems this is an intractable problem.

Many-Body Problem

Make Born-Oppenheimer approximation:

$$\begin{aligned}
 \hat{H} = & \underbrace{-\frac{\hbar^2}{2} \sum_I \frac{\nabla_I^2}{M_I}}_{T_n} + \underbrace{\frac{-\hbar^2}{2} \sum_i \frac{\nabla_i^2}{m_e}}_{T_e} + \underbrace{\frac{1}{8\pi\epsilon_0} \sum_{i \neq j} \frac{e^2}{|\vec{r}_i - \vec{r}_j|}}_{V_{ee}} \\
 & + \underbrace{\frac{-1}{4\pi\epsilon_0} \sum_{i,I} \frac{e^2 Z_I}{|\vec{R}_I - \vec{r}_i|}}_{V_{en}} + \underbrace{\frac{1}{8\pi\epsilon_0} \sum_{I \neq J} \frac{e^2 Z_I Z_J}{|\vec{R}_I - \vec{R}_J|}}_{V_{nn}} \\
 = & T_e + V_{ee} + V_{ext}
 \end{aligned}$$

Hohenberg-Kohn Theorem

- For a system in the ground state, there is a one-to-one correspondence between the ground state density and V_{ext} . As a corollary:

$$\hat{H} = \hat{T}_e + \hat{V}_{ee} + \hat{V}_{ext}$$

$$E = \langle \Psi | \hat{H} | \Psi \rangle$$

$$\begin{aligned} E_{V_{ext}} &= \underbrace{\langle \Psi | \hat{T}_e + \hat{V}_{ee} | \Psi \rangle}_{F_{HK}[\rho]} + \langle \Psi | \hat{V}_{ext} | \Psi \rangle \\ &= F_{HK}[\rho] + \int d^3r \rho(\vec{r}) V_{ext}(\vec{r}) \end{aligned}$$

where $F_{HK}[\rho]$ is the Hohenberg-Kohn density functional.

Kohn-Sham Equations

- Reformulate the many-electron system into an equivalent one of non-interacting electrons. The energy functional is then given by:

$$E_{V_{ext}}[\rho] = T_0[\rho] + \int d^3r \rho(\vec{r}) \left(V_{ext}(\vec{r}) + \frac{V_H(\vec{r})}{2} \right) + E_{xc}[\rho]$$

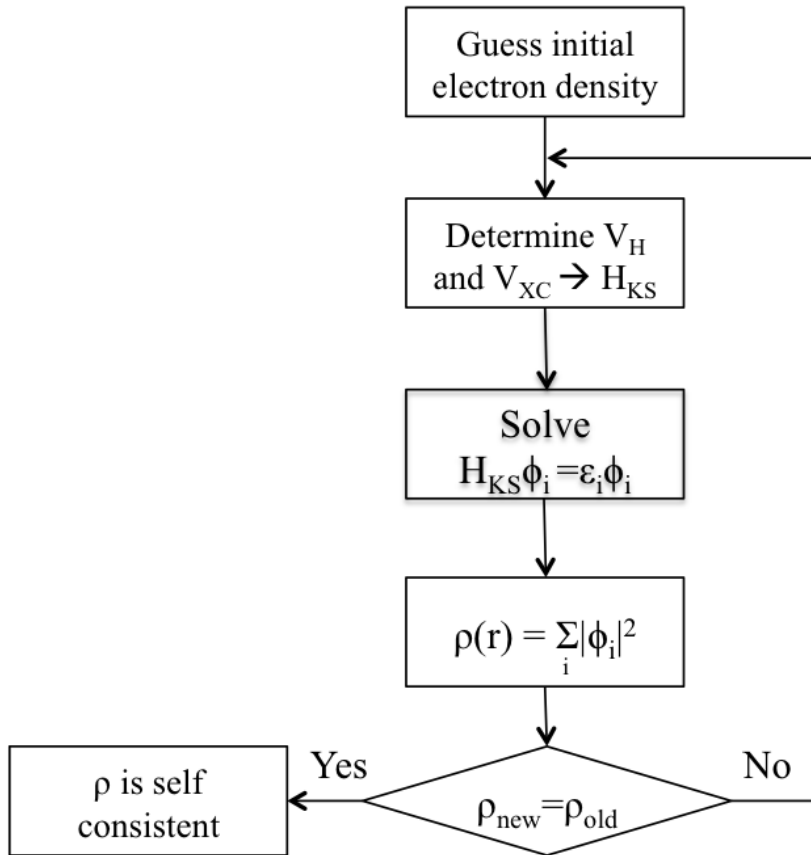
- The Kohn-Sham Hamiltonian is then given by:

$$\hat{H}_{KS} = T_0 + \frac{V_H}{2} + V_{xc} + V_{ext}$$

- This can be solved using:

$$\hat{H}_{KS}\phi_i = \epsilon_i\phi_i \qquad \rho(\vec{r}) = \sum_i^N |\phi_i(\vec{r})|^2$$

Solving KSE Self Consistently



Fully relativistic
Scalar relativistic
Non-relativistic

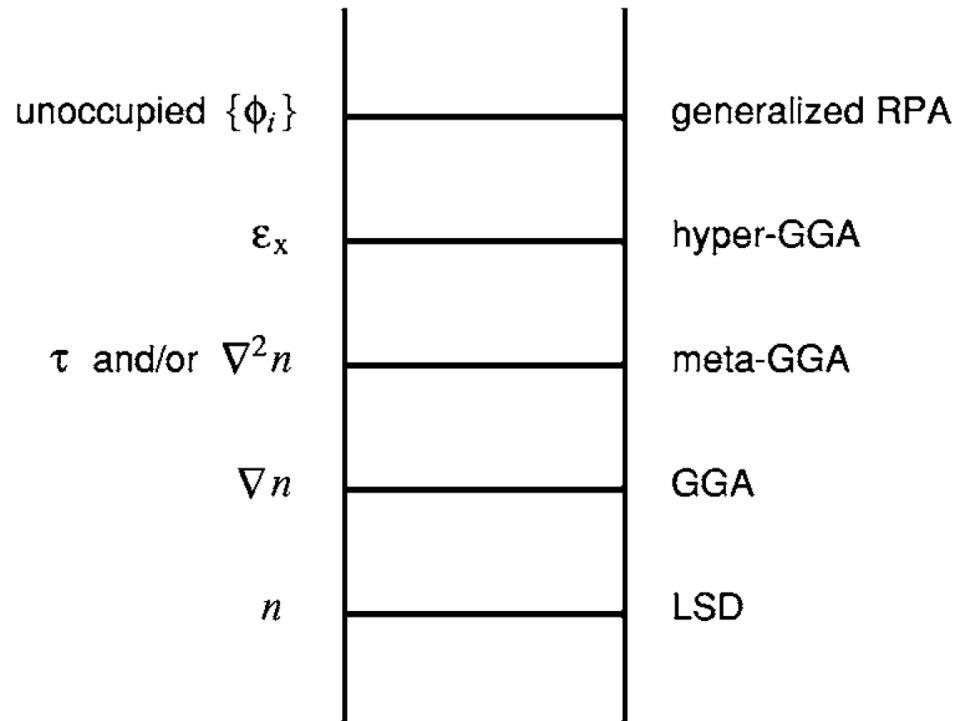
All-electron full potential
Pseudopotential

$$\left(T_0 + \frac{V_H}{2} + V_{xc} + V_{ext} \right) \phi_i = \epsilon_i \phi_i$$

Plane wave
Linearized augmented plane wave
LCAOs

Exchange-Correlation Functionals

HEAVEN OF CHEMICAL ACCURACY



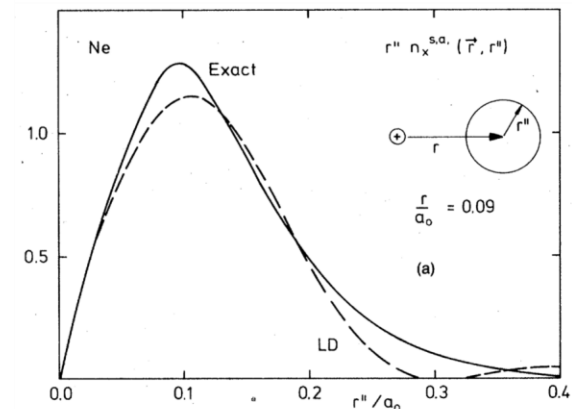
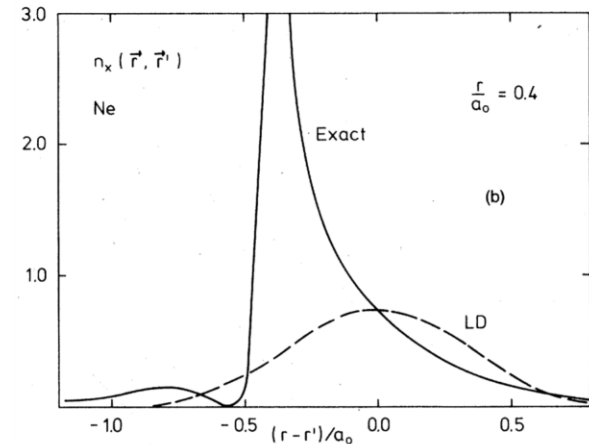
HARTREE WORLD

Local Density Approximation

- Exchange-correlation functional is given by:

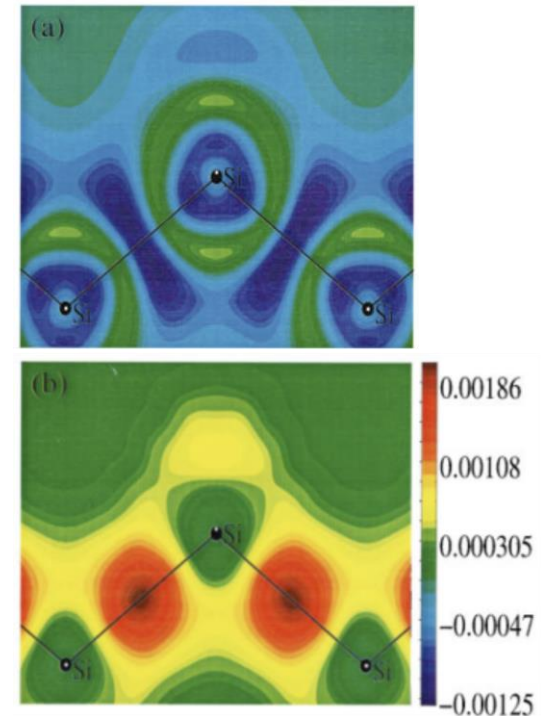
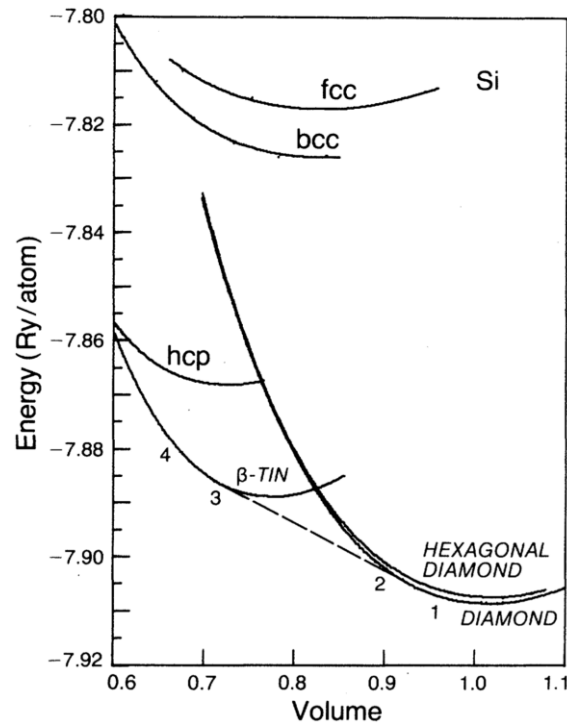
$$E_{xc}^{LDA}[\rho_{\downarrow}, \rho_{\uparrow}] = \int d^3r \rho(\vec{r}) \epsilon_{xc}^{unif}(\rho_{\downarrow}, \rho_{\uparrow})$$

- The energy depends only on the local density and thus describes localized features, such as the exchange-correlation hole in Ne, quite poorly
- The spherical average of the of atomic exchange-correlation holes is well described



Local Density Approximation

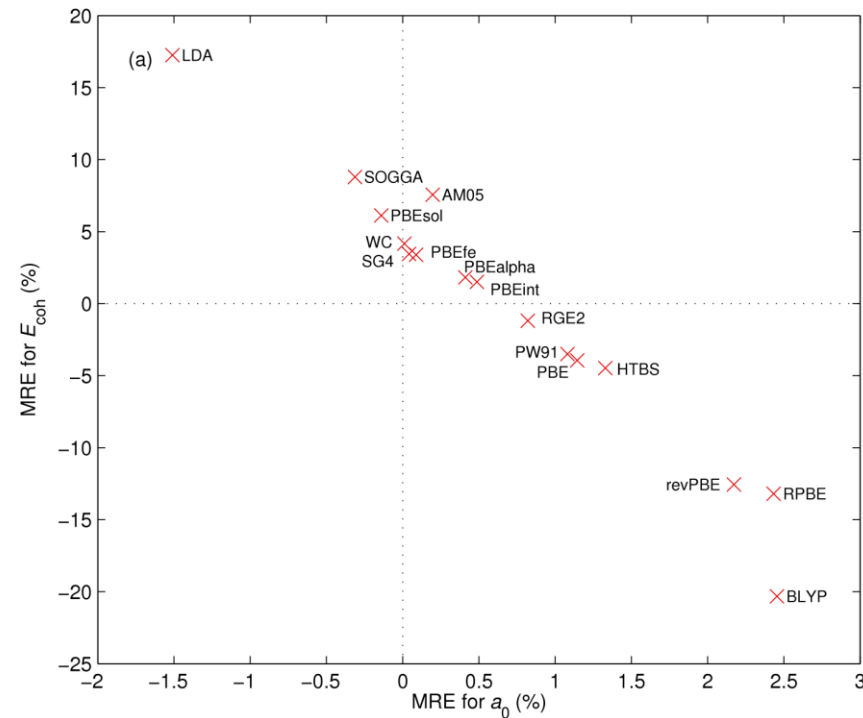
- Diamond phase of Si correctly predicted to be lowest energy. Lattice constant and bulk modulus are within 1% of experiment
- This is due in part due to a fortuitous cancellation of errors in the exchange and correlation energies
- Error in atomization energy of molecules is 70-100 kcal/mol



Generalized Gradient Approximation

$$E_{xc}^{GGA}[\rho_{\downarrow}, \rho_{\uparrow}] = \int d^3r \rho(\vec{r}) \epsilon_{xc}^{GGA}(\rho_{\downarrow}, \rho_{\uparrow}, \nabla \rho_{\downarrow}, \nabla \rho_{\uparrow})$$

- After the LDA, there are empirical and non-empirical functionals.
- WIEN2k supports the 1996 PBE and PBEsol formulations of the GGA

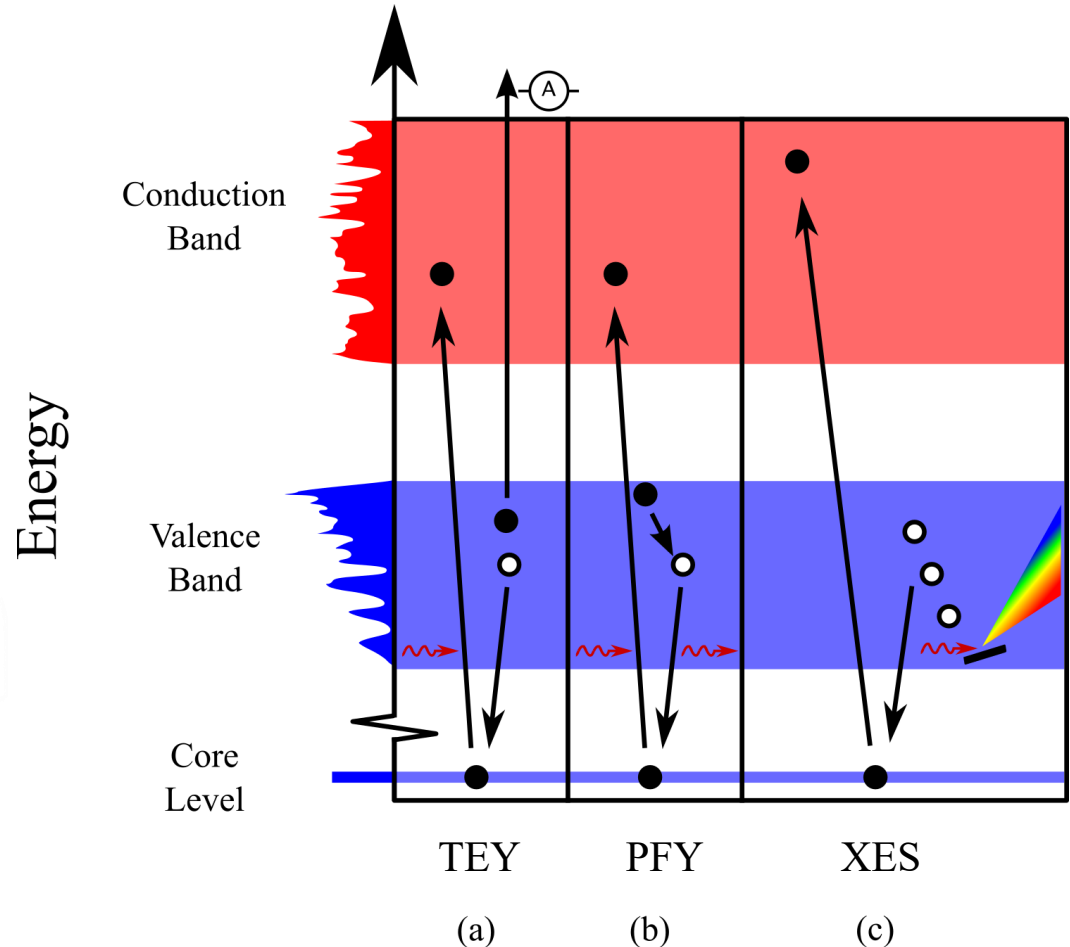


Modelling X-ray Absorption and Emission Spectroscopy

- XAS (XES) are sensitive to the unoccupied (occupied) partial density of states
- Element, character selective owing to binding energy and dipole selection rules

$$T_{i \rightarrow f} = \frac{2\pi}{\hbar} |\langle \Psi_f | H' | \Psi_i \rangle|^2 \rho_f$$

- Spectral weight depends on the final state of a particular measurement



Case Study: Effect of a core hole in graphite

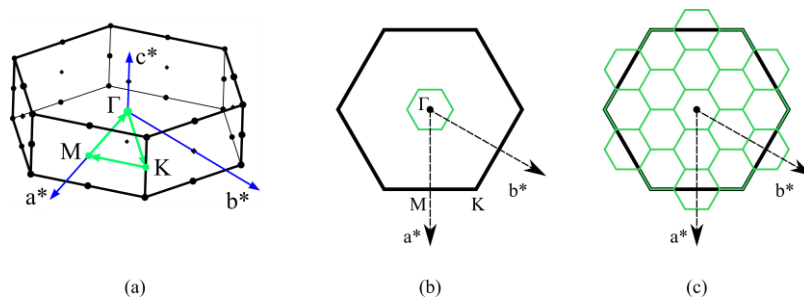


Figure 1: (a) The Brillouin zone of AB-stacked graphite, with the reciprocal axes as shown. A selected path through is shown in green, with the critical points labelled as indicated. (b) A projection of the AB-stacked graphite Brillouin zone. The same projection for a $4 \times 4 \times 1$ supercell is shown in green. (c) A mapped version of the supercell is shown, showing how points in momentum space can be mapped between the original unit cell and a supercell

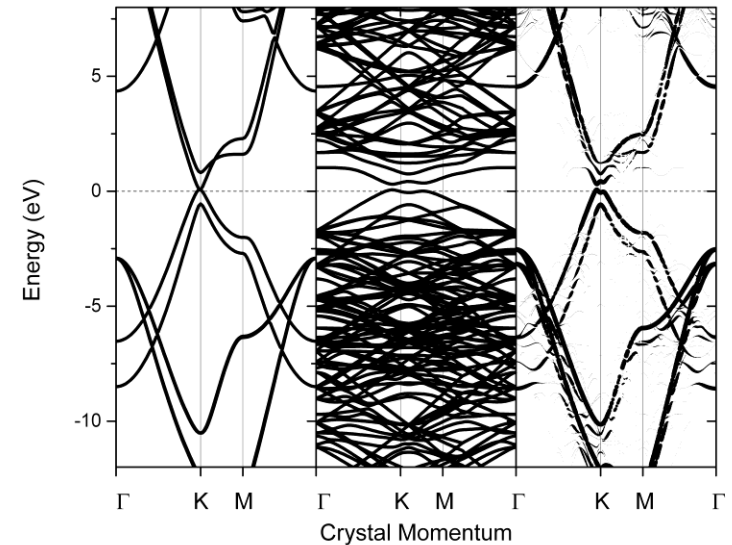
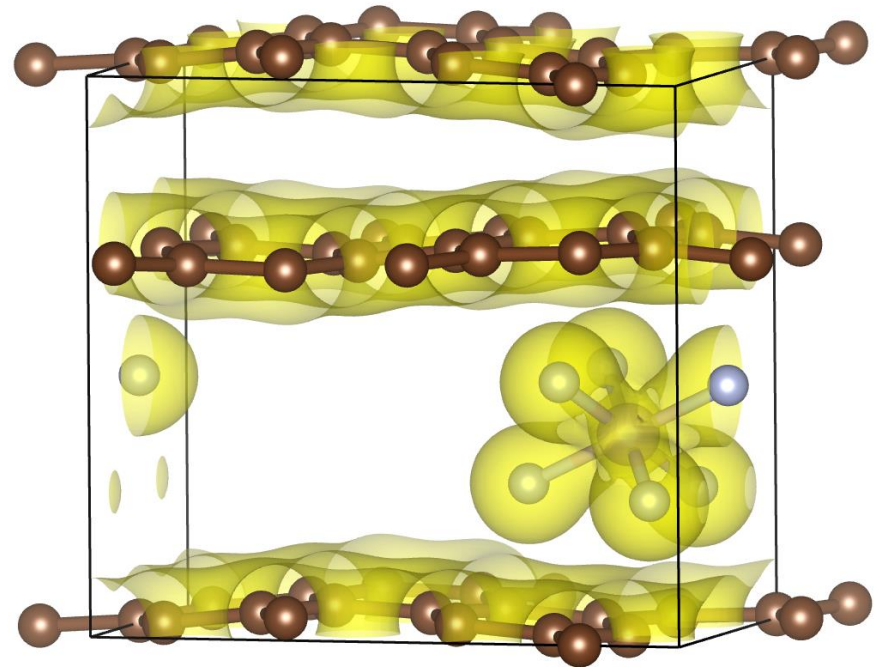


Figure 2: (left) Band structure diagram of AB-stacked graphite. (middle) Band structure diagram of a $3 \times 3 \times 1$ supercell of AB-stacked graphite perturbed by a core hole. (right) Band structure diagram of $3 \times 3 \times 1$ supercell folded to the original Brillouin zone using a Bloch Spectral weight approach.

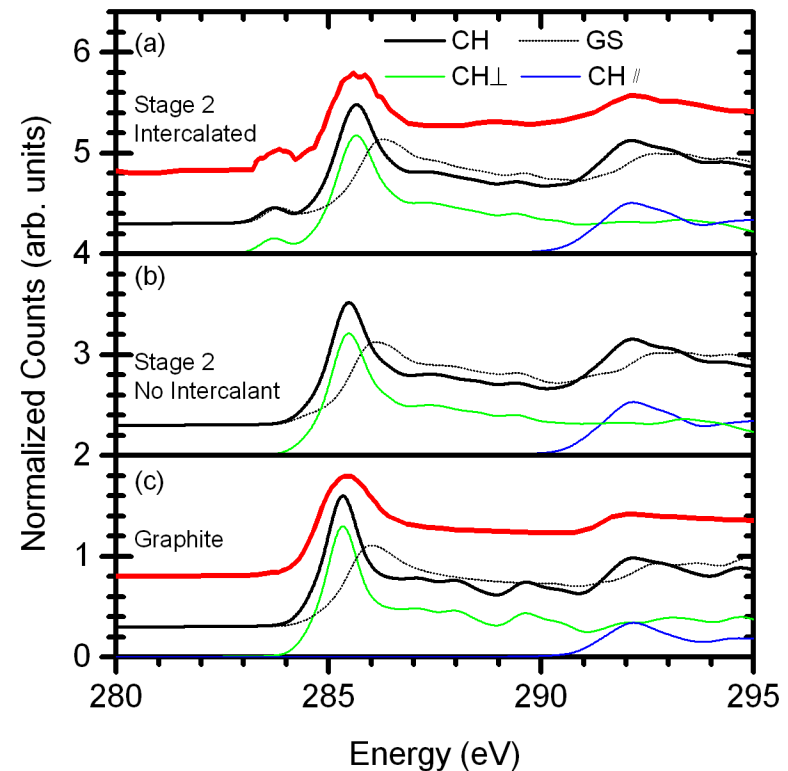
Motivation: Understand anion intercalation in graphite

- PF_6 -intercalated graphite has been proposed for use as a cathode in a dual carbon battery cell owing to favorable properties:
 - High storage capacity
 - High discharge rate
- Important aspects of this system are controversial or unresolved:
 - Staging index
 - How the electronic and physical structure of the host graphite lattice are perturbed by the intercalant
- A novel spectroscopic XAS feature (a pre- π^* peak) has been observed, the origin of which was unknown prior to this study



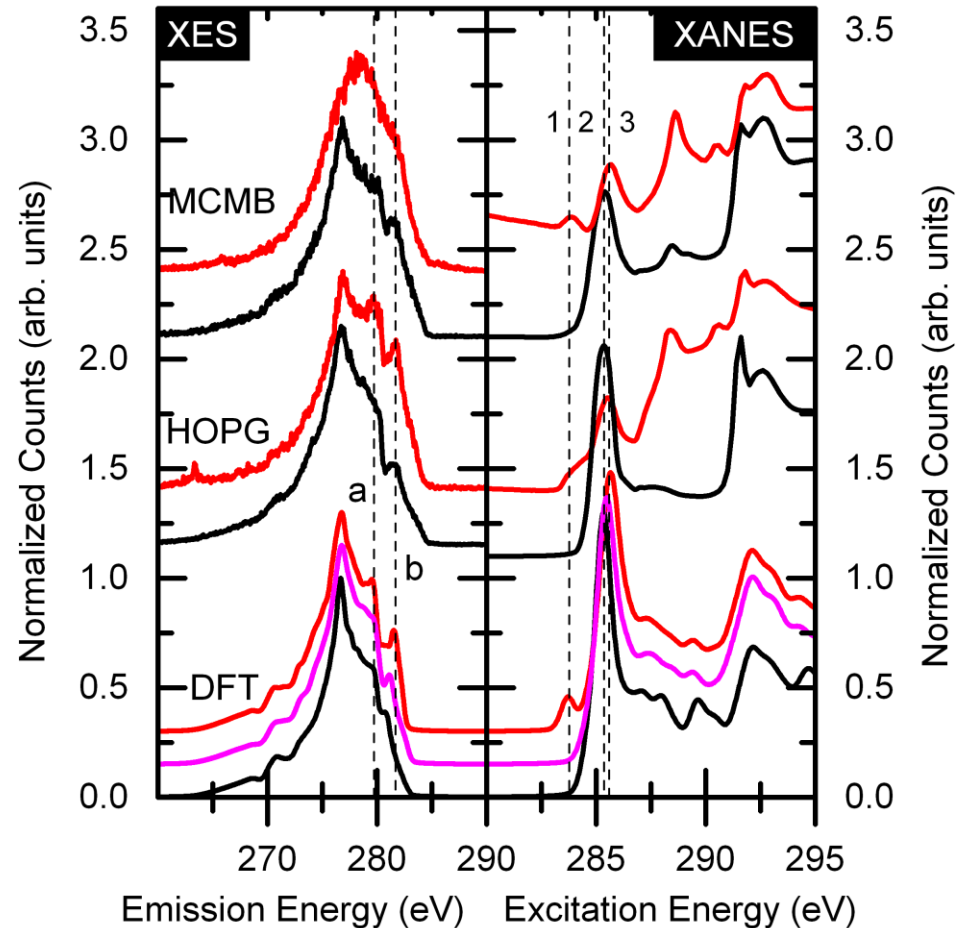
Case Study: Effect of a core hole in graphite

- The electronic density is perturbed by the presence of a core hole.
- This is reflected in the calculated C K XAS spectra
- In the case of PF_6^- intercalated graphite, Two key differences are apparent:
 - The emergence of a pre- π^* feature
 - A slight shift in the π^* feature



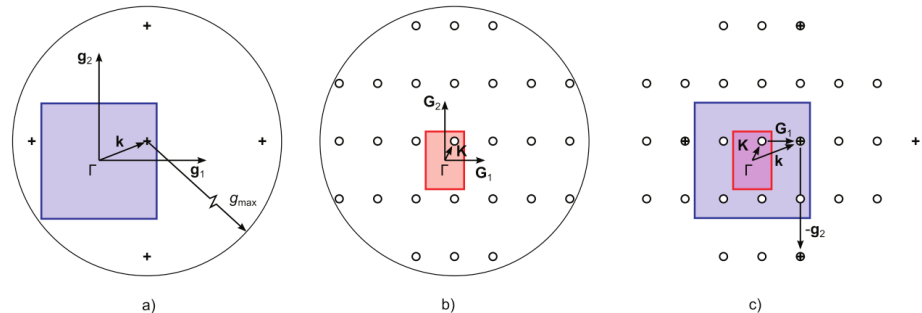
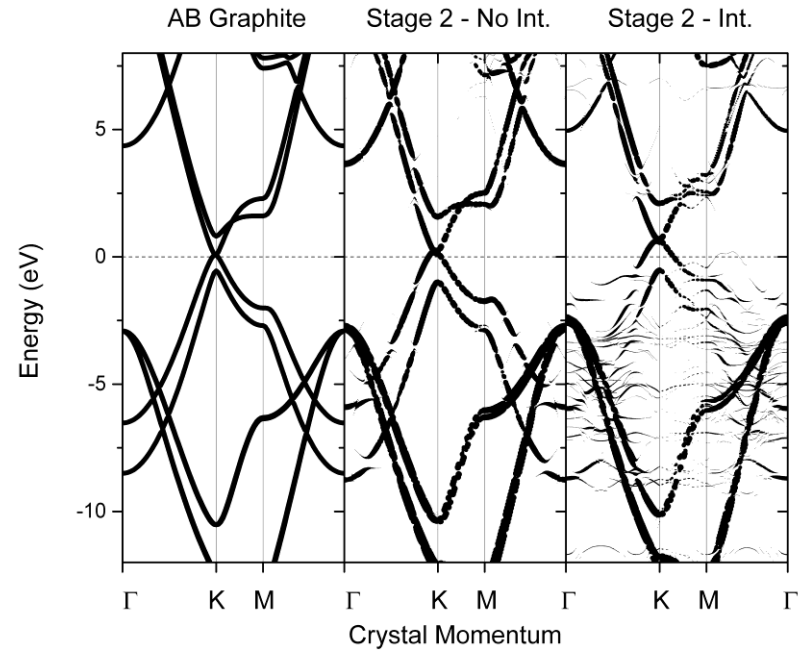
Results – XES/XANES

- In the TEY spectra:
 - A similar pre- π^* feature is observed
 - A similar shift is seen in the main π^* peak
 - Additional features between the π^* and σ^* peaks are observed, which increase monotonically with intercalant concentration.
- In the XES spectra, the spectral weight is increased at the high energy shoulder. This trend is reproduced by our calculations



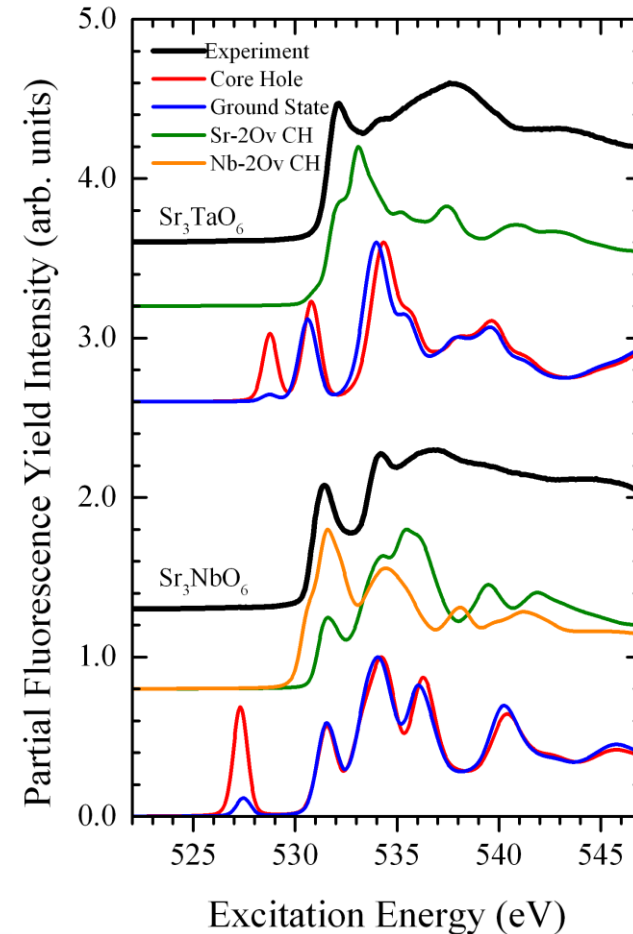
Results - Theory

- The XES, XRS results can be understood by considering the energy-crystal momentum diagram.
- AB-stacked graphite has an approximately linear dispersion at E_F .
- Considering the intercalated structure without intercalant, although the bands are distorted, no change in E_F is observed.
- Introducing the intercalant to the lattice results in two key changes:
 - The emergence of localized states associated with the intercalant.
 - A lowering of the E_F .
- According to a Bader analysis, this results in an effective transfer of charge from the graphite host to the intercalant atoms. This allows us to intuitively understand the changes in the XES, XRS spectra.



Case Study: Sr_3TaO_6 , Sr_3NbO_6

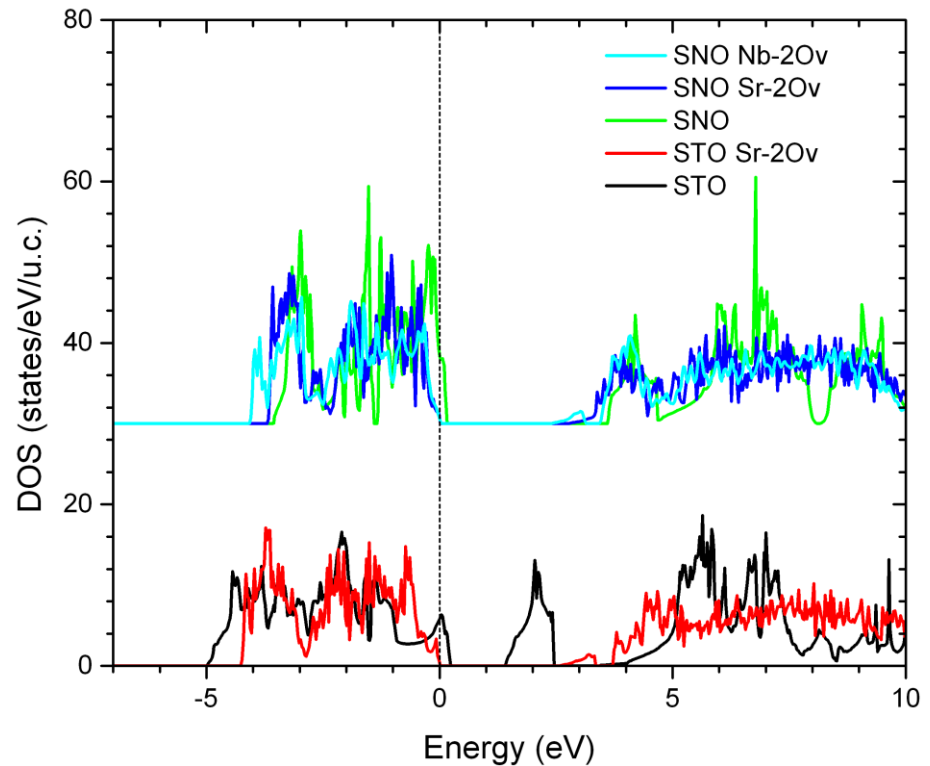
- Sr_3TaO_6 (STO) and Sr_3NbO_6 (SNO) are double perovskites which show potential as highly efficient red emitting pc-LED materials.
- Comparing O K XAS measurements with calculated spectra reveals poor agreement with the nominal XRD-derived structure.
- Introducing double vacancies around the cation sites significantly improves the overall agreement.
 - For STO, the 528 eV and 530.5 eV features are gone, better matching experiment.
 - For SNO, in the Sr-2O_v and Nb-2O_v cases the 528 eV feature is gone, better matching experiment.
- These spectral differences can be better understood by considering the DOS



Case Study: Sr_3TaO_6 , Sr_3NbO_6 - DOS

To better understand the origin of differences between the defected and 'pristine' DFT spectra we can consider the total DOS.

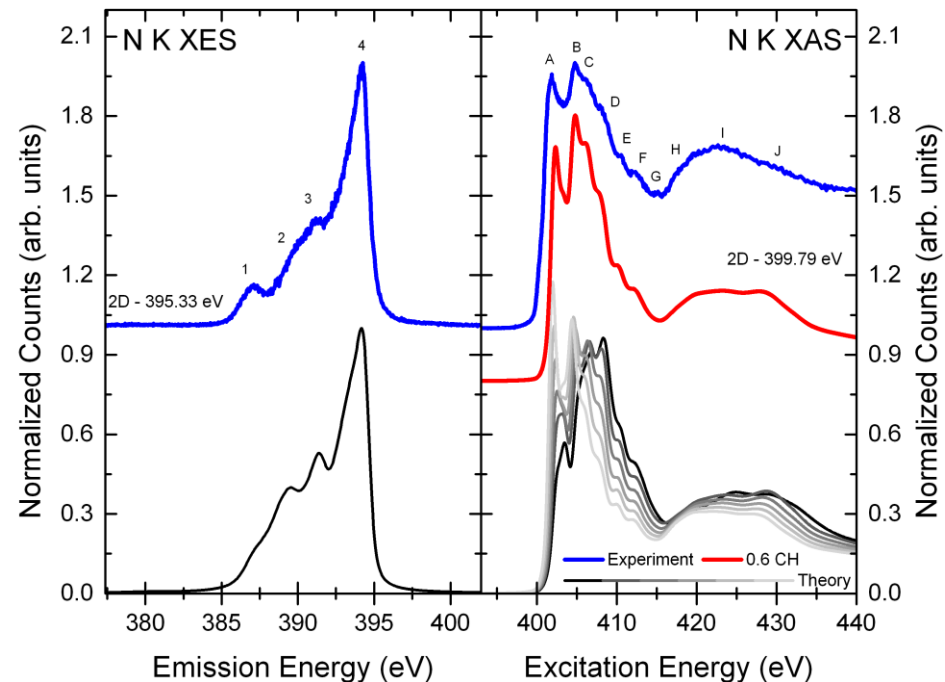
- For SNO, the compensation of the oxygen vacancies can be readily seen in the total DOS, in which case the Fermi energy level coincides with the valence band edge; this suppresses the spurious calculated 528 eV O K XAS feature
- Comparing SNO and STO, a significant difference the total DOS is observed. For STO, a 'mid-gap' conduction band present centered at 2 eV is present.
- The fact that STO is metallic and has this 'mid-gap' conduction band explains the origin of the calculated 528 and 530.5 eV features.
- With the introduction of oxygen vacancies, this mid-gap band is suppressed, and the system is no longer metallic.



Energy is relative to Fermi energy level

Case Study: ZnSiN₂

- Recent developments in synthesis have made resulted in freestanding crystals using ammonothermal synthesis
 → Otherwise impossible except using molecular beam epitaxy
- XES-XAS separation of 4.56 eV and a core hole shift of 0.15 eV yields an overall 4.70 ± 0.20 eV band gap (MBJ: 4.51 eV)
- Best agreement for 0.6 fractional CH concentration
- Disagreement with calculated XES spectra is due to hybridization with Zn d states which are poorly described using DFT

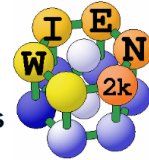


WIEN2k Installation

[WIEN2k](#)[\(L\)APW+lo](#)[FEATURES](#)[HARD+SOFT](#)[ORDER INFO](#)[PAPERS](#)[REG USERS](#)[WORKSHOPS](#)

Adding a new dimension to DFT calculations of solids ...

WIEN2k



P. Blaha, K. Schwarz, G. K. H. Madsen, D. Kvasnicka, J. Luitz, R. Laskowski, F. Tran and L. D. Marks

Institute of Materials Chemistry, TU Vienna

The program package WIEN2k allows to perform electronic structure calculations of solids using density functional theory (DFT). It is based on the full-potential (linearized) augmented plane-wave ((L)APW) + local orbitals (lo) method, one among the most accurate schemes for band structure calculations. WIEN2k is an all-electron scheme including relativistic effects and has many [features](#). It has been licensed by more than 3600 user groups and has about 19000 citations on Google scholar (Blaha WIEN2k). A recent extensive overview on WIEN2k is given in:

[WIEN2k: An APW+lo program for calculating the properties of solids.](#)

P. Blaha, K.Schwarz, F. Tran, R. Laskowski, G.K.H. Madsen and L.D. Marks, J. Chem. Phys. 152, 074101 (2020)

The current version is

WIEN2k_23.2

and was released on 7. February 2023. Version 23.2 contains an important bug fix for cubic symmetries introduced in WIEN2k_23.1. Upgrading from version 23.1 is very important, results for cubic systems in WIEN2k_23.1 are unreliable. [Upgrading](#) from WIEN2k_21 (or earlier) is highly recommended too.

We proudly announce that the

3000th license of WIEN2k

was granted free of charge to

Dr. Daniel Ion Bilc, Babeş-Bolyai University, Romania

We would also like to take the opportunity to thank all WIEN2k users for their continuous interest and the lively discussions on the WIEN2k-mailinglist. In particular we want to [acknowledge](#) all who have contributed to this package. This international cooperation is largely responsible for the success of WIEN2k.

WIEN2k Installation

- After purchase, download source code, transfer to computer
- Move WIEN2k_XX.tar to a dedicated WIEN2k directory
- Then (from the terminal) unzip using:
 - `tar -xvf wien2k XX.tar`
 - `gunzip *.gz`
 - `chmod +x ./expand lapw`
 - `./expand lapw`

WIEN2k Installation

- Once this is complete we can configure the compilation settings with:
`./siteconfig lapw`
- On DRAC/Compute Canada the ifort+mkl libraries can be used with slurm. You will be prompted to specify the following:
 - System type is 'LS'
 - Default compilers of ifort/cc/
 - Parallel execution:
 - Shared Memory: No;
 - No specific command is needed to bind jobs to specific nodes
 - MPI_REMOTE set to 0
 - Remote shell is ssh
 - Remote copy is scp
 - Finegrained parallel: No
- If using a computing cluster, generally these are not shared memory machines
- When configuring FFTW, we need to set:
 - FFTWROOT:
`/cvmfs/soft.computecanada.ca/easybuild/software/2020/avx2/Compiler/intel2020/fftw/3.3.8/`
 - FFTW architecture: lib
 - FFTW library name: fftw3
- Set the TEMP path to scratch or another folder you can write to

WIEN2k – DRAC/CC Settings Reference

```
*****
*                               *
*               W I E N         *
*             site configuration *
*                               *
*****

Last configuration: Tue 02 May 2023 12:34:17 PM EDT
Wien Version:      WIEN2k_21.1 (Release 14/4/2021)
System:           linuxifs

S  Specify a System
C  Specify Compiler
O  Compiling Options (Compiler/Linker, Libraries)
P  Configure Parallel Execution
D  Dimension Parameters
R  Compile/Recompile
U  Update a package
L  Perl Path (if not in /usr/bin/perl)
T  Temp Path

Q  Quit

Selection:  
```

Compiling Options



```
*****
*                               *
*               Compiler and linker options *
*                               *
*****

Since intel changes the name of the mkl-libraries from version to version,
you may find the linking options for the most recent ifort version at
http://software.intel.com/en-us/articles/intel-mkl-link-line-advisor/

Recommended options for system linuxifs are:
OpenMP switch:      -qopenmp
Compiler options:  -O -FR -mp1 -w -prec_div -pc80 -pad -ip -DINTEL_VML -traceback -assume buffered_io -I$(MKLRROOT)/include
Linker Flags:      $(FOPT) -L$(MKLRROOT)/lib/$(MKL_TARGET_ARCH) -lpthread -lm -ldl -liomp5
Preprocessor flags: '-DParallel'
R_LIB (LAPACK+BLAS): -lmkl_intel_lp64 -lmkl_intel_thread -lmkl_core

Current settings:
M OpenMP switch:      -qopenmp
O Compiler options:  -O -FR -mp1 -w -prec_div -pc80 -pad -ip -DINTEL_VML -traceback -assume buffered_io -I$(MKLRROOT)/include
L Linker Flags:      $(FOPT) -L$(MKLRROOT)/lib/$(MKL_TARGET_ARCH) -lpthread -lm -ldl -liomp5
P Preprocessor flags: '-DParallel'
R R_LIBS (LAPACK+BLAS): -lmkl_intel_lp64 -lmkl_intel_thread -lmkl_core
F FFTW options:      -DFFT3 -DFFTW_OMP -I/cvmfs/soft.computecanada.ca/easybuild/software/2020/avx2/Compiler/intel2020/fftw/3.3.8/include
FFTW-LIBS:          -L/cvmfs/soft.computecanada.ca/easybuild/software/2020/avx2/Compiler/intel2020/fftw/3.3.8/lib -lfftw3 -lfftw3_omp
X LIBC-LIBS:
LIBX-LIBS:

PO Parallel options
```

```
*****
*                               *
*               FFTW Settings *
*                               *
*****

Your current FFTW options are:
FFTW_OPT:          -DFFT3 -DFFTW_OMP -I/cvmfs/soft.computecanada.ca/easybuild/software/2020/avx2/Compiler/intel2020/fftw/3.3.8/include
FFTW_LIBS:         -L/cvmfs/soft.computecanada.ca/easybuild/software/2020/avx2/Compiler/intel2020/fftw/3.3.8/lib -lfftw3 -lfftw3_omp

which are derived from following settings:
R FFTWROOT:        /cvmfs/soft.computecanada.ca/easybuild/software/2020/avx2/Compiler/intel2020/fftw/3.3.8/
V FFTW_VERSION:    FFTW3
L FFTW_LIB:        lib
M FFTW_LIBNAME:    fftw3

RS Reset complete FFTW setup
X Delete all settings

B Back to parallel options

Selection:  
```

FFTW Settings



To run from scratch, run 'siteconfig_lapw -first'

WIEN2k Installation

- Compile WIEN2k (this may take an hour)
- Once this is completed, run
 `userconfig_lapw`
- This will configure environment variables and aliases
- Set `$OMP NUM THREADS` to 1
- Once this is done, either exit and reconnect to the computer or run `'source ~/.bashrc'`

WIEN2k Installation – w2web

The main interface to WIEN2k is a web-based interface to configure. To configure/launch run from the terminal:

w2web

On the first launch it will prompt for:

- username: admin
- password:password
- port: choose a number between 8000-20000
- For hostname press enter
- This is the master node

Metadata about cases is organized by login node, so being consistent is key!

```
[yme980@gra-login2 ~]$ w2web
#####
# w2web starter                                     #
# Copyright (C) 2001 luitz.at                       #
#####
w2web installer on host gra-login2.graham.sharcnet

#####
# w2web installer                                     #
# Copyright (C) 2001 luitz.at                       #
#####

Checking for Installation in /home/yme980/.w2web/gra-login2.graham.sharcnet

Creating /home/yme980/.w2web/gra-login2.graham.sharcnet
conf directory does not exist - creating it.
logs directory does not exist - creating it.
sessions directory does not exist - creating it.
tmp directory does not exist - creating it.

Installing w2web files ...
Please answer these questions for proper installation.
Just press enter for the default value of (in brackets).

Please enter the username: [admin] admin
Please enter the password: [password] password
admin:password
Remember these. You will need them when you log in.

Select the port to run on: [7890] 7890
Running on port 7890

Please enter this system's hostname: [gra-login2.graham.sharcnet]
Using gra-login2.graham.sharcnet

Is this your master node?: [y] y
Installing... Attempting to start now...

Trying to start /home/yme980/WIEN2k211/SRC_w2web/bin/w2web
w2web server started, now point your web browser to
http://gra-login2.graham.sharcnet:7890

done.
```

WIEN2k Resources

- Density Functional Theory and the Family of (L)APW-methods: A Step-By-Step Introduction, S. Cottenier ISBN 978-90-807215-1-7 (2013).
- WIEN2k User's Guide, P. Blaha et al. ISBN 3-9501031-1-2 (2023).
- WIEN2k FAQ:
http://susi.theochem.tuwien.ac.at/reg_user/faq/
- WIEN2k Mailing List:
<https://www.mail-archive.com/wien@zeus.theochem.tuwien.ac.at/>
- WIEN2k Workshop Lecture Notes and Videos:
<http://www.wien2k.at/events/>
- Useful tools:
VESTA - <https://jp-minerals.org/vesta/en/>
xcrysden - <http://www.xcrysden.org/>

Summary


- DFT is a widely used approach to solving the quantum many-body problem
- Choice of functional will depend on accuracy required, resources available
- DFT can describe well a range of systems including metals, semiconductors and Mott-Hubbard insulators

WIEN2k – Practical Cases

- How to create, initialize and run a test case (AB-stacked graphite)
 - Using StructGen in w2web
 - Using VESTA or a cif file
- A consideration of core leakage
- Submitting a job to slurm
- How to calculate XES, XAS spectra
- How to make a supercell and initialize a core hole calculation

Worked Example: AB-Graphite

- Each WIEN2k case should reside in a separate directory
- Each 'case' takes the name of the directory it is in
- The session and case names can be different



Session: [\[AB-Graphite \]](#)
/home/tid927/WIEN2k/AB-Graphite

StructGen™

View only mode --> [\[edit STRUCT file \]](#)

Title:

Lattice:
Spacegroup: 194_P63/mmc

[\[Spacegroups from Bilbao Cryst Server \]](#)

Splitting of equivalent positions not available.
To split you must select a lattice type

Lattice parameters in

a= b= c=
 α= β= γ=

Inequivalent Atoms: 2

Atom 1: Z= RMT=

Pos 1: x= y= z=

Pos 2: x= y= z=

Atom 2: Z= RMT=

Pos 1: x= y= z=

[\[Execution >> \]](#)
[\[StructGen™ \]](#)
[\[initialize calc. \]](#)
[\[run SCF \]](#)
[\[single prog. \]](#)
[\[optimize\(V,c/a\) \]](#)
[\[mini. positions \]](#)

[\[Utils. >> \]](#)

[\[<< Tasks \]](#)
[\[El. Dens. \]](#)
[\[DOS \]](#)
[\[XSPEC \]](#)
[\[TELNES3 \]](#)
[\[OPTIC \]](#)
[\[Bandstructure \]](#)

[\[Files >> \]](#)
[\[struct file\(s\) \]](#)
[\[input files \]](#)
[\[output files \]](#)
[\[SCF files \]](#)

[\[Session Mgmt. >> \]](#)
[\[change session \]](#)
[\[change dir \]](#)
[\[change info \]](#)

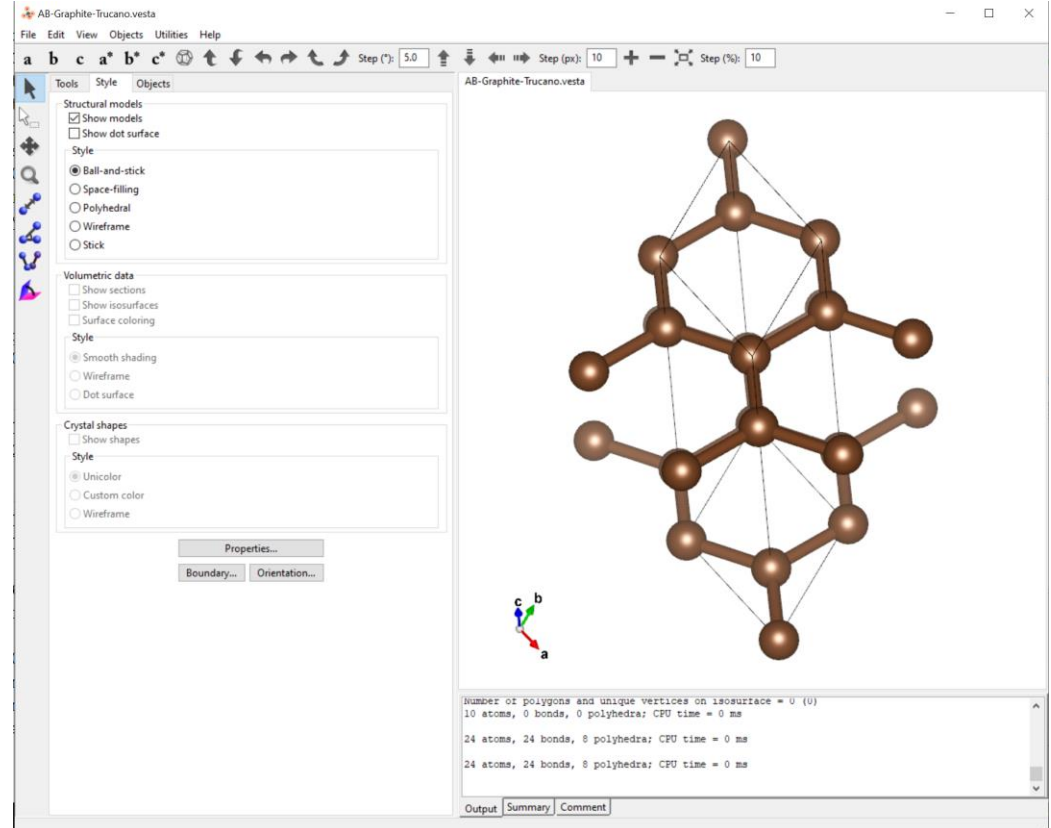
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idea and realization by
www.wien2k.at 001-2006

We can connect to w2web with 'ssh -L port:localhost:port user@cluster'
and accessing localhost:port in a web browser

Using Vesta to generate input structure



Calculating X-ray Spectra

- X-ray spectra are calculated using the XSPEC utility
- Input file is case.inxs
- Output file is case.xspec, case.txspec
- Spectra must be calculated individually for each atom and edge

Input for Absorption Spectra:

```

----- top of file: case.inxs -----
NbC: C K      (Title)
2            (number of inequivalent atom)
1            (n core)
0            (l core)
0,0.5,0.5    (split, int1, int2)
-2,0.1,30    (EMIN,DE,EMAX in eV)
ABS          (type of spectrum)
0.5          (S)
0.25        (gamma0)
----- bottom of file -----
  
```

Spectrum	n	l
<i>K</i>	1	0
<i>L_{II,III}</i>	2	1
<i>M_V</i>	3	2

Table 8.123: Quantum numbers of the core state involved in the x-ray spectra

Consideration: k-point energy convergence

- When is a calculation sufficiently accurate?
- One consideration is how the energy converges as a function of k-mesh density:

Input:

```
grepline :ENE '*.scf' 1
```

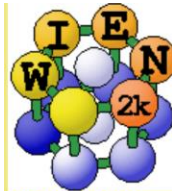
Output:

```
SnO2_500kpt.scf::ENE : ***** TOTAL ENERGY IN Ry = -25305.85703249  
SnO2_800kpt.scf::ENE : ***** TOTAL ENERGY IN Ry = -25305.85693307  
SnO2_1000kpt.scf::ENE : ***** TOTAL ENERGY IN Ry = -25305.85691537  
SnO2_1500kpt.scf::ENE : ***** TOTAL ENERGY IN Ry = -25305.85683928  
SnO2_2000kpt.scf::ENE : ***** TOTAL ENERGY IN Ry = -25305.85694803  
SnO2_5000kpt.scf::ENE : ***** TOTAL ENERGY IN Ry = -25305.85694006
```

- For more exercises see section 7.2 of S. Cottenier

Consideration: Charge Leakage, Core Levels

- For core levels, if charge leakage occurs, this can be addressed by adjusting the RMT sphere radii or running with core density superposition (run touch .lcore in project folder)
- Ensure that the core energy cutoff retains the desired energy levels as core levels



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Session: [\[ZSN_REIXS\]](#)
/globalhome/tld927/HPC/WIEN2k/ZSN_REIXS

Atomic configuration for atom: Si		Z= 14.00					
	E-up (Ry)	E-dn (Ry)	Occupancy		q/sphere	core-state	
1S	-131.237875	-131.227304	1.00	1.00	1.0000	T	
2S	-10.237696	-10.225965	1.00	1.00	0.9957	T	
2P*	-7.041595	-7.026053	1.00	1.00	0.9929	T	
2P	-6.994011	-6.978511	2.00	2.00	0.9927	T	
3S	-0.835703	-0.712146	1.00	1.00	0.1977	F	
3P*	-0.340961	-0.221156	1.00	0.00	0.1041	F	
3P	-0.338616	-0.218883	1.00	0.00	0.1029	F	

```

:WARNING:      0.052 Si   CORE electrons leak out of MT-sphere !!!!
:WARNING: touch .lcore and run scf-cycle with core density superposition
:WARNING: Or: rerun lstart with lower E-core separation energy
:WARNING: ORBITAL: 2S   -10.238  -10.226
:WARNING: ORBITAL: 2P*  -7.042   -7.026
:WARNING: ORBITAL: 2P   -6.994   -6.979
  
```

Atomic configuration for atom: N		Z= 7.00					
	E-up (Ry)	E-dn (Ry)	Occupancy		q/sphere	core-state	
1S	-28.235803	-28.124002	1.00	1.00	1.0000	T	
2S	-1.460886	-1.124777	1.00	1.00	0.7387	F	
2P*	-0.610907	-0.304313	1.00	0.00	0.6777	F	
2P	-0.609451	-0.303080	2.00	0.00	0.6770	F	

```

LSTART ENDS
0.209u 0.004s 0:00.58 34.4%      0+0k 4768+3624io 21pf+0w
  
```

Continue with

Slurm Submission

- Most jobs will be submitted to a job scheduler using a batch script (file on right)
- Fields that need to be modified are highlighted in yellow
- To see how much memory is required we can use 'htop -u user'
- To kill a process: 'killall processName'

```
#!/bin/tcsh
#SBATCH -J ZSN
#SBATCH --mail-user=tristan.deboer@usask.ca
#SBATCH --mail-type=ALL
#SBATCH --ntasks=20
#SBATCH --mem-per-cpu=3G
#SBATCH --time=3:00:00
#SBATCH --get-user-env
```


```
echo "NTASKS = $SLURM_NTASKS"
setenv SCRATCH /home/tld927/WIEN2k/ZSN/
echo DIRECTORY = $SLURM_SUBMIT_DIR
echo WIENROOT = $WIENROOT
echo SCRATCH = $SCRATCH
echo "Got $SLURM_NTASKS cores"
echo nodelist "$SLURM_JOB_NODELIST"
srun hostname -s >slurm.hosts
set proclist=`cat slurm.hosts|sort`
set nproc=$SLURM_NTASKS
set nproc0=$nproc
```

```
rm .machines
set i=1
while ($i <= $nproc0)
echo "1:$proclist[$i]" >>.machines
@ i ++
##@ i ++ # uncomment if you want to use only every second proc
end
echo "granularity:1" >>.machines
echo "extrafine:1" >>.machines
echo ' ' >>.machines
```

```
##Create .processes
x lapw1 -p -d >&/dev/null
#lapw1para_lapw lapw1.def
```

```
#####
## Now put you wien2k command like:
run_lapw -NI -p -ec 0.0001 -cc 0.01 -j 500
##x lapw2 -p -gtl
```

Making a Supercell



Session: [\[AB-Graphite \]](#)
/home/ld927/WIEN2k/AB-Graphite

Single Programs

Programs for initialisation

nn sgroup symmetry instgen_lapw
 lstart kgen dstart afminput

SCF Programs

lapw0 lapw1 lapwso lapw2
 lapwdm orb lcore mixer

Other programs

aim clmcop clminter dipan
 filtvec irrep joint lapw3
 lapw5 lapw7 optic pairhess
 qtl spaghetti supercell symmetso
 telnes3 tetra txspec xspec

Options: (help)

complex iterative noHinv spinorbit
 spin polarized: spin up spin down orb
 parallel nohns qtl band
 super fermi efg grr
 lcore copy nmat_only only def-file

Type of execution: background Execute!

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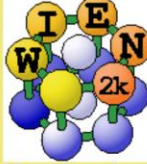
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Session: [\[AB-Graphite \]](#)
/home/ld927/WIEN2k/AB-Graphite

Filename of original struct file: AB-Graphite.struct

Number of cells in x direction: 2
Number of cells in y direction: 2
Number of cells in z direction: 1

Optional shift of all atoms (fractional coordinates)

in x direction: 0.0
 in y direction: 0.0
 in z direction: 0.0

Enter your target lattice type: P v

(Some choices are restricted by symmetry)

For surfaces or isolated molecules: (for P lattice only)

Vacuum in x-direction [bohr]: 0
 Repeat atoms at x=0: N v

Vacuum in y-direction [bohr]: 0
 Repeat atoms at y=0: N v

Vacuum in z-direction [bohr]: 0
 Repeat atoms at z=0: N v

Execute!

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Initializing a core hole calculation

- Ensure a 'unique' atom is designated in StructGen
- Add a core hole by editing case.inc
- Add compensating background charge in case.inm
- The k-mesh should be scaled down by the change in cell dimension
- Run 'x dstart'
- Run calculation as normal

Acknowledgements

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Thank you for your attention!