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Analyzing and post-processing abinit output data

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Best softwares for data analysis

- Xmgrace, gnuplot: for plotting everything you need to plot. Choose your side. Available on the internet.
- XCrysDen: for visualizing charge densities and Fermi surfaces. Available on the internet.
- Cut3d: for converting abinit output files into a bunch of different formats. Included with abinit.
- QAgate: for pretty much everything else, a.k.a. your new best friends for years to come. Available on the internet.

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I. BAND STRUCTURE

Eigenvalues
Fermi Surface
Density of States (DOS)
Projected DOS

Band structure

- Friendly reminder:
  - Electrons in a solid is a many-body problem.
  - DFT : independent electrons moving in an effective potential $U(\mathbf{r})$ and satisfying the single-electron Schrödinger equation.
  - The potential $U(\mathbf{r})$ is periodic.

- Bloch theorem: such electrons are called Bloch electrons. The associated wave functions can be expressed as plane waves:

$$\psi_{n\mathbf{k}} = e^{i\mathbf{k}\cdot\mathbf{r}} u_{n\mathbf{k}}(\mathbf{r})$$

  where $u(\mathbf{r})$ has the same periodicity as the Bravais lattice

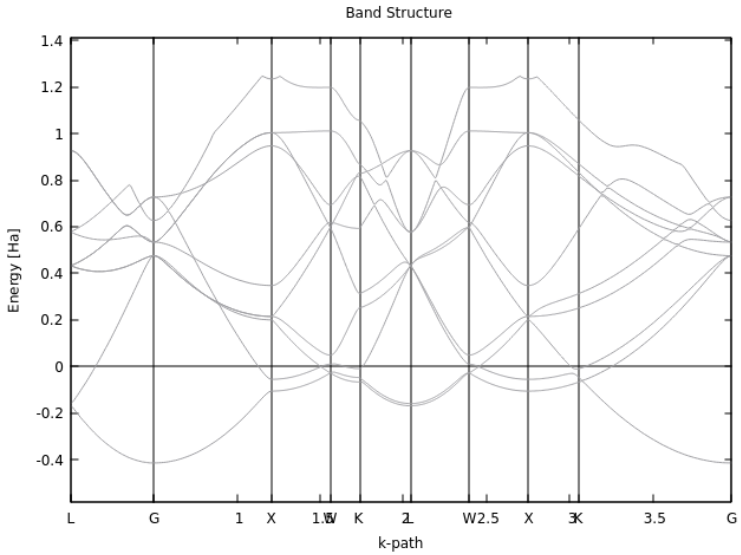
- $\mathbf{k}$ is the wave vector. n is the band index: for each value of $\mathbf{k}$, there is an infinite set of solutions of the Schrödinger equation.

- Energy levels of one electron in a periodic potential: $\epsilon_n(\mathbf{k}) \rightarrow$ band structure of the solid.

Band structure

- **How To** – Plot a band structure:
  - In the first dataset, run a regular ground state (GS) calculation.
  - In the second dataset, run a non self-consistent calculation (iscf -2): read the GS charge density (getden -1) and define the $\mathbf{k}$-point segments (kptopt, kptbounds, ndivk) .
  - Typical $\mathbf{k}$-point segments for a fcc structure: $L-\Gamma-X-W-K-L-W-X-K-\Gamma$. Available on the abinit website.
  - Plot the single electron eigenvalues $\epsilon_n(\mathbf{k})$ using your favorite tool (xmgrace, gnuplot, …)

- Example: aluminum. For each wave vector $\mathbf{k}$, there are nband bands.

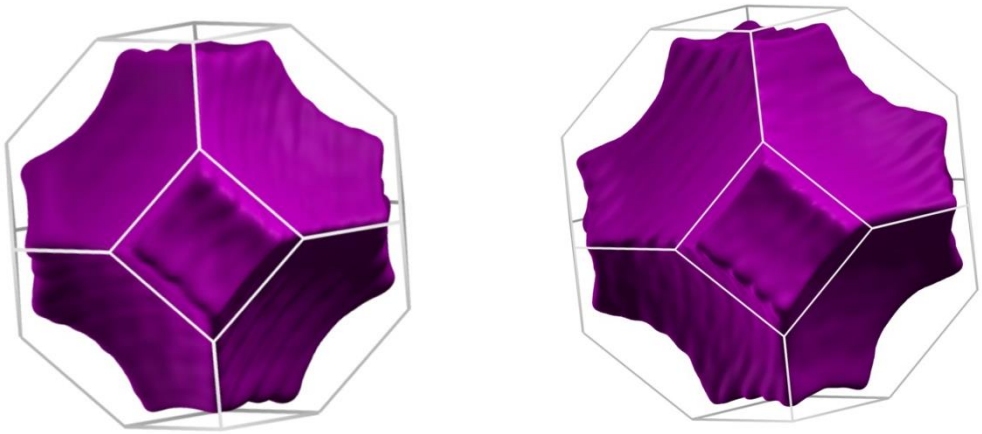


Band structure

- Fermi surface : surface that separates occupied from unoccupied states.
  - N non-interacting free electrons : the Fermi sphere.
  - N non-interacting electrons in a periodic potential : Fermi surface usually not spherical.
  - Fermi surface: constant energy surface in the $\mathbf{k}$ space.
  - Several material properties depend on the geometry of the Fermi surface.

- **How To** – Visualize a Fermi surface:
  - Run a regular GS calculation with prtfsurf 1. Fine $\mathbf{k}$-point grid required!
  - A _BXSF file is printed at the end of the calculation. Use it to draw the Fermi surface with xcrysden

- Example: aluminum.



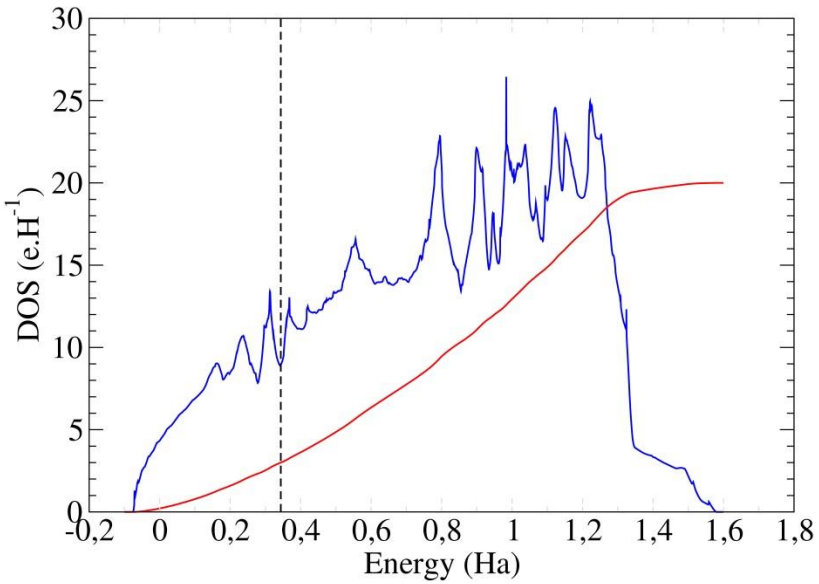
Band structure

- Density of states (DOS) $g_n(\epsilon)$: number of electronic states in the n^{th} band around ϵ.

- Integrating the whole DOS up to the Fermi level yields the total number of electrons.

- **How To** – Plot the density of states:
  - Run a regular GS calculation with prtdos 2. Fine $\mathbf{k}$-point grid required!
  - Plot the DOS using your favorite tool (xmgrace, gnuplot, …)

- Example: aluminum.



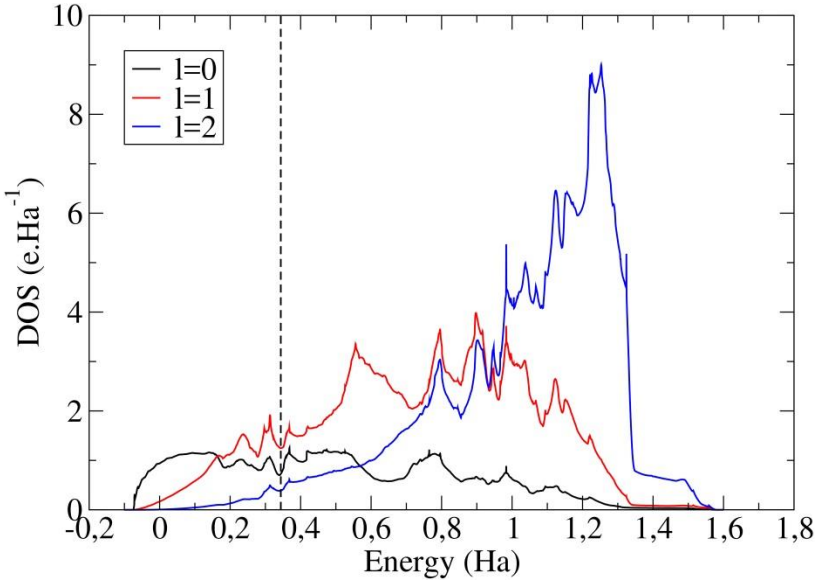
Band structure

- Projected DOS: decomposition of the DOS by atom and l quantum number
  - $l = 0 \rightarrow s, l = 1 \rightarrow p, l = 2 \rightarrow d, l = 3 \rightarrow f$.
  - Contribution of each atomic orbital to the total DOS.

- **How To** – Plot the l-decomposed DOS:
  - Run a regular GS calculation with prtdos 3. Specify the number (natsph) and index (iatsph) of the atoms to be considered.
  - Plot the DOS using your favorite tool (xmgrace, gnuplot, …)

- Example: aluminum, one atom.

- Careful: Only electrons in PAW spheres are accounted for.



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II. CHARGE DENSITY

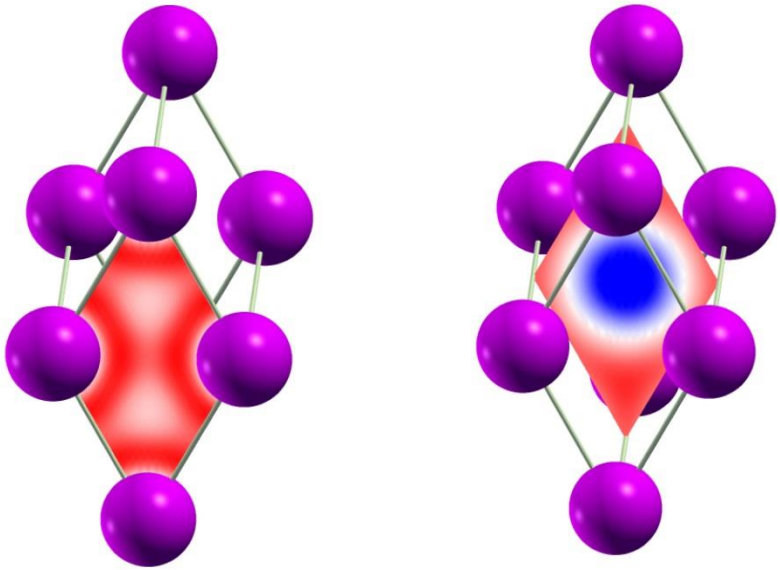
Charge Distribution
Magnetic Moments

Charge density

- Friendly reminder:
  - DFT: the charge density instead of the wave functions.

- **How-To** – Visualize the charge density in the cell:
  - Run a regular GS calculation, this will output by default the charge density file _DEN.
  - Use cut3d to convert the charge density file into an xcrysden .xsf file.
  - Use xcrysden to open the .xsf file and visualize the charge density. Requires a bit of practice!

- Example: aluminum.



Charge density

- Integrating the charge density inside PAW spheres yields, if any:
  - The atomic magnetic moments.
  - The Bader charges.

- **How-To** – Get atomic magnetic moments:
  - Run a regular GS calculation including spin-polarization (nsspol 2). This will take twice more time!
  - Search for the string "Diff" at the end of the output file.
  - Diff(up-dn) column shows the atomic magnetic moments.

```
 Integrated electronic and magnetization densities in atomic spheres:
 ---------------------------------------------------------------------
 Note: Diff(up-dn) is a rough approximation of local magnetic moment
 Atom    Radius     up_density    dn_density  Total(up+dn)  Diff(up-dn)
    1   1.90363      0.393496      0.393496      0.786991    -0.000000
 ---------------------------------------------------------------------
```

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III. QAGATE

Installation
Features

Animemd

- Qagate is the ultimate tool for abinit. You can:
  - Visualize crystal structures, get space group, …
  - Calculate bond distance and angles.
  - Plot total energy, pressure, temperature, stress, etc. with respect to time step, image, etc.
  - Visualize phonon modes and condense unstable modes.
  - Build supercells for studying defects.
  - Visualize diffusion pathways.
  - And much more!

- **How-To** – Install qagate (Linux only):
  - Add the repository to your repository list:

    sudo add-apt-repository ppa:piti-diablotin/abiout

    sudo apt-get update
  - Install qagate:

    sudo apt-get install abiout