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1 Density of states

We already talked about the density of states (DOS) of the homogeneous electron gas and its definition in general (see exercise sheet 2). Now we want to calculate it *ab inito* for different materials like insulators, semi-conductors and metals.

1. Perform ground state calculations for silicon, aluminum and sodium chloride (optional: gallium arsenide, iron). Plot the density of states for each material using

   ```
   en, dos = si.calc.get_dos(spin=0, npts=201, width=0.1)
   ```

   and study their differences. What can you tell about the DOS at the Fermi level $D(E_\mathrm{F})$?

   Note: Especially for metals, you need a rather dense k-grid. Once your code works without errors, you should use a BZ sampling of $12 \times 12 \times 12$ points and a plane wave cut-off of $800\,\mathrm{eV}$.

2. What can you conclude for the bandstructure just from looking at the DOS plots?

3. What is the result of integrating the DOS of non-metals a) over the entire computed range and b) up to the Fermi energy? What changes if you vary the `nbands` parameter?

   Hint: For finding the index of the energy nearest to E_F, slicing the DOS-array at E_F and plotting a vertical line at E_F, you can use this snippet:

   ```
   idx = np.abs(en - efermi).argmin()
   dosUpToEf, enUpToEf= dos[:(idx+1)], en[:(idx+1)]
   plt.axvline(x=efermi, ls="--", alpha=0.5)
   ```

2 Projected density of states

As briefly mentioned in last lab's sheet, there is a method to project the DOS onto a set of atomic orbitals in order to calculate the so-called *projected* density of states. It is sometimes used by researchers for bonding analysis and can be motivated as follows:

We start with the definition of the DOS and add a "one" of the form $1 = \langle \psi_n | \psi_n \rangle$, where $\{|\psi_n\rangle\}$ is the set of (orthonormalized) Kohn-Sham eigenstates (= auxiliary states used in DFT),

$$D(E) = \sum_n \langle \psi_n | \psi_n \rangle \, \delta(E - E_n) \,. \tag{1}$$

Now we can insert identity again using the completeness property of bases,

$$\mathbb{1} = \sum_k |k\rangle \langle k| = \int \mathrm{d}^3 \boldsymbol{x} \, |\boldsymbol{x}\rangle \langle \boldsymbol{x}| = \sum_i |\phi_i^a\rangle \langle \phi_i^a| \,, \tag{2}$$

where $\{|\phi_i^a\rangle\}$ is again a set of orthonormal, but *atomic* eigenfunctions corresponding to atom a. This transforms the DOS into

$$D(E) = \sum_{n,i} |\langle \phi_i^a | \psi_n \rangle|^2 \, \delta(E - E_n) = \sum_i D_i(E) \,, \tag{3}$$

where the individual PDOS functions are now simply defined as

$$D_i(E) = \sum_n |\langle \phi_i^a | \psi_n \rangle|^2 \, \delta(E - E_n) \,. \tag{4}$$

The total density of states "TDOS" is then reobtained by summing over all PDOS,

$$D(E) = \sum_i D_i(E) \,. \tag{5}$$

A nice summary of this topic can be found in the GPAW documentation:
https://wiki.fysik.dtu.dk/gpaw/tutorialsexercises/electronic/pdos/pdos.html

You can use the function

```
calc.get_orbital_ldos(a=atomID, spin=0, angular=orbital, width=0.3, npts=2001)
```

to calculate the DOS projected on wave functions of atom with index a (e. g. 0 and 1 for As and Ga in GaAs or Si #1 and Si #2 for Si in diamond structure) and orbital `'s'`, `'p'`, `'d'` or `'f'`. The parameter `width` is again a smearing factor which is used to smooth out the resulting plot.