



Presenting DFT results:
the Methods section

The methods section: general principles and goals

- It should allow the reader to understand what calculation was performed, to assess how the results were obtained
Example: you find a heavily underestimated band gap; this is normal if you have used DFT-PBE; this is strange if you have used Hartree-Fock
- It should allow to reproduce the calculation
If the reader has access to the code, does the reader have all information to reproduce it?

The methods section: which information is crucial (1)

- to understand what calculation was performed,
- to reproduce the calculation
- Obvious information (not necessarily in this order):
 -) basis set (linearised augmented plane-waves + local orbitals, plane waves, Gaussians, numerical orbitals,...)
 -) exchange and correlation functional
 -) code used (Wien2K,...)
 -) Core states vs. valence states (see next slides)
 -) k-points (shifted/unshifted)

The methods section: which information is crucial (2)

- Obvious information (not necessarily in this order):
 -) other parameters that regulate precision/convergence (e.g. cutoff energy)
 -) occupation scheme for Kohn-Sham eigenstates (smearing scheme, smearing width)
 -) convergence criteria for the selfconsistent cycle, and in case for relaxation
 -) structure and simulation cell (see next slides)
 - [-) for molecular dynamics: ensemble, thermostat, bariostat, temperature, pressure]

REFERENCES!

The methods section: core, semi-core and valence

report explicitly which states were treated as valence (sometimes it is enough to report the number of valence electrons)

for Wien2K, state also which states were treated as semi-core

for pseudopotential codes, report also kind of pseudopotential, and also database/specific name

The methods section: structure and simulation cell

Also in this case, there should be enough information to identify the structure of crystal/surface/molecule:

one could specify also the ICSD or COD code, space group + Wyckoff sites + all free parameters;

or .cif file in the supporting information;

gaining ground: put structures, or the whole input files, in public repositories, either on personal spaces (github) or on public databases (e.g. Zenodo by CERN)

Specific for wien2k:

wien2k version 23.2

initialization with `-prec 0-3(n)`

defines HDLO basis and several computational parameters:

$R_{\min} K_{\max}$ (plane-wave cutoff)

RMTs for all atoms

GMAX (Fourier series for charge density/potential)

FFTfactor (additional factor for XC-potential FFT mesh)

L-vns (max l for $H_{\text{non-spher.}}$)

E-cut (or charge-cut) for core-valence separation, or better an explicit list of core states, semicore (treated with LOs) and valence states. Explicit list for HDLOs (or HELOs)

The methods section: more details on the Hamiltonian

For a simple Kohn-Sham Hamiltonian, specification of the exchange and correlation functional is sufficient

However, more sophisticated Hamiltonians require further specifications:

-) Hubbard U correction comes in different flavours
-) spin-orbit coupling
-) hybrid functionals
-) van der Waals potentials/functionals
-) ...

The methods section: less crucial parameters

For example, details of how selfconsistency is reached (preconditioning, mixing) affect speed of convergence, but 'usually' not the final result.

However, there might be difficult cases where this information is important to reach selfconsistency at all (magnetic systems...)