Ab initio methods in solid state physics

XIV. Toolbox

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Computational Solid State Toolbox

- Low level
  - Kinds of ab-initio codes
  - You get what you pay for?
- High level
  - Individual interfaces
  - Umbrella codes
  - Post processing tools
  - Computing environments
  - Visualisation

Ab Initio programs (by method)

- plane wave (VASP, AbInit, QE, ...)
  - Long range interactions, expensive vacum, high accuracy, bed scaling
- localized orbitals (Siesta, OpenMX, ...)
  - linear scaling, low acuracy, free vacum
- LAPW (GPAW, Elk, Fleur, ...)
  - Expensive, good for electronic structure
- Gaussian (gaussian, nwchem, ...)
  - chamistry
- Mixed (GM/MM, Wien2K, ...)
  - often specialized codes
- Many more:
  - Wikipedia: List_of_quantum_chemistry_and_solid-state_physics_software
  - ASE: https://wiki.fysik.dtu.dk/ase/ase/calculators/calculators.html

Ab initio programs - other classifications

- Non-free
  - CASTEP, Gaussian, Mopac, ...
  - VASP, Wien2k, ONETEP, ...
- Gratis
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- Gratis
  - AbInit, QE, Siesta, GPAW, ...
- Closed source
  - CASTEP, Mopac, ...
- Open source
  - VASP, Wien2k, ONETEP, ...
- Free software
  - AbInit, QE, Siesta, GPAW, ...

Free/Gratis/Open/Close ???

Why is source important?

- You need to know what you are doing!
- Do you want to tell the referee: *I do not know. I just push this button.* ?
- **REPRODUCIBILITY**
- Eventually, you will need to change or inspect the code to get your idea working.
- Sharing your results

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Why price is *less* important

- Your equipment is usually more expensive (Wien2k is 400EUR, VASP 5000EUR)
- Sometimes even your one conference trip
- You can use your grant money for this
- Sometimes *it is worth it* - not always

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- Interfacing
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  - Electronic structure (WANNIER90, BandUP, ...)
  - Other (XtalOpt, BoltzTraP, Elastic, ...)
  - Good scripting language (Python, Rust, Julia, Go, ...)
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- Writing
  - Plain text is **The King**
  - Give Markdown a try, if you need formating (these slides are MD+Quarto)!