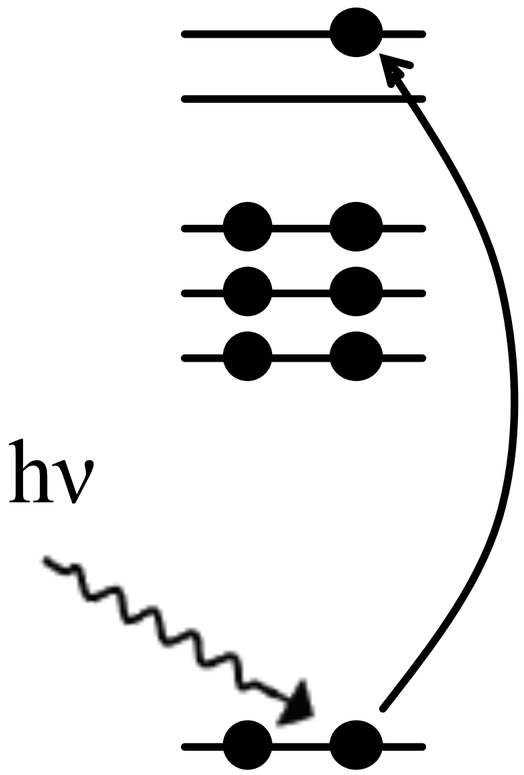
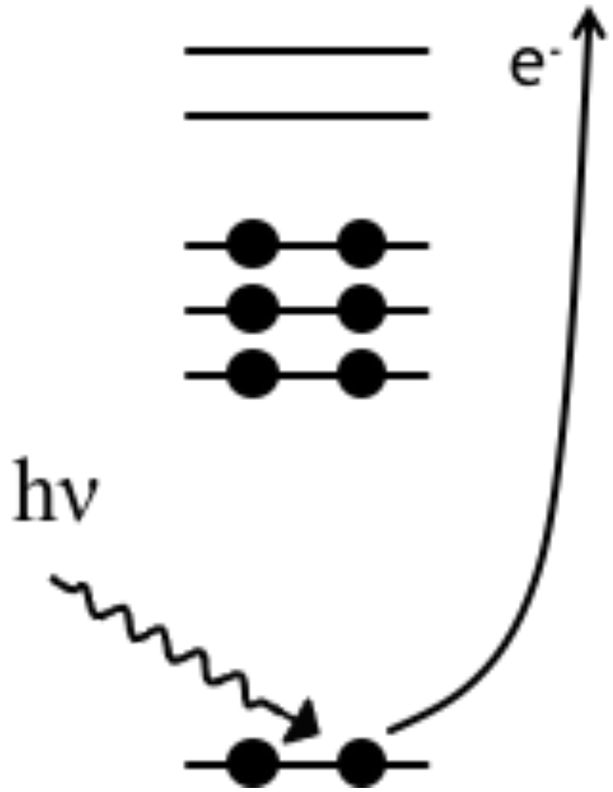
XPS with ADF



XAS



XPS
Core electron binding energy

- Experts: Mauro Stener, Del Chong
- ADF: Erik van Lenthe
- NEXAFS / XANES exercise also available

Calculating XPS peaks

Compare binding energy of neutral system with core hole state (+1)

In ADF we set explicit core holes with IRREPOCCUPATIONS

Choose frozen cores for all other elements, so it’s easier to identify the orbital we want to de-occupy for the all-electron element(s).

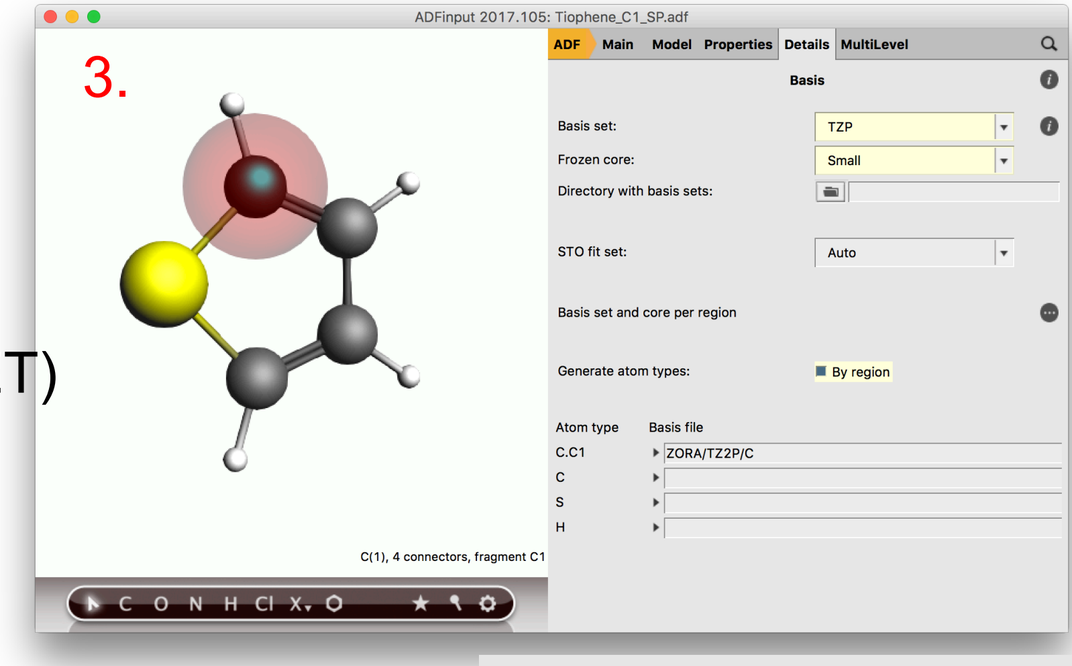
In the GUI: run a Single Point, unrestricted, to easily set the occupations

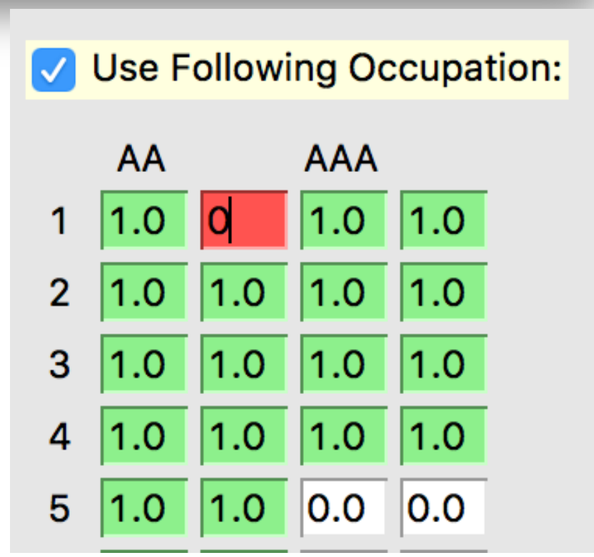
Workflow XPS

1. Optimize your molecule (e.g. BP/TZP-small core)
2. Select ‘unrestricted’
3. Select the atom of interest and make it a region
4. Define a large AE basis set for it (TZ2P, QZ4P, or ET)
5. Save as other, Run as single point
6. Model => Spin & Occupations
7. Remove a core beta electron (1.0=>0.0)

   Check ADFlevels / output to see which orbital if its ambiguous

   You may have to go to ‘Details => Run script’ and explicitly set occupations
8. Save as other & Run
9. Compare the Bond energies (logfile) between 5. and 8.
10. Repeat for cores of other atoms





Command-line: just set regions, explicit basis sets and the occupations

See also: Example for Core Energy Binding Energies by using core-hole fragments

Example: Thiopene C1 & C2 (inputs), compare with literature