



Topics of exercises

Basic tasks with w2web: setup, scf, DOS, bandstructure, electron density
Volume optimization, Optimization of free atomic positions, optimization of
lattice parameters
Cohesive energies
Supercells, surfaces, adsorption energies
Commandline interface
Parallelization
Magnetism
meta-GGAs, mBJ and hybrid-DFT
DFT+U and EECE
Optical properties
Valence photoelectron spectra
Xspec (XANES), EELS and XPS
Phonons
Atoms-in-molecules
Hyperfine interactions (EFG, NMR chemical shifts)
Wannier functions, Polarization, Born effective charges
Topology, Chern number, Weyl points
Effective masses
Thermoelectric properties
Impurities, fold2Bloch