wien2k goodies: Utility scripts:

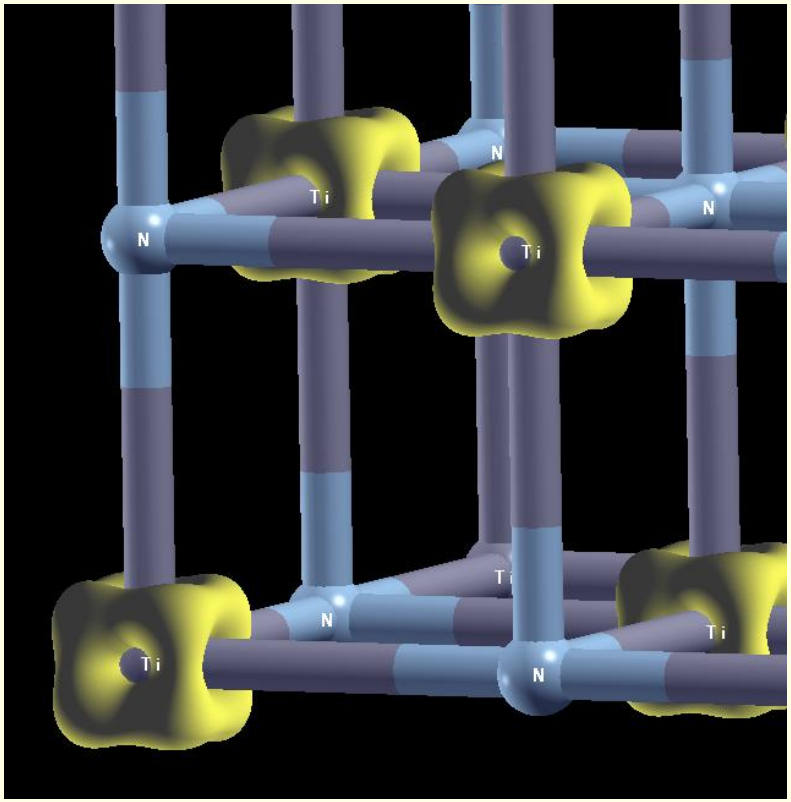
- **hex2rhomb**
  - *converts hexagonal to rhombohedral coordinates needed for R cells. (Remember: WIEN2k uses hexagonal a,c; but rhombohedral atomic positions for R spacegroups)*
- **x struct2cif**
  - *writes a cif file from your optimized structure*
- **x xyz2struct**
  - *converts POSCAR to struct file*
- **run123_lapw**
  - *runs initialization+scf with different precisions*
- **clean_lapw**
  - *removes temporary and large files once a case has been finished to save disk space*

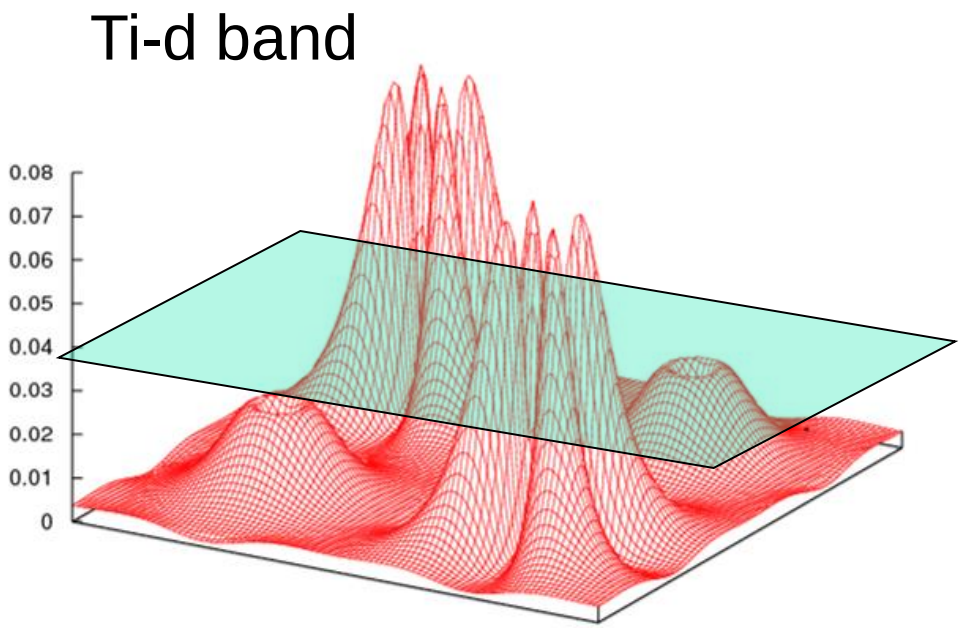
Utility scripts

- **migrate_lapw** [FLAGS OPTIONS] [user@]host:path/case-dir
  - *-put -> transfer of files to a remote host (default)*
  - *-get -> transfer of files from a remote host*
  - *-all -> the complete directory is copied*
  - *-start -> only files to start an scf cycle are copied (default for put)*
  - *-end -> only new files resulting from an scf cycle are copied (default for get)*
- **create_add_atom_clmsum_lapw**
  - *The script creates a better starting density for a case, where you already have a scf-solution for a "similar" case (differs by ONE atom).*
- **reduce_rmt_lapw** [-r XX / -a XX:Rxx,YY:Ryy,... -sp -vxc X]
  - *when touching spheres occur during structure optimization, use this script to reduce RMTs and extrapolate the density*
- **min_lapw** (**+mini**): alternative position optimization, can also do (limited) MD (molecular dynamic)

wien2k goodies: programs

- x 3ddens
  - *creates 3D electron densities (XSF file), useful for empty structures/surfaces, convenient for STM simulations*





wien2k goodies: programs

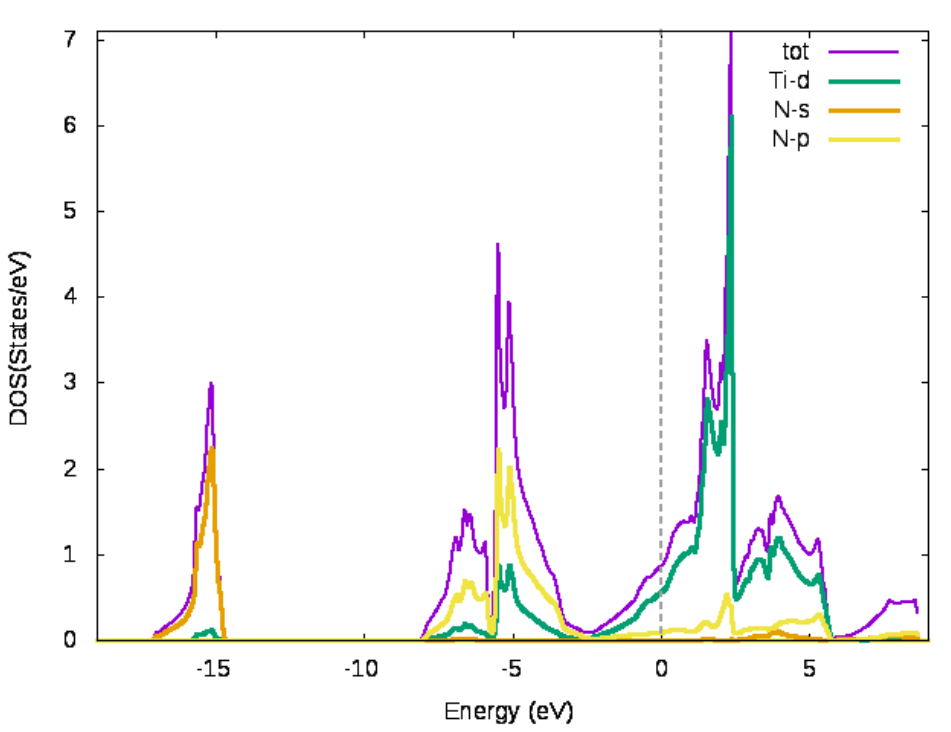
- x rendos
  - *creates renormalized partial DOS (sum of PDOS = total DOS; no interstitial) by a least squares fit and optimizing the orbital localization*

Orbital	*fract (outputst)*	*fract (opt.)*	*charge-tot*	*charge-tot (opt.)*
Ti3d	*0.78*	*0.91*	*1.70*	*1.85*
Ti4s	*0.11*	*0.26*	*0.13*	*0.48*
Ti4p	*0.30*	*0.24*	*0.25*	*1.05*
N 2s	*0.81*	*0.96*	*1.49*	*1.55*
N 2p	*0.74*	*0.80*	*3.13*	*3.92*
Sum of spheres (should be: 9.00)			*6.70*	*8.86*

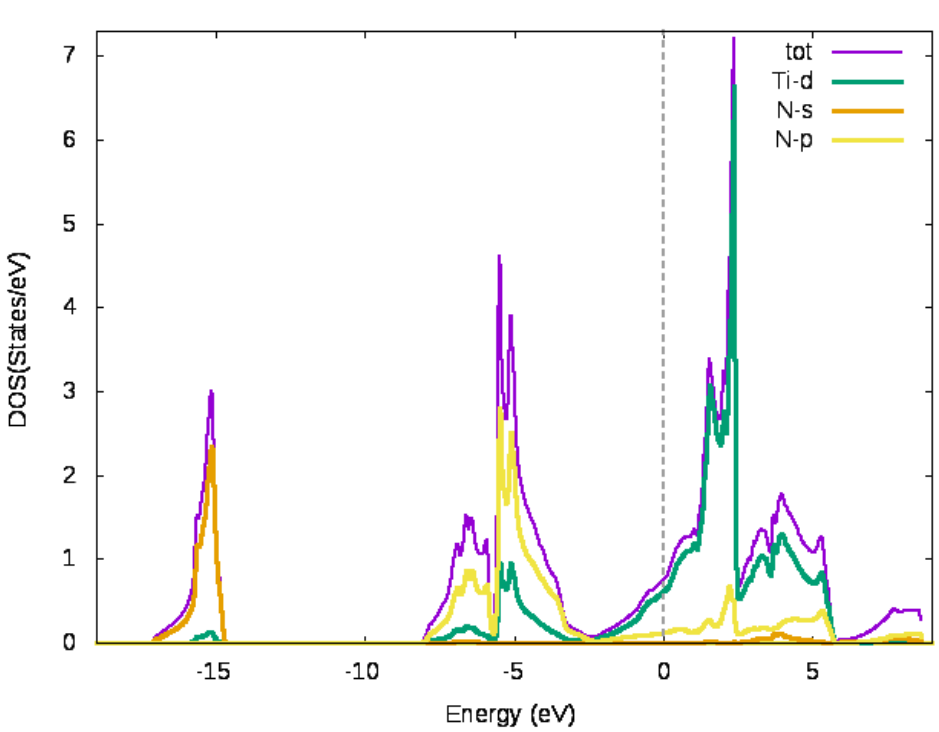
  - *2.3 e from interstitial → increased atomic charges*

rendos

DOS



renormalized DOS

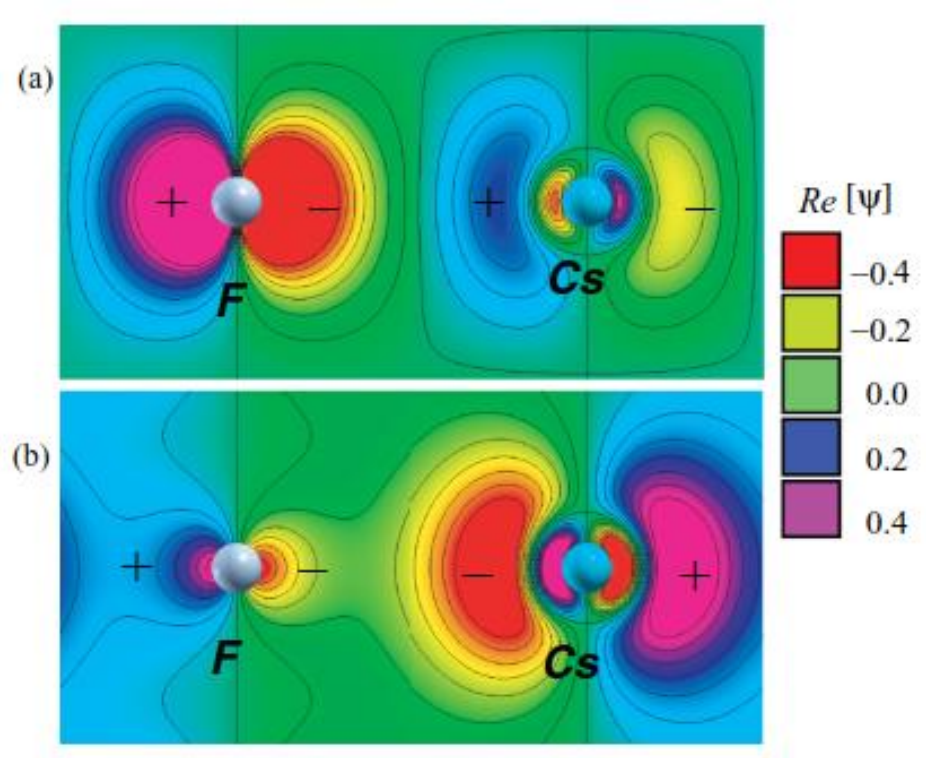


wien2k goodies: programs

- x dipan
  - *This program calculates the magnetic dipolar hyperfine field and the dipolar magnetocrystalline anisotropy by a direct lattice summation over the magnetic moments of all sites.*
- elast - Irelast
  - *elastic constants for different crystal structures*
- x fsgen
  - *2D Fermi surface plots in various planes of the BZ*
- x lapw3
  - *X-Ray structure factors (Fourier transformation of the density)*

wien2k goodies: programs

- x lapw7
  - *2D plot of wavefunktion (modulus, real or imag.part) of one eigenvalue at one k-point (bonding – antibonding analysis because of sign)*

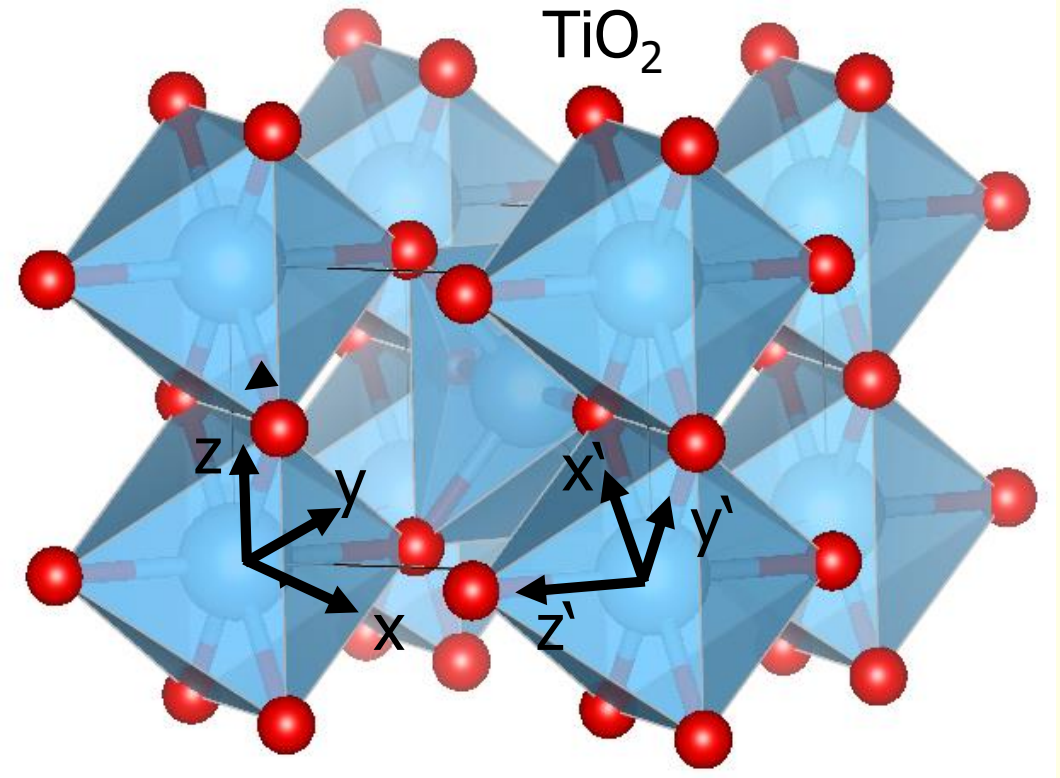


antibonding wavefunction at X in F-p band

bonding wavefunction at X in Cs-p „semicore"-band

wien2k goodies: programs

- x qtl
  - *partial charges for f-electrons,*
  - *in different coordinate systems (octahedra for e_g/t_{2g} analysis),*
  - *for spin-orbit analysis (p-1/2 – 3/2; ...);*
  - *„cross" partial charges for telnes3*



wien2k goodies: programs

- x telnes3
  - *simulation of core-electron energy loss spectra (EELS), can include non-dipole transitions (needs some knowledge of the experimental setup). Valence-EELS available in „optics".*
- x tetra
  - *DOS for 1 k-point by Gaussian (Lorentzian) broadening.*
  - *summation over different PDOS (eg. sum all O atoms in a structure)*
- x animxsf
  - *creates an animated xsf file from the scf file of a position-optimization, displayed by: xcrysden --xsf case.xsf (or VESTA)*
- x arrows
  - *allows to display the "**forces acting on all atoms**" or*
  - *the "**differences between two structures**"*
  - *using arrows in Xcrysden (see UG)*

structeditor

- octave: helpstruct
  - *a2adist* * calculates distance between atoms
  - *mina2adist* * calculates minimum distance between atoms
  - *addatom* * adds an atom to the structure
  - *addeqatom* * adds an atom and all equivalent
  - *copyatom* * creates a copy of an atom
  - *getaname* * converts atomic number into atomic symbol
  - *getar0* * calculates r0 from atomic number
  - *getazz* * converts atomic name into atomic number
  - *loadstruct* * reads Wien2k structfile
  - *makeconventional* * converts structure into the conventional form
  - *makeprimitive* * converts structure to the primitive form
  - *makesupercell* * creates supercell
  - *makesurface* * creates surface
  - *mergestruct* * merges two structures
  - *movealla* * moves all atoms with vector vec

structeditor

- *replaceatom* * replaces an atom with other atom
- *replaceeqatoms* * replaces an atom and all equivalent with other atoms
- *rescale_c* * rescales c for surface cell (vacuum in the middle)
- *rescale_c_2* * rescales c for surface cell (vacuum above)
- *rescale_c_3* * rescales c for surface cell (vacuum outside)
- *rmatom* * removes an atom
- *rmeqatoms* * removes an atom and all equivalent
- *rotateall* * rotates all atoms around z with a given angle
- *rotateatomlist* * rotates specified atoms around z with a given angle
- *rotatethreedim* * rotates specified atom around vector with given angle
- *savestruct* * saves crystal structure
- *shiftatomlist* * shifts specified atoms by a vector
- *showequivalent* * outputs list of equivalent atoms
- *showstruct* * displays structure (using xcrysden)
- *smultatom* * creates symmetry equivalent positions
- *sshift* * symmetric shifts of equivalent atoms

- *help command* * gives help

unsupported software

- **WIENNCM**: noncollinear magnetism code (free for registered users)
  - *spin-spirals (no spin-orbit)*
  - *fully non-collinear WIEN2k*
- **BSE** code (free for registered users)
  - *valence and core excitons, including spin-orbit core states*
- **GAP2-GW** code from Hong Jiang
  - *state of the art quasiparticles, band gaps*
- **CFP** by Pavel Novak
  - *crystal field parameters in 4f systems*
- **DMFT** Dynamical mean field theory (for correlated electrons)
  - *TRIQS*
  - *DFT+eDMFT (By K. Haule)*

unsupported software

- **SKEAF** by P.M.C. Rourke.
  - *Extracts **quantum oscillation frequencies** and **effective masses** from **fermi surfaces (De Haas-van Alphen)***
- **ATAT@WIEN2k** by M. Chakraborty et al.
  - *Interface between WIEN2k and the "Alloy Theoretic Automated Toolkit" (ATAT), which is a cluster expansion package for simulations of phase diagrams of alloys*
- **ElaStic** (and similar tools, see wien2k.at)
  - *for elastic constants (of various lattices)*
- **VESTA** (visualization program)
  - *displays also partial unitcells and atoms outside the unit cell if part of a coordination polyhedra; (transparent) coordination polyhedra, multiple bonds (thick and thin rods for small and larger distances); can plot xsf files; allows manipulation of the structure (VESTA → cif → struct)*