(Spin) bulk band structure calculations with SFHIngX

Session D3
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Workshop on application of Density-Functional Theory in Condensed-Matter Physics, Surface Physics,Chemistry, Engineering, and Biology
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Fritz-Haber-Institut der Max-Planck-Gesellschaft,
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Talk / session flow

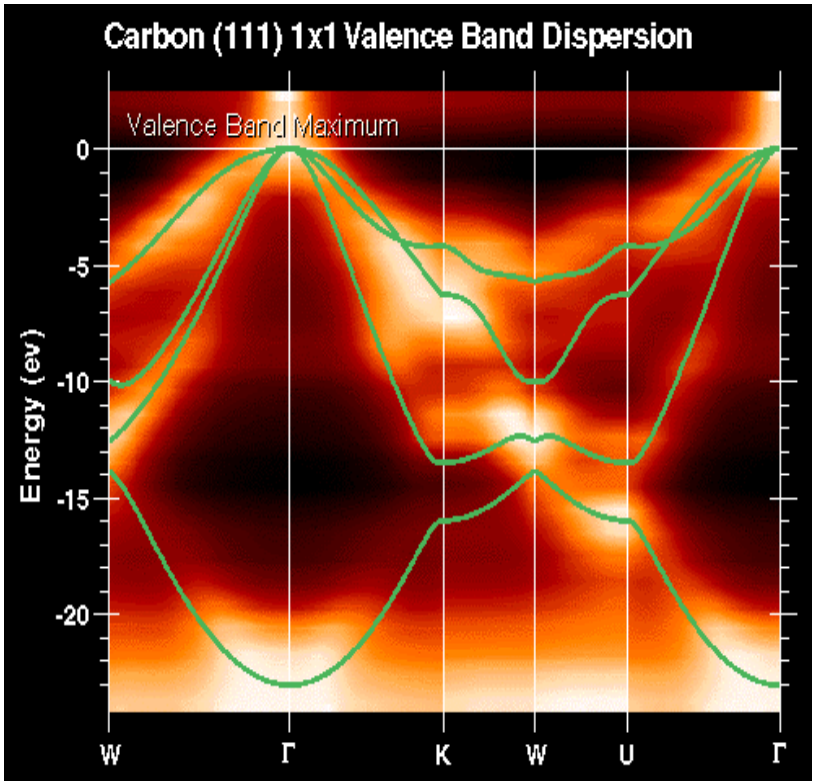
List of tasks:

- Recall how to setup SCF run
- Learn how to setup band structure calculations
- Learn how to analyze band structure output

- Magnetic systems
- How to setup initial magnetic structures
- Band structure for magnetic system

Why should one care about band structure?

- Understanding of physics at nanoscale
- Deep understanding of material properties à engineering of new materials, feasibility of its application in industry (optical / electronic / magnetic / spintronic / catalytic devices)
- Direct comparison with experiment à



Comparison between angle-resolved photoelectron spectroscopy and theoretically predicted band structure *

*Taken from http://www-als.lbl.gov/als/science/sci_archive/diamond.html

How to obtain band structure?

1 • Have full description of the system = know Hamiltonian operator

In frame of Kohn-Sham theory means to get converged ground-state charge density

SCF charge density
SCF wave-functions

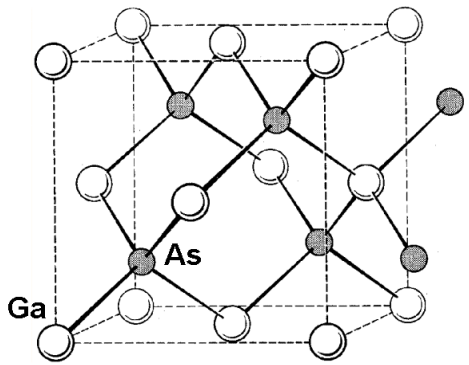
2 • Diagonalize Hamiltonian employing specified k-point set →

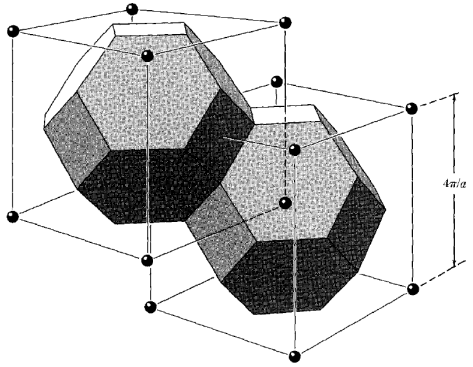
One-particle eigenspectrum (band structure)

3 • Density of allowed states in given energy interval (TDOS)

4 • Atom resolved contributions to density of allowed states in given energy interval (PDOS)

1 • How to get full description of the system?



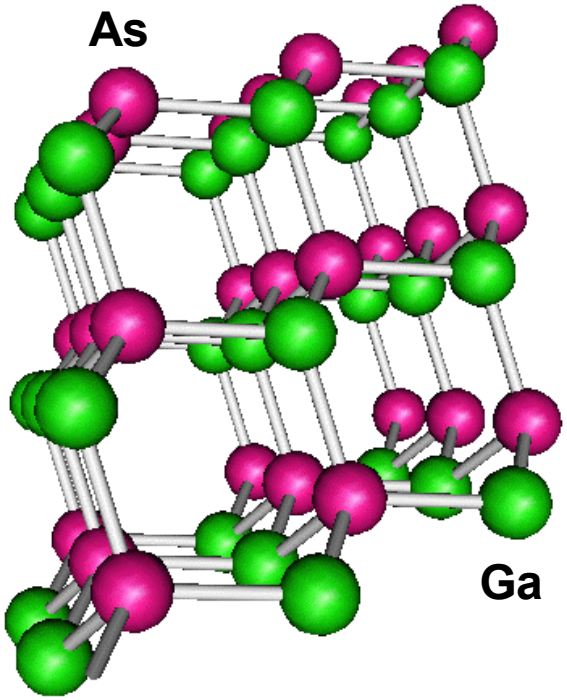


GaAs crystal structure
and corresponding
(fcc) Brillouin zones

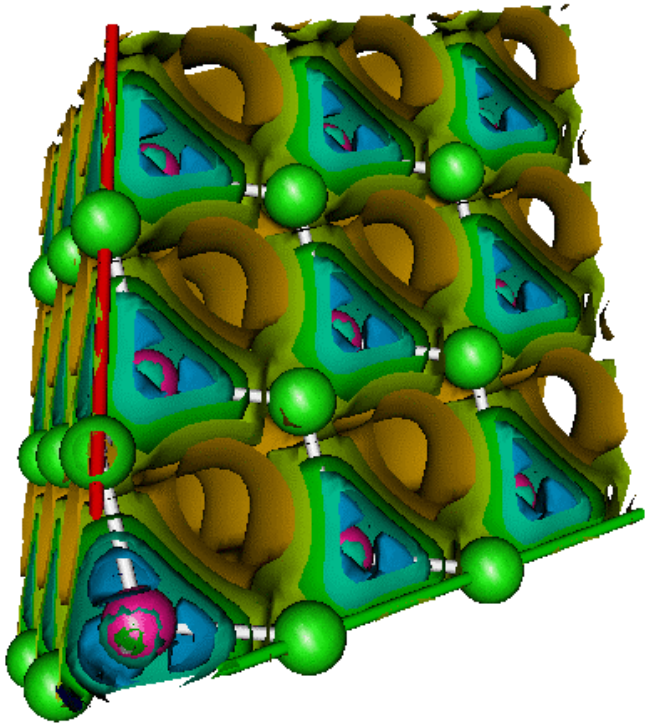
```
structure { … }      ß  Can be checked with pxviewer
basis {                                        Converged
  eCut    = 10; // Ry
  kPoint { coords = [1/2, 1/2, 1/2]; weight = 1; relative; }
  folding = [4, 4, 4];
}
Hamiltonian { … }
initialGuess { … }
main {
  DIIS_CCG {                    Updates charge density
  …
  dEnergy      = 1e-04; // Hartree
}
}
```

Schematic structure of input.sx (SCF)

What one gets after SCF calculation?



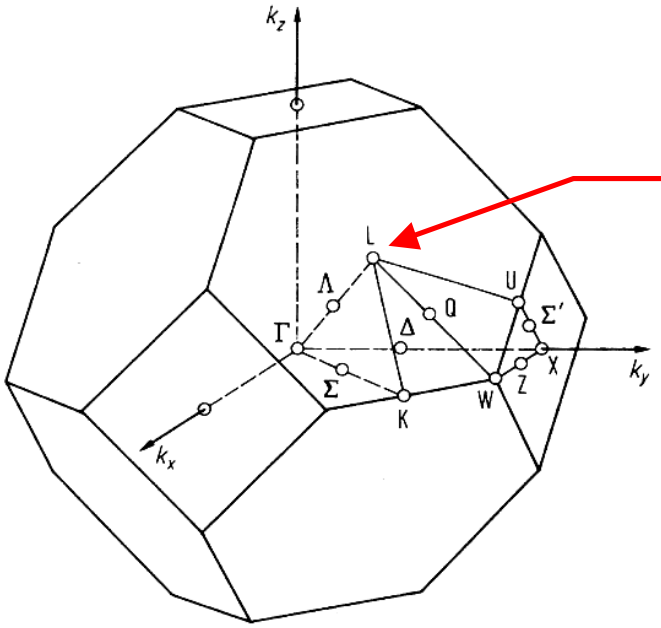
GaAs atomic structure



GaAs SCF charge density

Self-consistent (SCF) converged charge density
Set of SCF wave-functions
Fermi energy and occupations

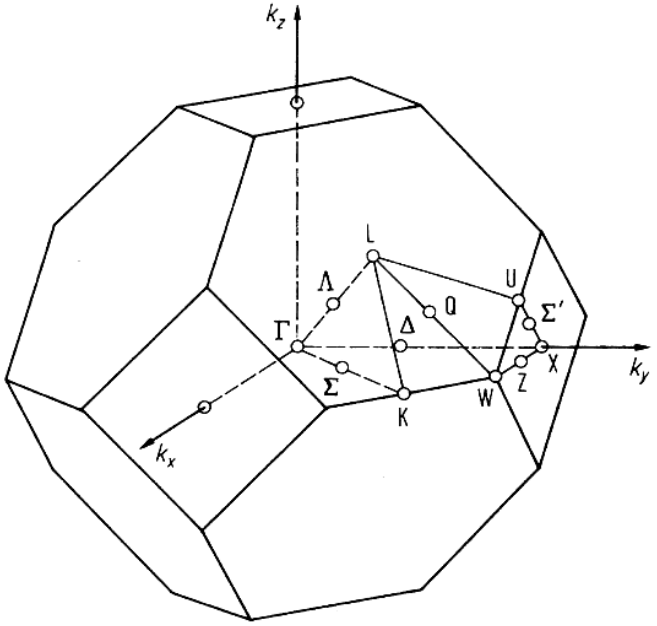
How to diagonalize SCF Hamiltonian?



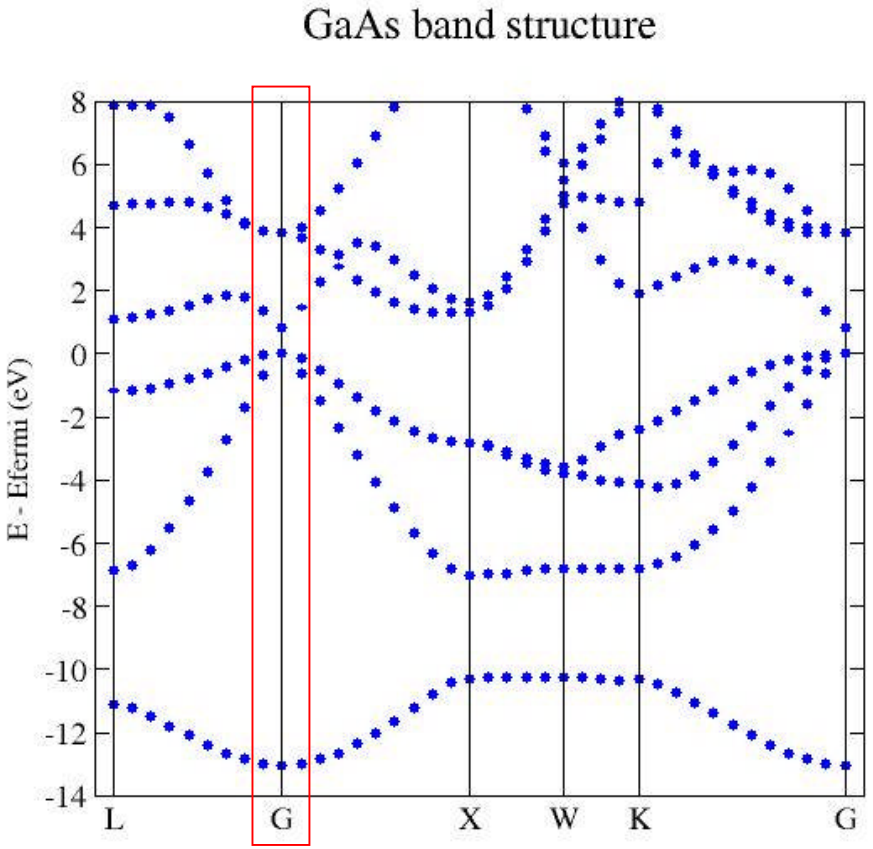
GaAs crystal structure and corresponding (fcc) Brillouin zone

```
structure  { … }      ß  Can be checked with pxviewer
basis  {
  eCut    = 10;  // Ry   ß  Must be as in SCF
  kPoints {                                          Any set
    from { coords = L; label = "L";}
    to     { coords = G; label = "Gamma"; nPoints = 9;  }
    …
    to     { coords = G; label = "Gamma"; nPoints = 11; }
  }
}
Hamiltonian  { … }
initialGuess  { rho = "scf-rho.sxb"; … }     Read-in SCF
main  {
  DIIS_CCG  {          Keep SCF charge density
  …
  keepRhoFixed;   ß VERY IMPORTANT
  dEnergy       = 1e-04;  // Hartree
  }
}
```

What we get after band structure calculation?



GaAs crystal structure
and corresponding
(fcc) first Brillouin zone

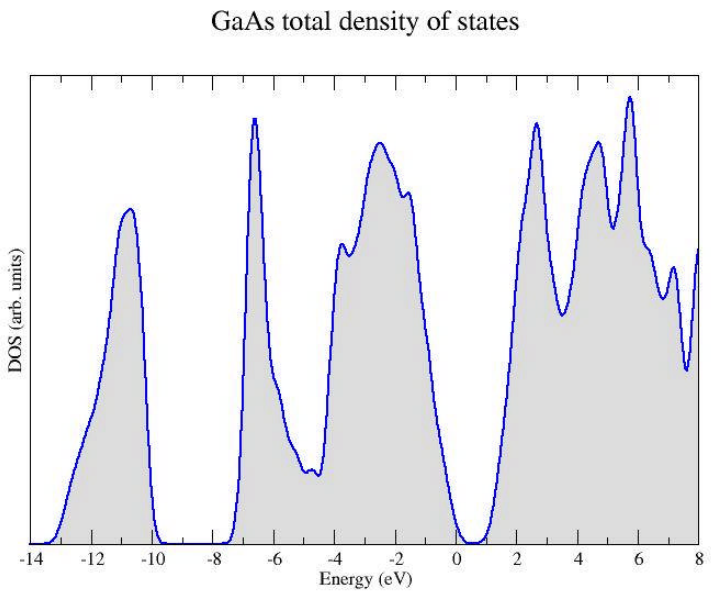


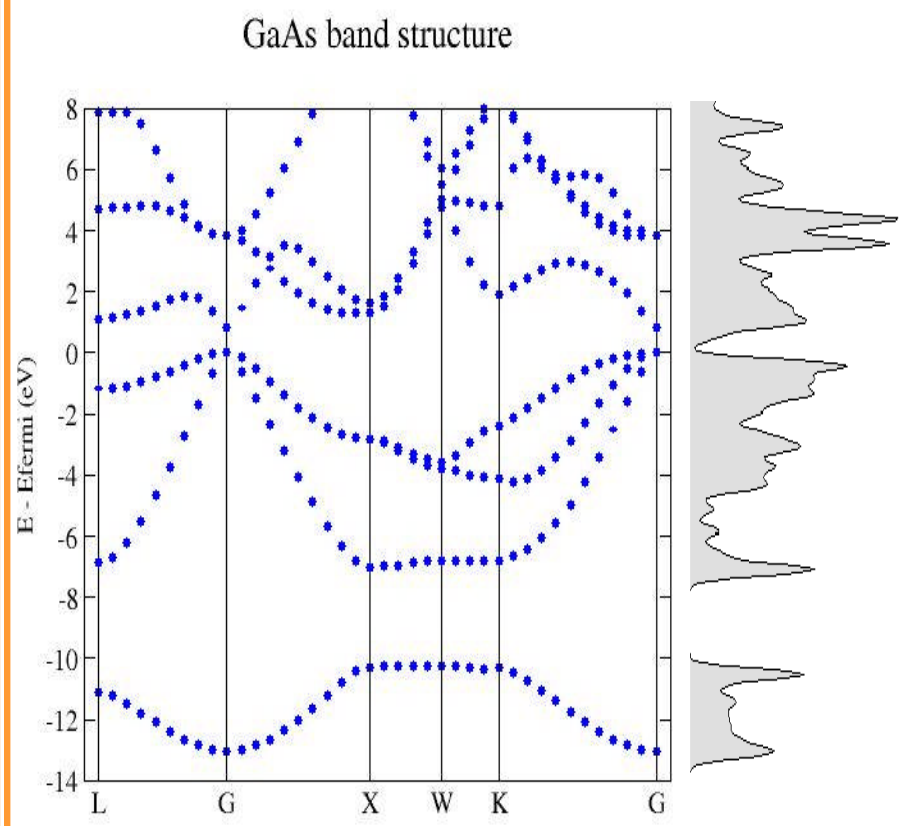
What we have discovered:
- Semiconductor
- Direct band gap
- Band gap width 0.90 eV

3 • Can one do more?

Total density of states (TDOS)
→number of available states
at given energy

$$TDOS(\mathrm{e}) = \sum_{i,k} w_k \, G(\mathrm{e} - \mathrm{e}_{ik})$$





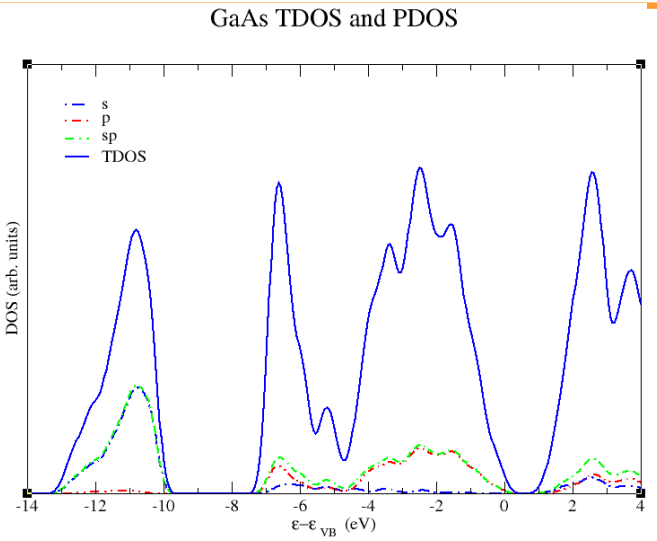
Band structure of GaAs at equilibrium

Attention – broadening is artificial → convergence tests needed

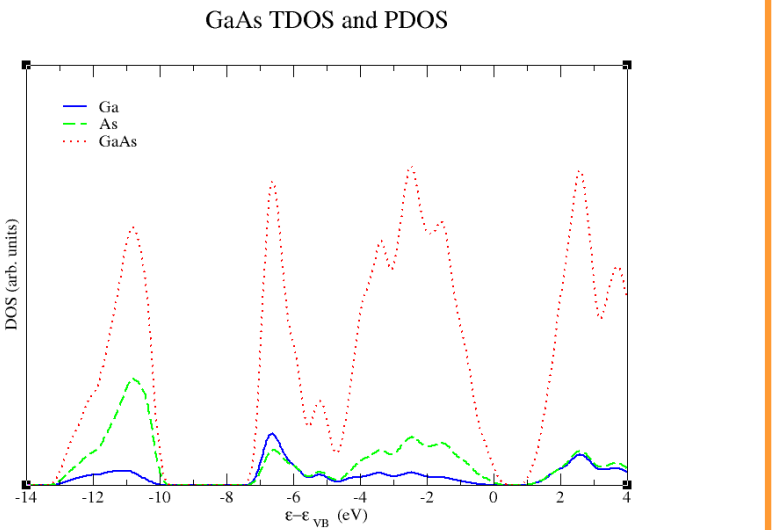
(3 • + 4 •) Can we learn more?

Projected density of states (PDOS)
→overlap of localized atomic orbitals with SCF wavefunction at given energy

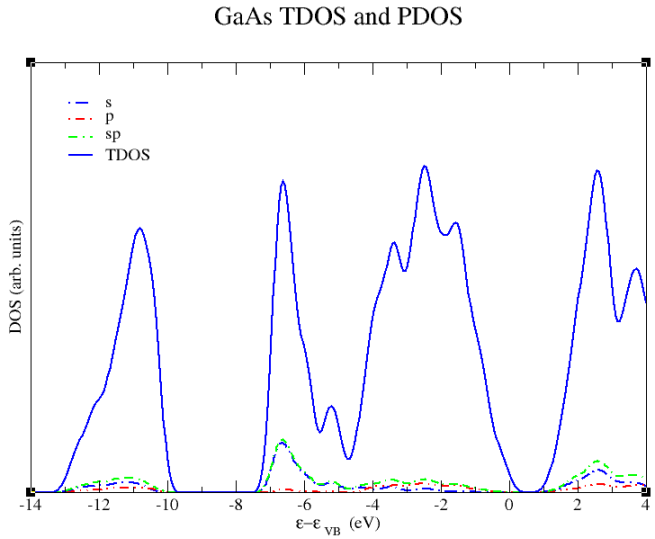
$$PDOS_{iOrb}(\mathrm{e}) = \sum_{i,k} w_k \, G(\mathrm{e} - \mathrm{e}_{ik}) \left| \langle \mathrm{m}_{iOrb} | R | \mathrm{y}_{ik} \rangle \right|^2$$



GaAs TDOS and As PDOS



GaAs TDOS and Ga and As PDOS



GaAs TDOS and Ga PDOS

Task on one's own

With the same machinery as applied to GaAs perform careful analysis of aluminum face-centered cubic structure, that is at thermodynamical equilibrium:

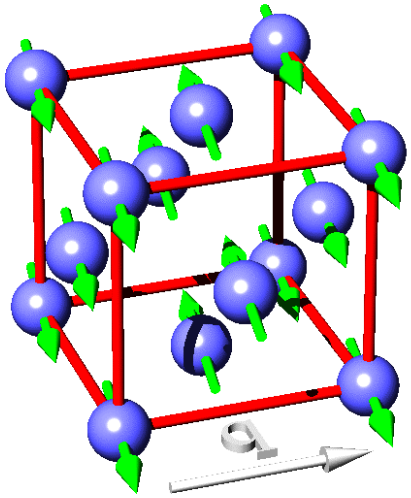
- Analyze atomic structure
- Obtain SCF charge density
- Visualize structure and SCF charge density
- Get aluminum band structure → answer question whether fcc-Al is metal or not?
- Calculate converged TDOS

Magnetism in SFHIngX

Current treatment of the magnetism in **SFHIngX**
- no spin-orbit coupling included
- only collinear magnetic structures can be treated → have only two spin channels – spin up and spin down

Questions to learn:

- Magnetic structure initialization
- Fixed magnetization calculations
- Spin-density visualization
- Magnetic electronic structure analysis



Picture from http://www.flapw.de/arthaupt_new.html

Magnetic structure initialization

How to switch spin on →

```
Hamiltonian {
  ...
  spinPolarized; ß
}
```

Initial magnetic structure initialized with LCAO

Total magnetization of the cell (all atoms are spin polarized)

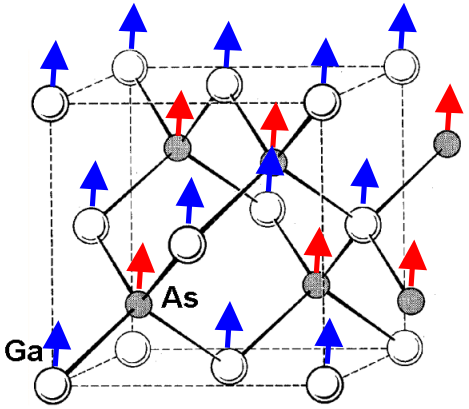
Mixed initialization (only part of atoms is spin-polarized)

Explicit occupation numbers for LCAO charge density

Magnetic structure initialization

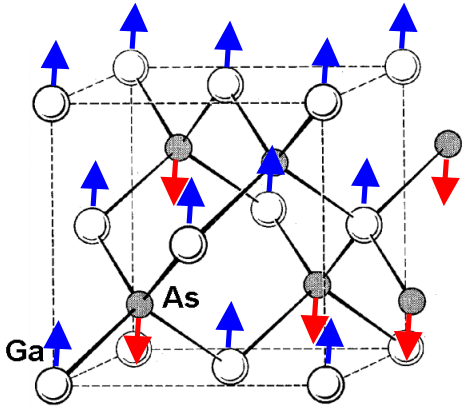
Total magnetization of the cell (all atoms are spin polarized)

```
initialGuess  {
  ...
  rho   { atomicOrbitals;  spinMoment = 1; }  ß
}
```



Explicit occupation numbers for LCAO charge density

```
species  {
  ...
  lcaoOrbitals       = [s,p,d];
  atomicRhoOcc   = [[1,2,0],[1,1,0]];   ß  (↑ s¹p²d⁰, ↓ s¹p¹d⁰)
  ...
}
```



Magnetic structure initialization

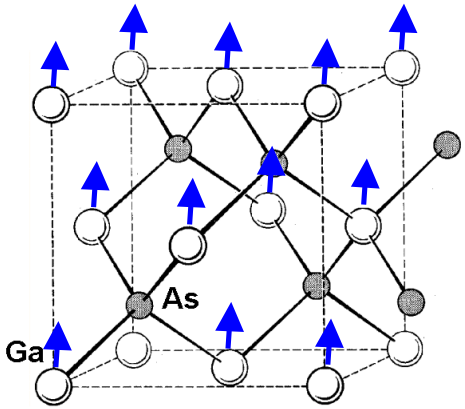
Mixed initialization

```
species  {
  …
  lcaoOrbitals      = [s,p,d];
  atomicRhoOcc      = [[1,2,0],[1,1,0]];
  …
}
species  {
  …
  lcaoOrbitals      = [s,p,d];
  atomicRhoOcc      = [2,3,0]];
  …
}
```

ß $\left(\uparrow s^1 p^2 d^0, \downarrow s^1 p^1 d^0\right)$

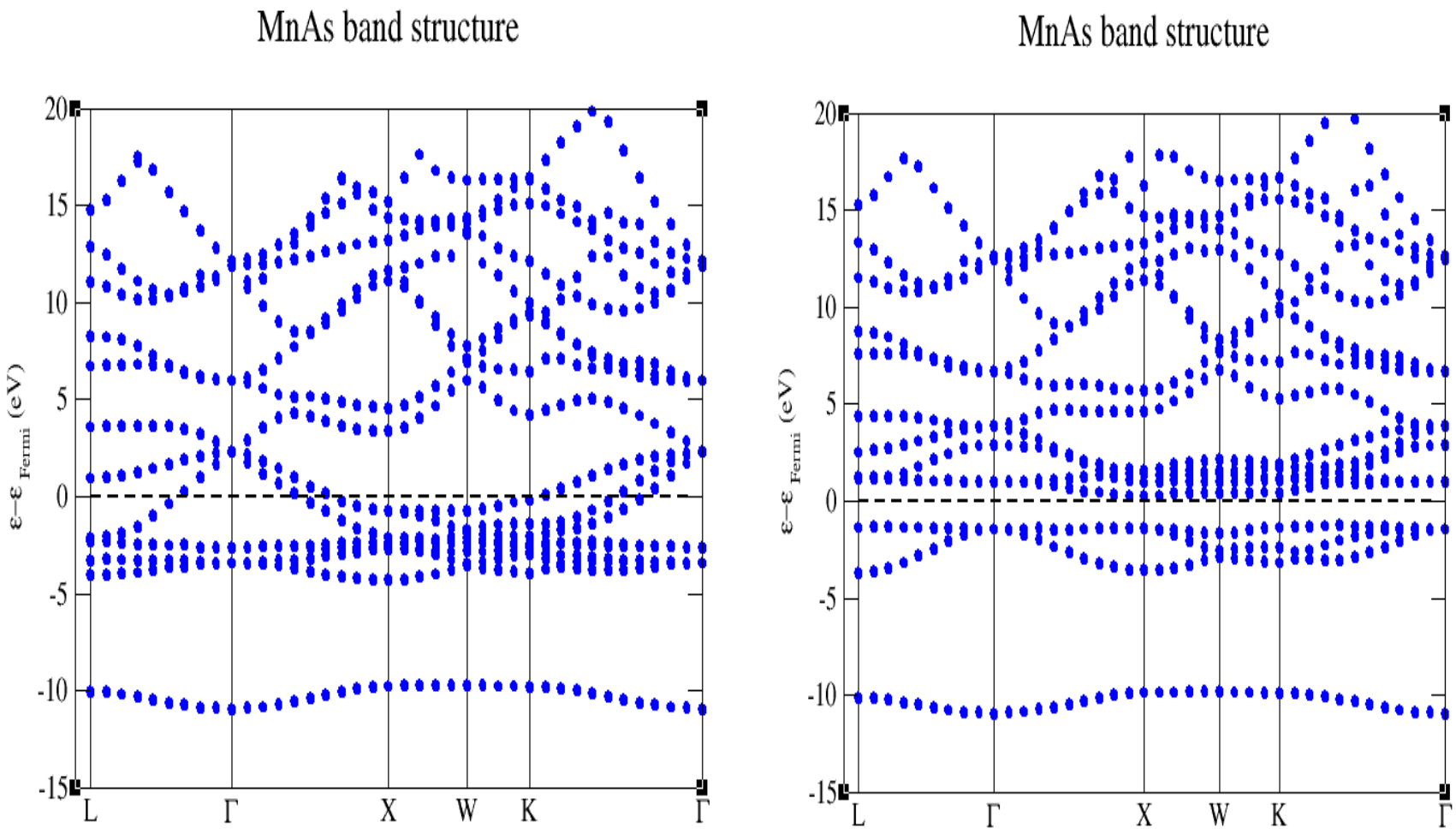
ß $\left(s^2 p^3 d^0\right)$

$\left(\uparrow s^1 p^{1.5} d^0, \downarrow s^1 p^{1.5} d^0\right)$



Hint: to get nonzero spin density system must be metallic → all-state-CCG can not be used

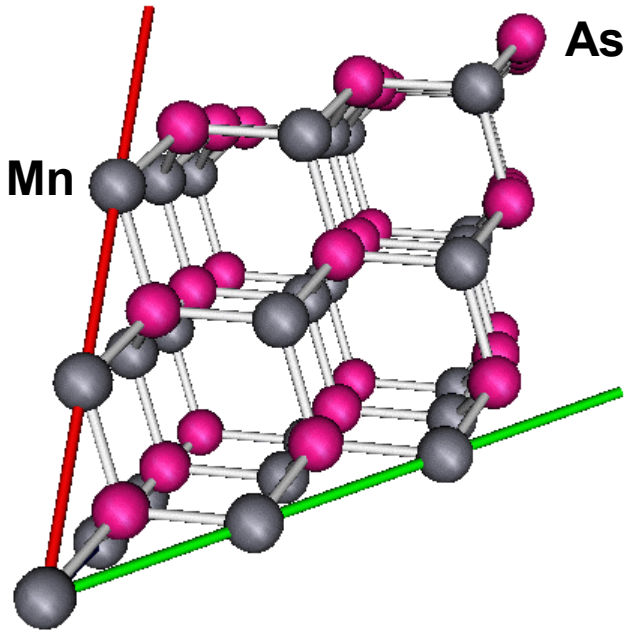
Magnetic structure analysis



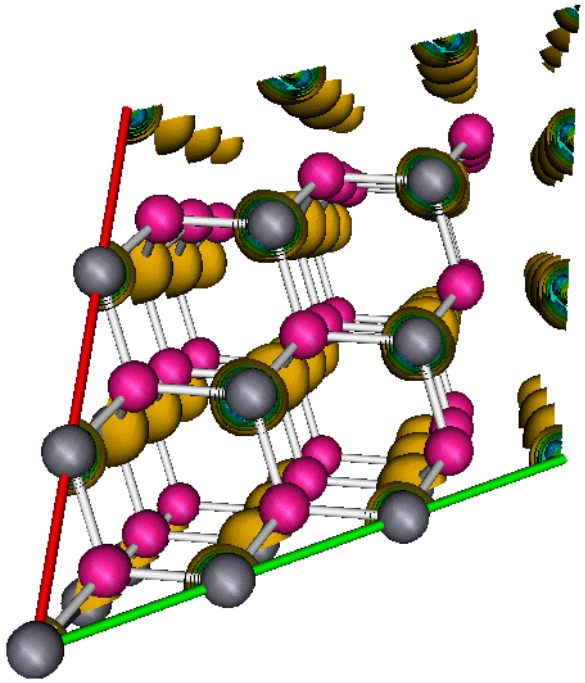
MnAs(zinc blende) band structure for majority and minority spin channels

Visualization of spin density

$$r_{SPIN}(\vec{r}) = r_{\uparrow}(\vec{r}) - r_{\downarrow}(\vec{r})$$



MnAs (zinc blende) atomic structure



MnAs (zinc blende) spin density

Tasks on one's own

Using different initial magnetic structure initialization schemes calculate:

- Isolated As atom (spin-polarized / spin-neutral)
- Isolated Ga atom (spin-polarized / spin-neutral)

Analyze obtained electronic structures (TDOS and PDOS) and draw conclusion about importance of spin-polarization

Perform analysis of MnAs (zinc blende) magnetic crystal:

- Analyze atomic structure
- Obtain SCF charge density
- Visualize structure and SCF charge density, spin density
- Get and analyze band structure
- Calculate converged TDOS

What one should learn in this session

- Setup nonmagnetic SCF run
- Setup band structure calculations
- Analyze band structure output

- Setup magnetic SCF run
- Different ways how to setup initial magnetic structures
- Visualization of spin density
- Band structure for magnetic system