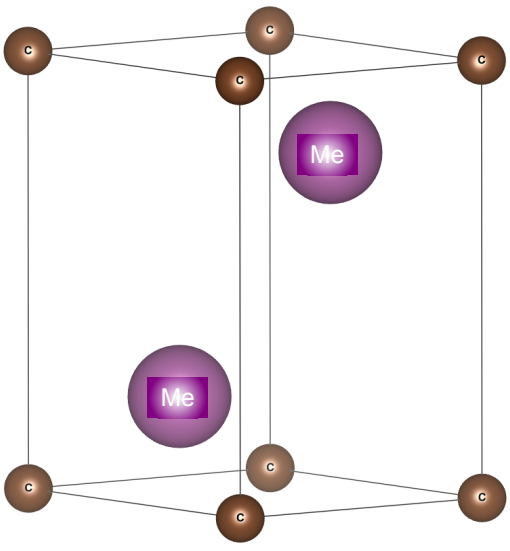
Computational Nano Science

Project:

Carbides:

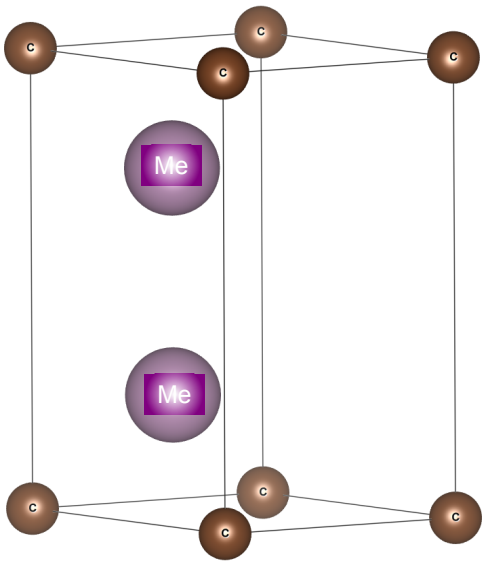
Geometry,
DOS and Band Structure

Carbides Me_2C



Me_2C (trigonal)

C: simple hexagonal
Me: approx. on cell diagonal



Me_2C (hexagonal)

C: simple hexagonal
Me: stacked

1. Preoptimization

- set up a unit cell for your system (use a = 3 Å and c = 6 Å as start lattice constants)
- for all following calculations use PBE (`GGA = PE`), `PREC = Accurate`, and `EDIFF = 1E-05`
- Find out whether your material is spin-polarized in the ground state:
  - Perform a full geometry optimization (atom positions + cell) with and without spin polarization adopting
    - a reasonable cutoff energy (!)
    - (10 x 10 x 5) **k**-mesh (Gamma)
    - Methfessel-Paxton smearing of order 1, σ = 0.2

  - ***Compare total energies***
  - ***What is the magnetization in case of the spin polarized calculation?***
  - ***Decide whether you need spin polarization for your material!*** *Use this setting in all remaining calculations!*

2. k-point convergence

- Perform single point calculations at the in **1.** obtained lattice constant(s) using the standard cutoff energy for Γ-including (N x N x N/2) **k**-meshes where N = 5, 10, 15, 20, 25 with
  - LT-C method
  - Methfessel-Paxton smearing of order 1 with σ = 1.0 ***and*** 0.2

- ***Tabulate and plot E($\sigma \rightarrow 0$) vs. N for the tested smearings (all in one graph)***
- ***Compare the convergence behavior of the three k-point integration schemes!***

3. Geometry Relaxation

- Perform a geometry relaxation (**`EDIFFG = -0.01`**) using
  - a reasonable cutoff energy
  - reasonable **`ISIF`**
  - Methfessel-Paxton smearing of order 1, σ = 0.2
  - a converged **k**-mesh (criterion: 1 meV per atom)

- ***Compare the optimized lattice constant(s) with the experimental values! Give the deviation in percent!***
- ***In case of spin polarization: What is the magnetization per unit cell?***

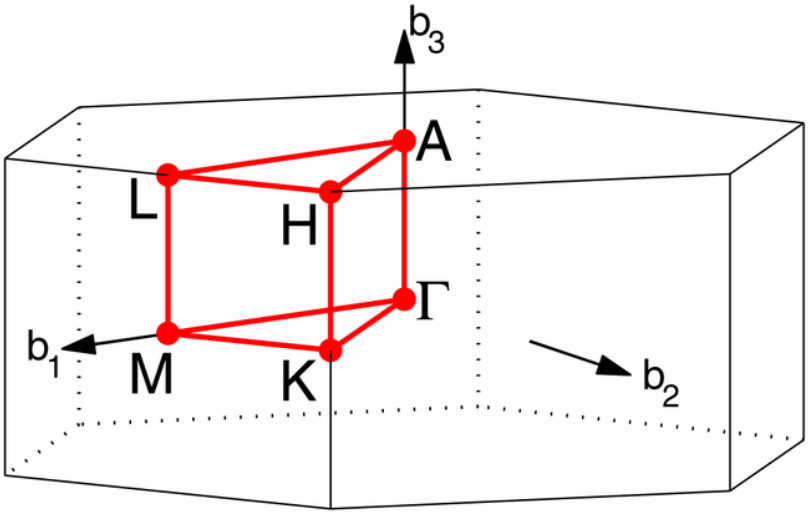
4. DOS and Band Structure

- Calculate the DOS for the optimized geometry of **3.**
  - keep **k**-mesh from geometry optimization for DOS
  - use LT-C smearing for DOS
  - set **`NEDOS = 1000`** in INCAR
  - you may reduce the energy cutoff to the standard value
- Calculate the band structure for the optimized geometry
  - use 20 **k**-points per line for the band structure
  - keep density from the DOS calculation fixed! (**`ICHARG = 11`**)
  - Band structure path (→ use xcrysden to determine coordinates):

    Γ–M–K–Γ–A–L–H–A | L–M | K–H

- ***Plot DOS and band structure for the valence states! (reasonable viewport!!)***
- ***Is the system metallic or non-metallic? Size of the band gap?***

k-path: Nomenclature



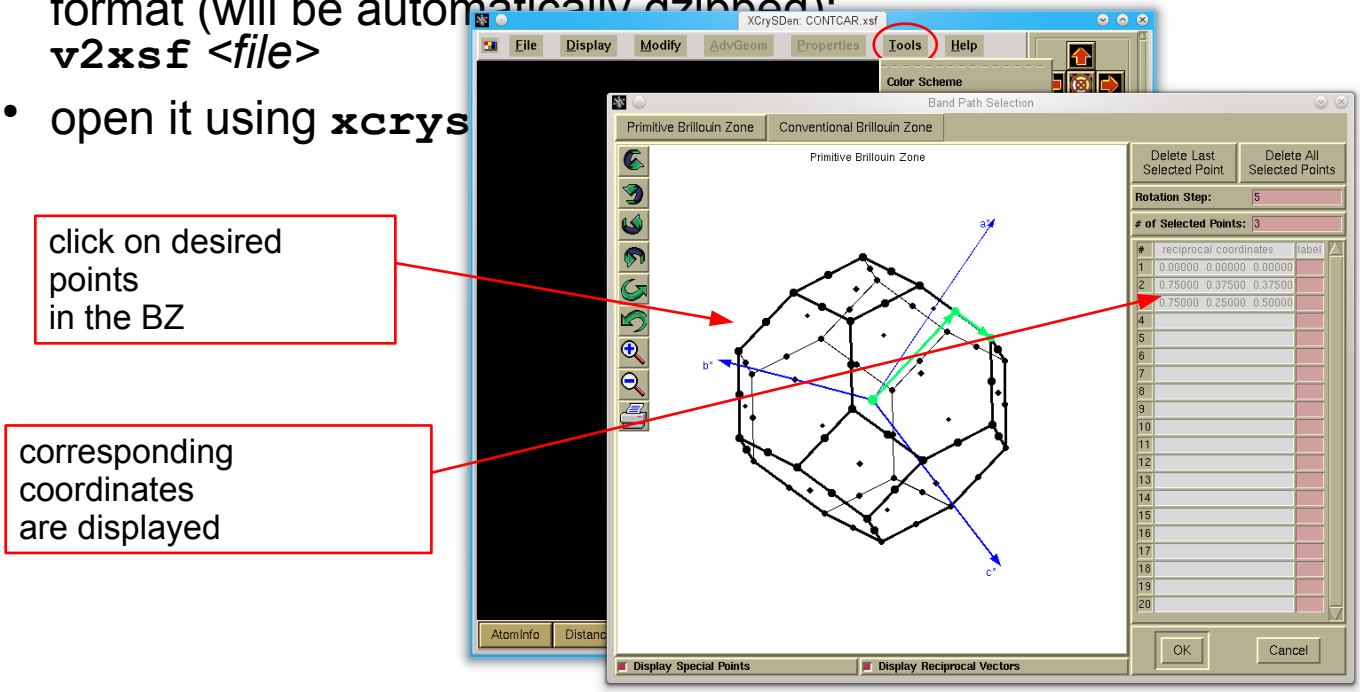
HEX path: Γ-M-K-Γ-A-L-H-A|L-M|K-H

Some final Tips...

- do not run more than two calculations at one time!
- **Protocol:**
  - **submit via StudON in pdf format!**
  - **Deadline: 5 June 2025**
  - Name, student-ID and calculated system on the front page!
    (but separate title page not needed)
  - short method section(s)
    - indicate all relevant information that someone else could reproduce your calculations based upon your report!
  - total energies: report 5 decimals
  - all points printed in ***italic*** on the preceding slides have to be addressed in the protocol!

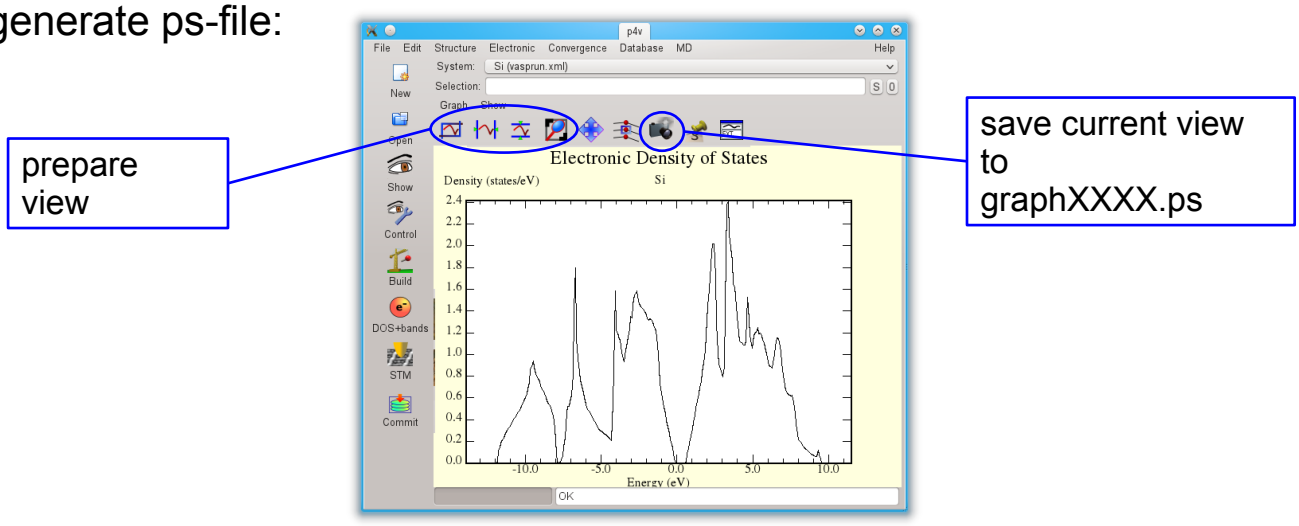
Selecting k-paths: xcrysden

- xcrysden offers a graphical interface to determine the coordinates of special points in the BZ
- use v2xsf to convert the CONTCAR (or POSCAR) file to xsf-format (will be automatically gzipped):
  `v2xsf` *<file>*
- open it using **`xcrys`**



p4v: Saving Graphs

- generate ps-file:



- convert to pdf format:

```
epstopdf graph0001.ps
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