

**Crystallography and Crystal Chemistry
X International School-Conference of
Young Scientists 2025**

Mini-lecture 3. Practice: VASP

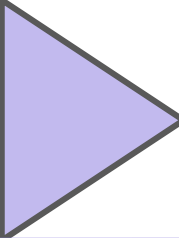
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VASP units

Mass	–	m_a
Energy	–	eV
Distance	–	Å
Force	–	eV/Å
Stresses	–	kBar, divide by 10 to get GPa
Charge	–	elementary charge
Dipole	–	electrons•Å
Temp	–	K
Time	–	fs (default, used in AIMD)

▶ How to use VASP

To run:

```
vasp_std > vasp.log
```

Note: *the following input files should be in the current directory:*

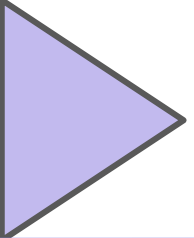
POSCAR – *contains crystal structure*

INCAR – *control parameters*

KPOINTS – *k-mesh in reciprocal space*

POTCAR – *PAW potential file*

```
Si          # just any name
1.000      # multiplier for vec
 0.00  2.71  2.71  # Lattice vec 1, Å
 2.71  0.00  2.71  # Lattice vec 2, Å
 2.71  2.71  0.00  # Lattice vec 3, Å
Si C
2 2        # N atom for each type
Direct     # type of coordinates
 0.00  0.00  0.00  # atom 1 Si
 0.25  0.25  0.25  # atom 2 Si
 0.00  0.00  0.00  # atom 1 C
 0.25  0.25  0.25  # atom 2 C
```



INCAR minimal

ENCUT = 300 # *eV, energy cut-off*

ISIF = 3 # *full optimization*

ISMEAR = 2 # *Smearing method, Methfessel-Paxton*

KSPACING = 0.1 # *spacing of k points, can be used instead of KPOINTS file*

▶ INCAR reasonable

```
SYSTEM = 2 Li; # name
EDIFF = 0.0001 # eV, stopping criteria of SCF
EDIFFG = -0.01 # eV/A, stopping criteria of relaxation
NSW = 20 # number of relaxation steps
ENCUT = 150 # eV, energy cut-off
IBRION = 1 # optimization algo
ISIF = 3 # full optimization
ISMEAR = 2 # Smearing method, Methfessel-Paxton
SIGMA = 0.2 # eV, smearing broadening
NBANDS = 4 # number of bands
```

INCAR for structural optimization of Si

```
ENCUT = 600      # eV, energy cut-off
EDIFFG = -0.01   # force stopping criteria, 0.01 eV/A or
ISIF = 3         # full optimization
IBRION = 2       # Quasi-Newton
NSW = 100        # Maximum Number of steps for optimization
ISMEAR = 0       # Smearing method, Gaussian
SIGMA = 0.1      # Smearing
LWAVE = .FALSE.  # do not save WAVECAR - usually huge ~1-10 GB
```

```
# EDIFFG reads as eV/A^3 for stresses. See "Total" in OUTCAR and
divide by  $N_{\text{at}}$ 
```

KPOINTS, normal calculation

Automatic Mesh

0

Monkhorst Pack

9 9 9

0 0 0

KPOINTS, band structure. CHGCAR required

kpoints for bandstructure L-G-X-U K-G

40 ! 40 intersections

line ! line mode

reciprocal ! type of coordinates

0.50000 0.50000 0.50000 !L

0.00000 0.00000 0.00000 !G

0.00000 0.00000 0.00000 !G

0.00000 0.50000 0.50000 !X

0.00000 0.50000 0.50000 !X

0.25000 0.62500 0.62500 !U

0.37500 0.7500 0.37500 !K

0.00000 0.00000 0.00000 !G

POTCAR - Potential file, with VASP

```
PAW_PBE Li 17Jan2003 # version
```

```
1.00000000000000000000 # N valence
```

```
parameters from PSCTR are:
```

```
VRHFIN =Li: s1p0 # electronic conf
```

```
LEXCH = PE # exch. cor PBE
```

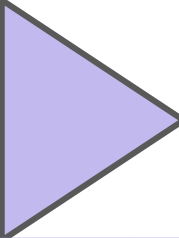
```
EATOM = 5.3001 eV # energy of atom in vacuum, it is  
subtracted from output total energy
```

Creating POTCAR for multiple elements

E. g. for SiC system you should run

```
cat Si/POTCAR C/POTCAR > POTCAR
```

The order should be the same as types of atoms follow in **POSCAR**



OUTPUT

- CONTCAR** - file with output structure, the same format as **POSCAR**
- OUTCAR** - main file with energies, etc.
- CHGCAR** - charge density file
- WAVECAR** - wave function file
- EIGENVAL** - Kohn-Sham energies at k - required for band structure plotting

And others. For more details, see [VASP manual](#).

▶ OUTCAR, check that is finished

```
grep reached OUTCAR
```

OUTPUT:

```
----- aborting loop because EDIFF is  
reached -----
```

▶ OUTCAR, read final energies

```
grep TOTEN OUTCAR
```

–Print total energy at each SCF step

```
grep 'energy without entropy' OUTCAR
```

–Print total energy after each relax step

use `energy(sigma→0)` extrapolated energy

OUTCAR, read stresses and forces

```
grep 'in kB' OUTCAR
```

- Print stress tensor after each relax step,
multiply by 100 to get MPa
residual stress of 100 MPa is OK for most solids

```
grep -A 3 TOTAL OUTCAR
```

- Print positions and forces
Why forces are zero?

OUTCAR, More

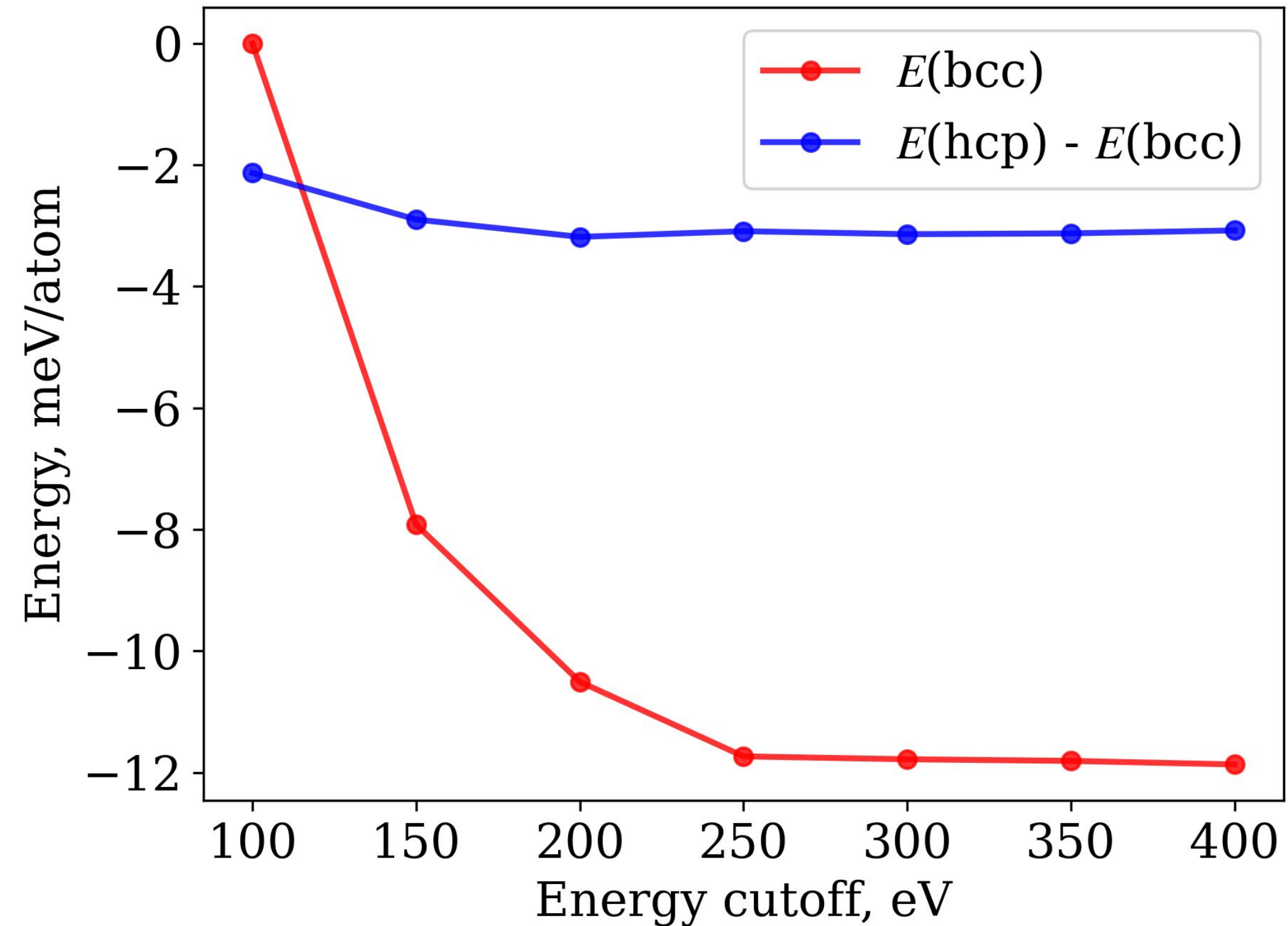
```
grep E-fermi OUTCAR
```

- Print Fermi energy in eV

residual stress of 100 MPa is OK for most solids

- Eigenvectors and eigenvalues of the dynamical matrix

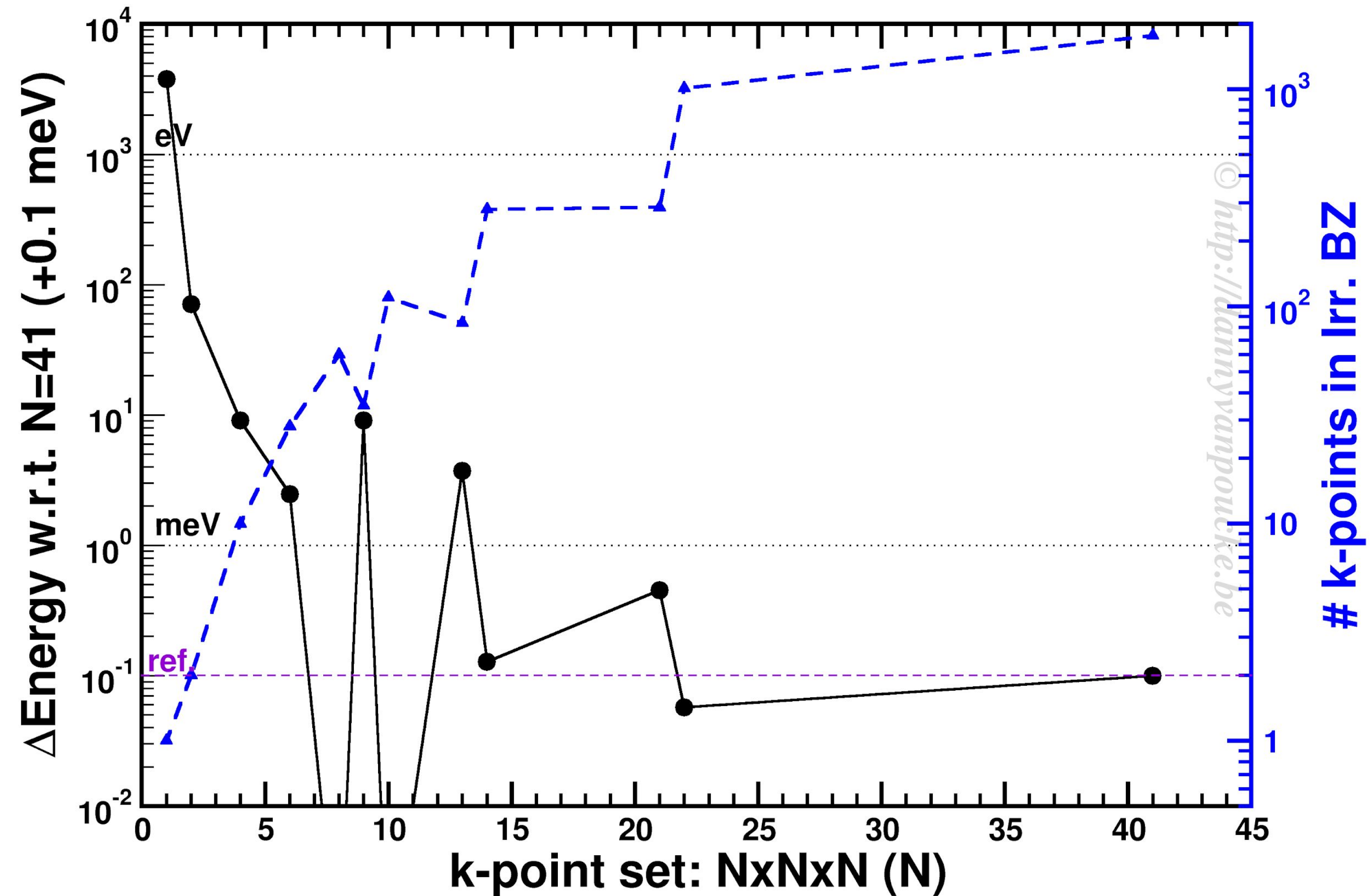
Convergence with respect to E-cut



Convergence of the energy cut-off for bcc Li and energy difference using the PBE functional and a 8x8x8 k-point grid for conventional cell.

- Make all calculations at fixed cut-off energy.
- The absolute energy has little sense, use differences.
- Check convergence for property of interest.

Convergence with respect to k-points and smearing



K-point convergence of alpha-Cerium using the PBE functional and ENCUT=500 eV.
<https://dannyvanpoucke.be/vasp-tutor-convergence-testing-en/>

Convergence with respect to k -mesh

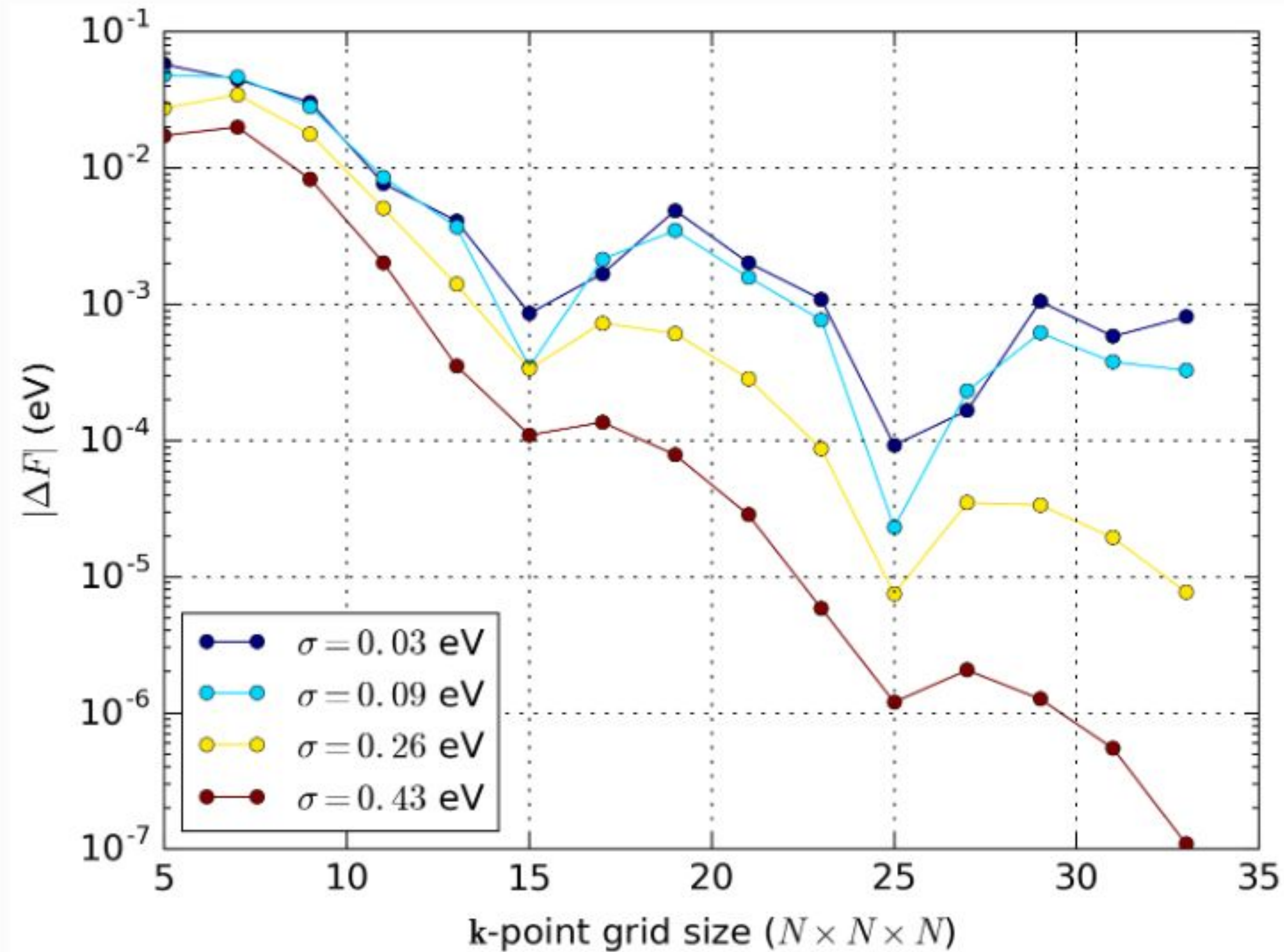
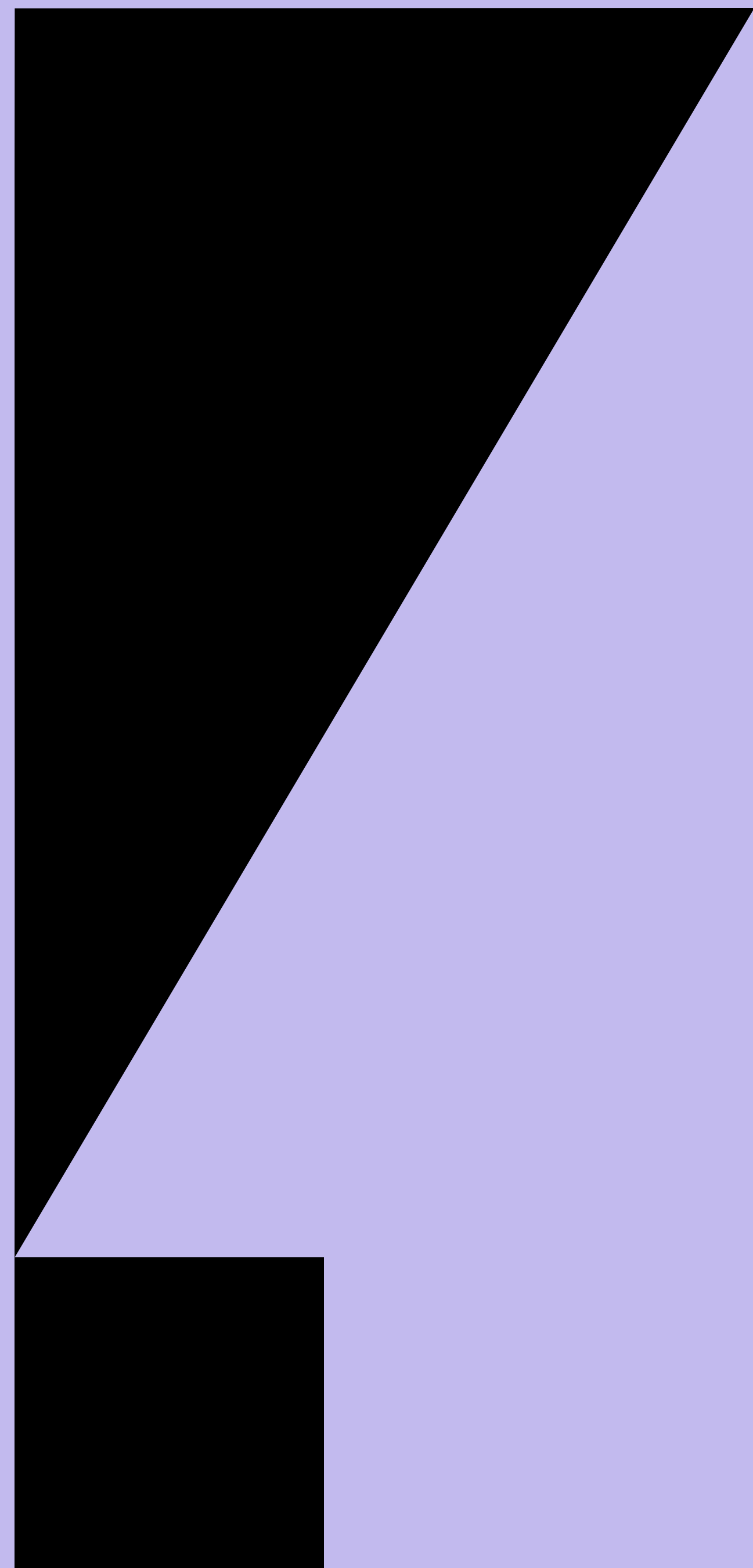


Fig. 105 Convergence of the free energy of bulk Aluminum with respect to the k -point sampling using the *Fermi-Dirac* occupation function with different broadenings. The free energy difference, ΔF , is calculated as the difference between the calculation at the given k -point sampling and one at $35 \times 35 \times 35$.

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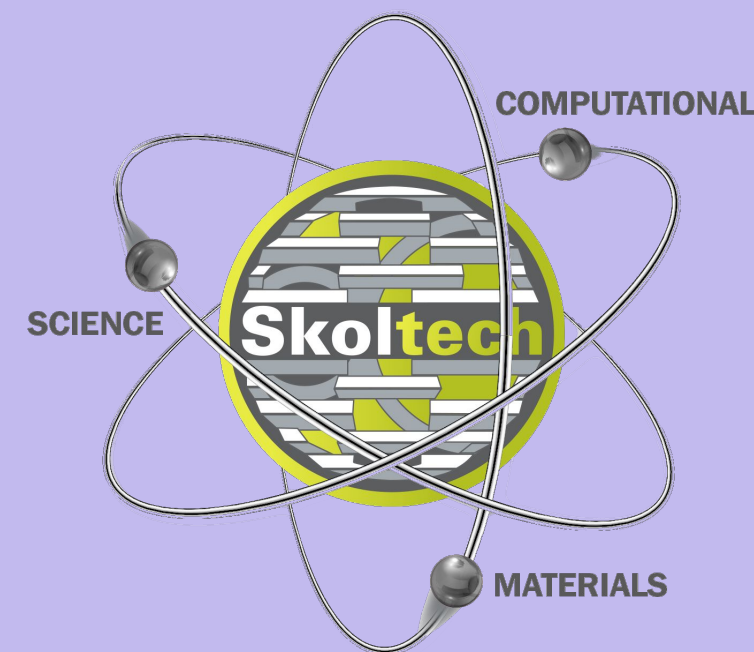
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Acknowledgement

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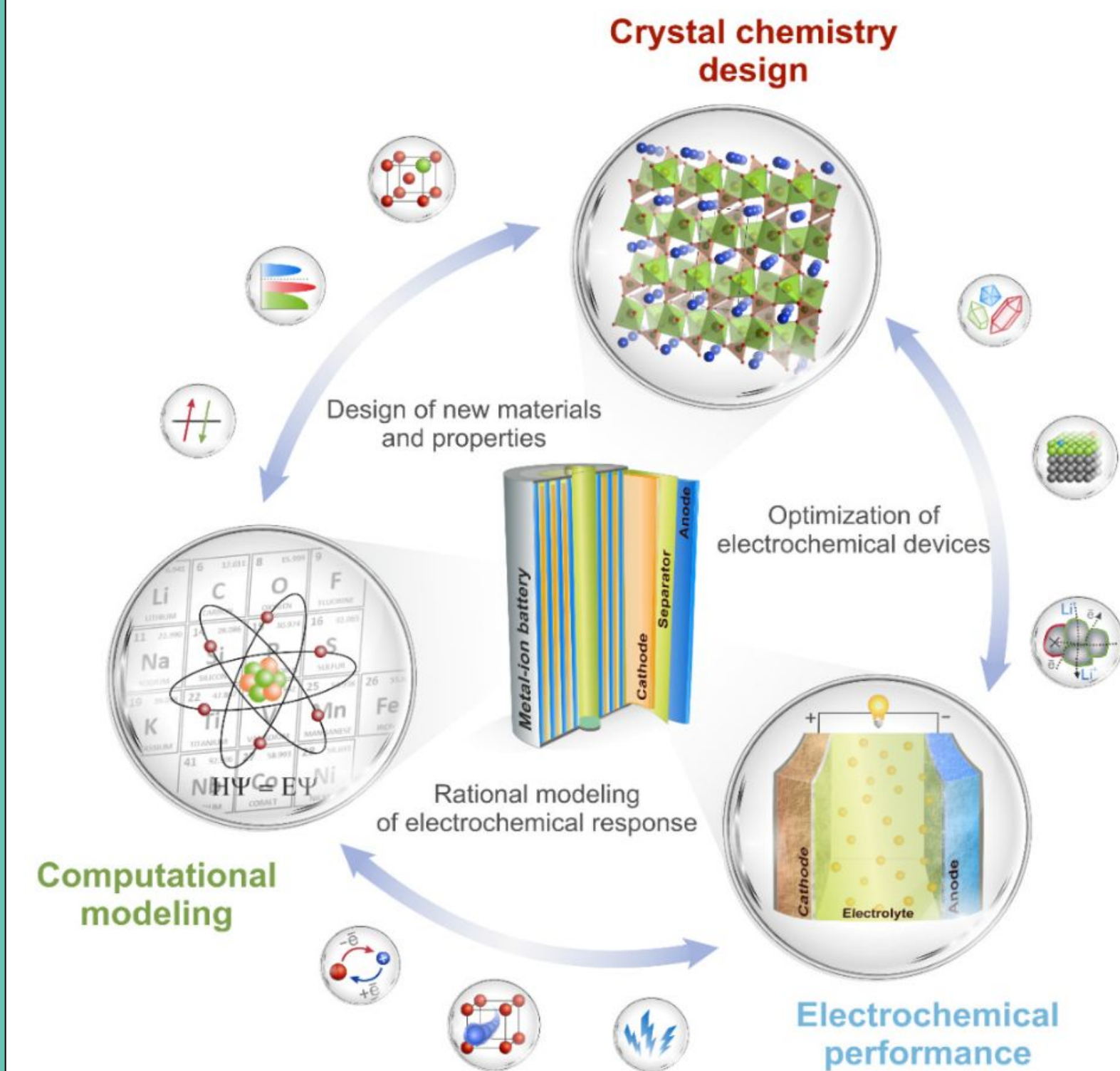


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★ [MatSolver](#) - a web-service for predicting materials properties.