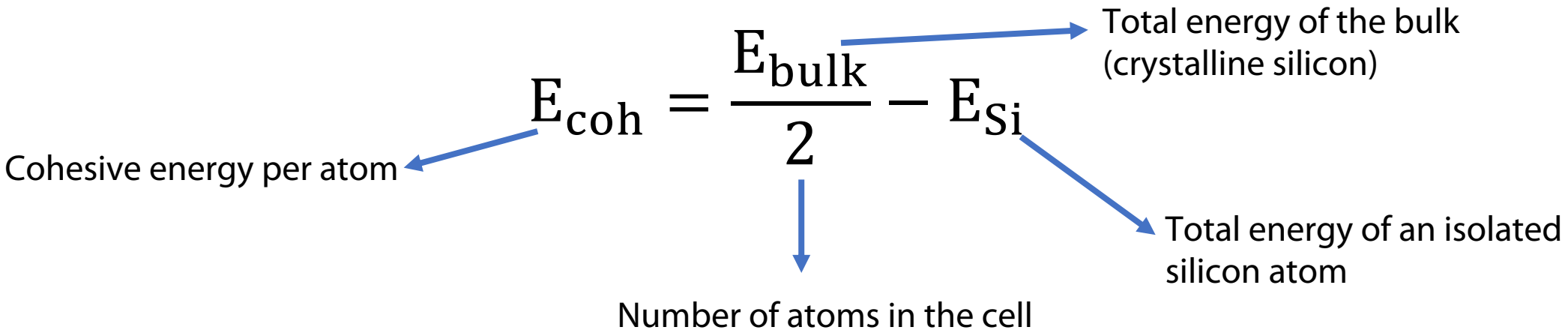
Cohesive energy

- The **cohesive energy** is defined as the heat of sublimation of a solid into its elements.
- In practice, you need to calculate difference between the total energy at the equilibrium lattice parameter and the total energy of each isolated atom



- The experimentally measured cohesive energy for silicon is ~4.6 eV.

Input files available at
https://github.com/AntimoMarrazzo/DFT_course_UniTS/tree/main/cohesive

The isolated atom

```
&SYSTEM
    ibrav              = 1
    celldm(1)          = 30
    ecutwfc            = 40.0
    ntyp               = 1
    nat                = 1
    nspin              = 2
    occupations        = 'smearing'
    degauss = 0.01
    tot_magnetization = 2
    nbnd = 5
/
&ELECTRONS
    conv_thr           = 1.d-12
/
ATOMIC_SPECIES
Si 28.086 Si.pbe_PseudoDojo.UPF
K_POINTS gamma
ATOMIC_POSITIONS alat
Si  0.0000000000 0.0000000000 0.0000000000
```

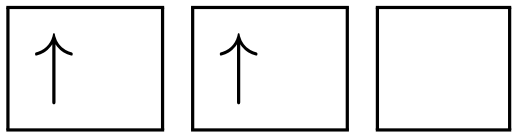
Cubic cell

30 Bohr

Spin-polarized calculations

We impose the total magnetization to be equal to 2 (Bohr magnetons)

Silicon outer shell is 3p and follows Hund's rules



Exercise & Homework

- **Exercise to do now**: converge the cohesive energy w.r.t to the wavefunction cutoffs. Does it converge faster than the total energy of the bulk?

- **Homework**: Calculate the cohesive energy of diamond and compare with its experimental value (~7.4 eV)

Electronic temperature (smearing)

- Why do we introduce smearing?

  To improve the convergence with respect to Brillouin zone sampling in metals (also to improve convergence with level crossing instabilities in the SCF)

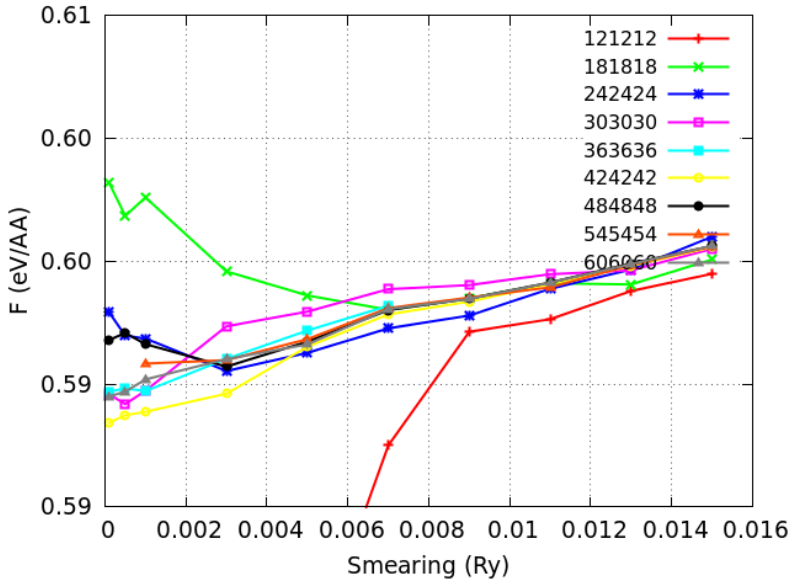
- Why does it work?:

  It **smoothens the discontinuous occupation function**, so k-space integrals can be integrated with higher accuracy at lower computational cost

- Side effects: you integrate the **wrong energy functional** E-TS (where T can be thousands of Kelvin), hence introducing a **systematic error**

- How to choose the temperature (and k-point sampling):

  1. decide what is the tolerated error (e.g. on the forces)
  2. choose a smearing such that the error is within tolerance
  3. For that smearing choose the smallest k-point sampling that correctly integrates the Brillouin zone.



SCF and bands of bulk nickel

- **Run a SCF and band-structure calculation for magnetic nickel:**
  1. SCF
  2. Bands
  3. Bands postprocessing: run **twice**, one for spin-up and one for spin-down bands.
  4. Plot spin-up and spin-down bands with gnuplot

Input files available at
https://github.com/AntimoMarrazzo/DFT_course_UniTS/tree/main/ni