INPUTS
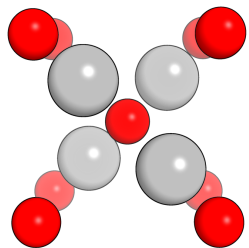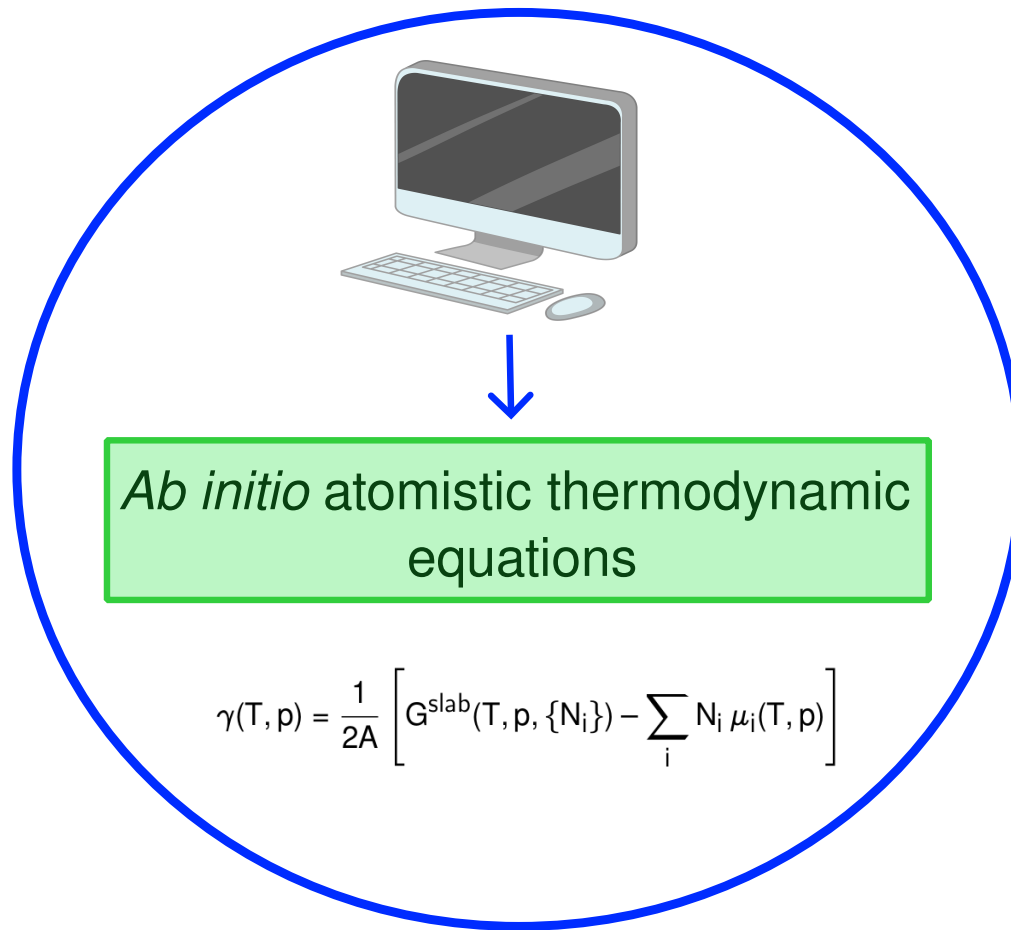
- DFT parameters

- Bulk structure

- Surface setup

TEROS Workflow

Ab initio atomistic thermodynamic equations

$$\gamma(T, p) = \frac{1}{2A}\left[G^{slab}(T, p, \{N_i\}) - \sum_i N_i\, \mu_i(T, p) \right]$$

OUTPUTS

Pressure (atm) @ 300 K
10^{-27} 10^{-24} 10^{-21} 10^{-18} 10^{-15} 10^{-12} 10^{-9} 10^{-6} 10^{-3} 1

Temperature (K) @ 1 atm
1100 1000 900 800 700 600 500 400 300

γ (J/m^2)

$\Delta\mu_O$ (eV)

$\Delta\mu_{Ag}$ (eV)

ln(p/p^0)

ST-C1
ST-C2

O rich

Ag poor — Ag rich

O poor

300 K

500 K

1200 K

$\Delta\mu_O$ (eV)