NOVEL MATERIALS DISCOVERY

European Centre of Excellence (CoE)

and something else…

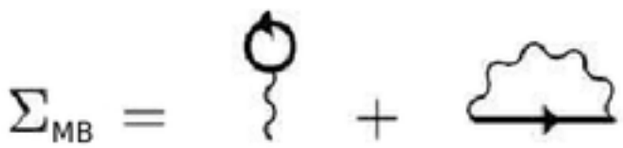
Mikkel Strange
(but presented by Karsten W. Jacobsen)

Overview of current projects

- Creating a big database for:
  DFT + Excited states + Molecular dynamics
  (writing parsers)

- Error bars in DFT calculations (finite basis set)
  Useful for comparing calculations, or not?

- Self-consistent
  hybrid functionals

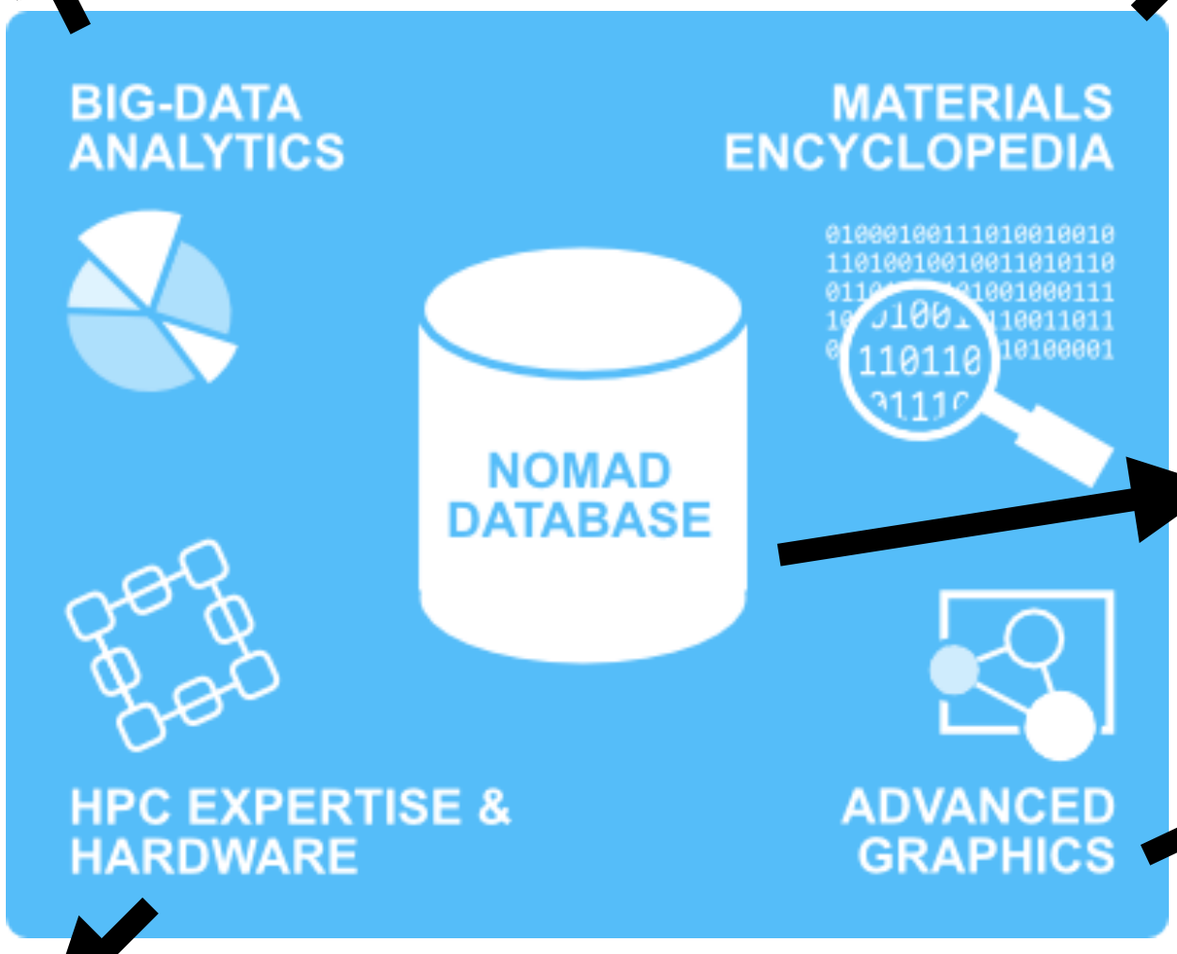


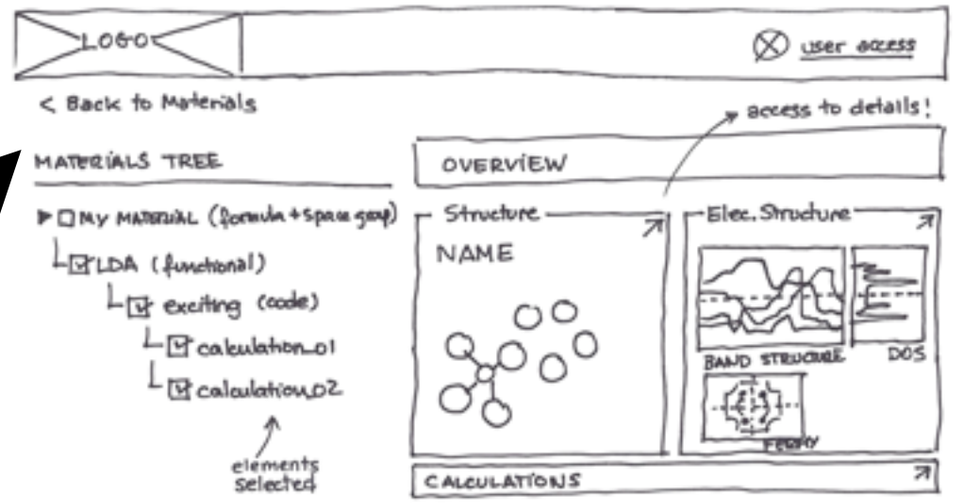
Outline

- Brief overview of the NOMAD project.
- “Parsers” that converts output from electronic structure codes to a common format
- “Error bars” from basis and k-point sampling
- Self-consistent hybrid functionals in GPAW

NOMAD overview

- Advanced analysis tools (machine learning etc)





3,027,865 calculations today

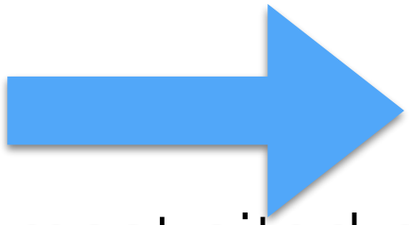
- Virtual reality (fx: exciton (r,r'))
- Remote visualisation (structures, wave-functions, etc)

- Stores your data for at least 10 years

Nomad: Producing data

Repository:
output files from all codes are welcome (file.gpw)

Conversion



50 most cited codes (GPAW, VASP, Gaussian, ASAP…)

Archive:
common data format (contains everything that is in the output files)

http://nomad-repository.eu/cms/

Big data analytics
Materials Encyclopedia
…

Nomad: Producing data

Parsers done at DTU for:

- GPAW | works
- MOPAC | works
- ASAP | works
- ATK | not started
- GROMACS | created

Start uploading your favourite GPAW gpw files come June 15th!

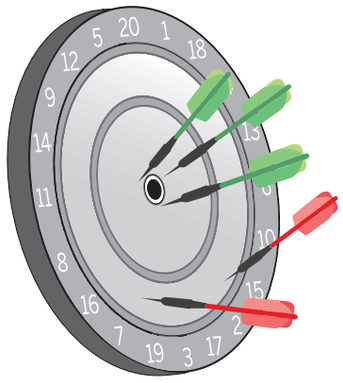
All data should be parsed:

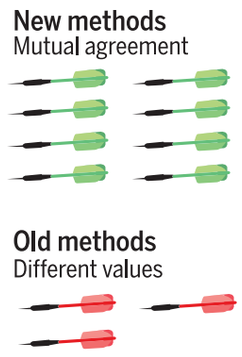
Structures
Energies
Electron density
Wave functions
SCF iteration time
Force field information
Constraints
…

Error bars project

Delta DFT:

DFT codes can be converged to good agreement





Scorecard

	0.3	0.3	0.6	1.0	0.9	0.3	1.5	0.6	0.9	0.4	1.0	0.4	0.4	6.3	13.5	1.1	2.1	0.7	1.4
0.3		0.1	0.5	0.9	0.8	0.2	1.5	0.6	0.8	0.4	1.0	0.5	0.3	6.3	13.4	1.1	2.1	0.7	1.4
0.3	0.1		0.5	0.9	0.8	0.2	1.5	0.6	0.8	0.4	0.9	0.5	0.3	6.3	13.4	1.1	2.1	0.7	1.4
0.6	0.5	0.5		0.8	0.6	0.4	1.5	0.6	0.8	0.6	1.0	0.7	0.5	6.3	13.2	1.0	1.9	0.6	1.3
1.0	0.9	0.9	0.8		0.9	0.9	1.8	0.9	1.3	1.0	1.4	1.0	0.9	6.4	13.0	1.2	1.8	1.0	1.6
0.9	0.8	0.8	0.6	0.9		0.8	1.7	0.7	1.1	0.8	1.3	1.0	0.8	6.5	13.2	1.1	1.8	0.8	1.5
0.3	0.2	0.2	0.4	0.9	0.8		1.5	0.5	0.8	0.3	1.0	0.5	0.3	6.2	13.4	1.0	2.0	0.6	1.4

Next step: something about the error due to:

- finite basis set
- k-point sampling
- other numerical settings?

Should be useful for judging the quality of data in the NOMAD database

Error bars project

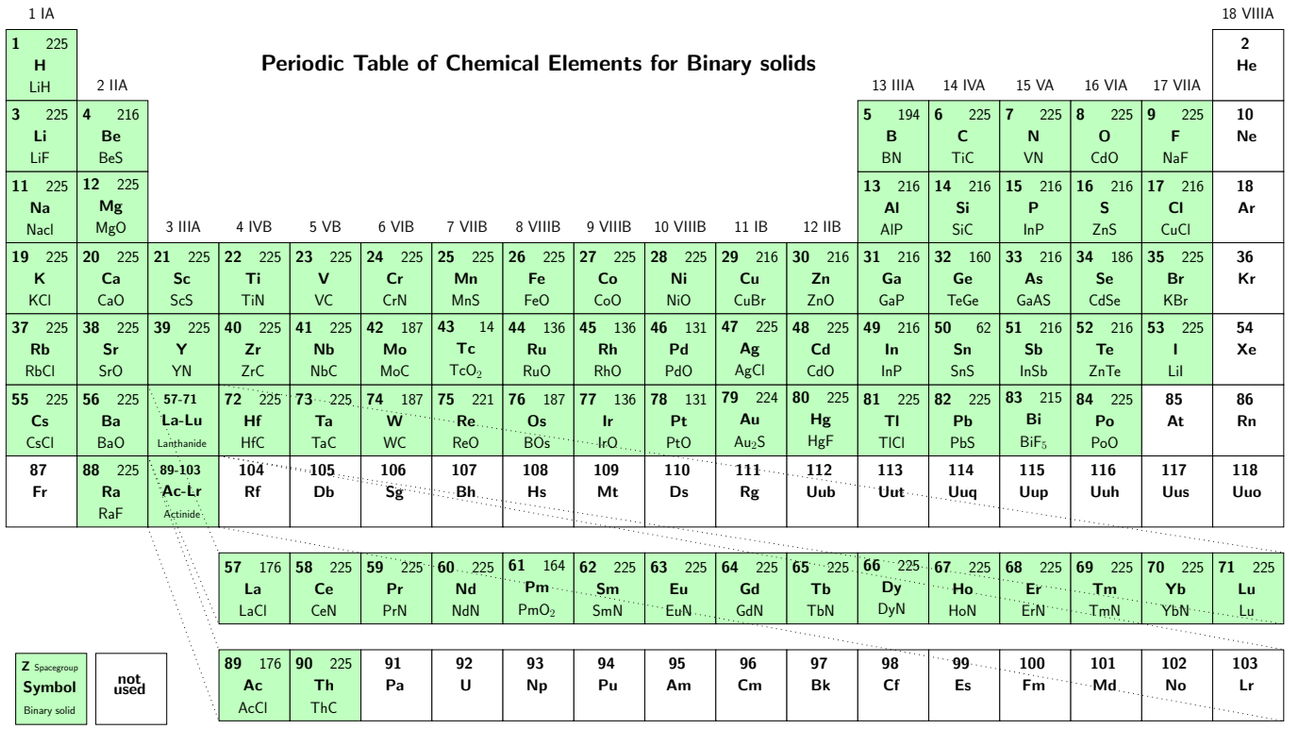
Some simple questions

- Is convergence with k-points and basis set independent?
- Can we give error estimates?

Error bars project

Codes:
GPAW | PW | DTU
VASP | PW | TU Graz
Exciting | LAPW | HU Berlin
AIMS | NAO | FHI Berlin

Properties:
Structures
Energies
Band gaps

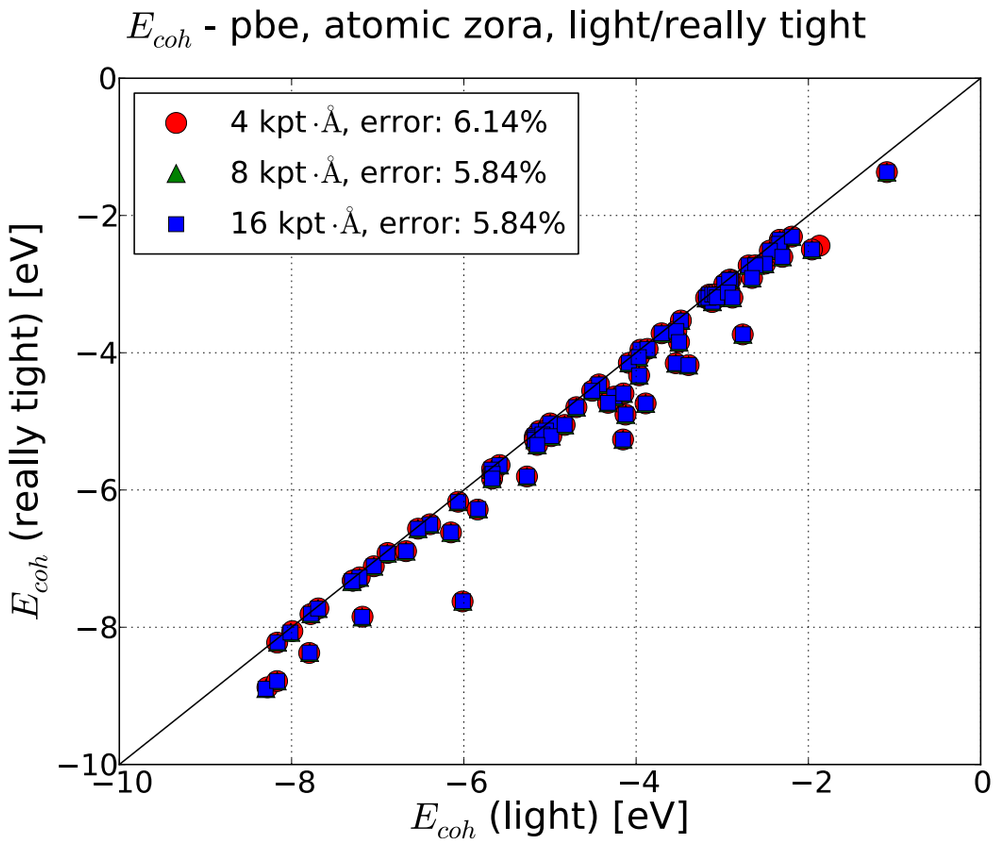


Functional: PBE and LDA
90 Binary solids
73 Elemental (from ΔDFT)
-> ~5000 calculations
(+ random systems
from the NOMAD database)

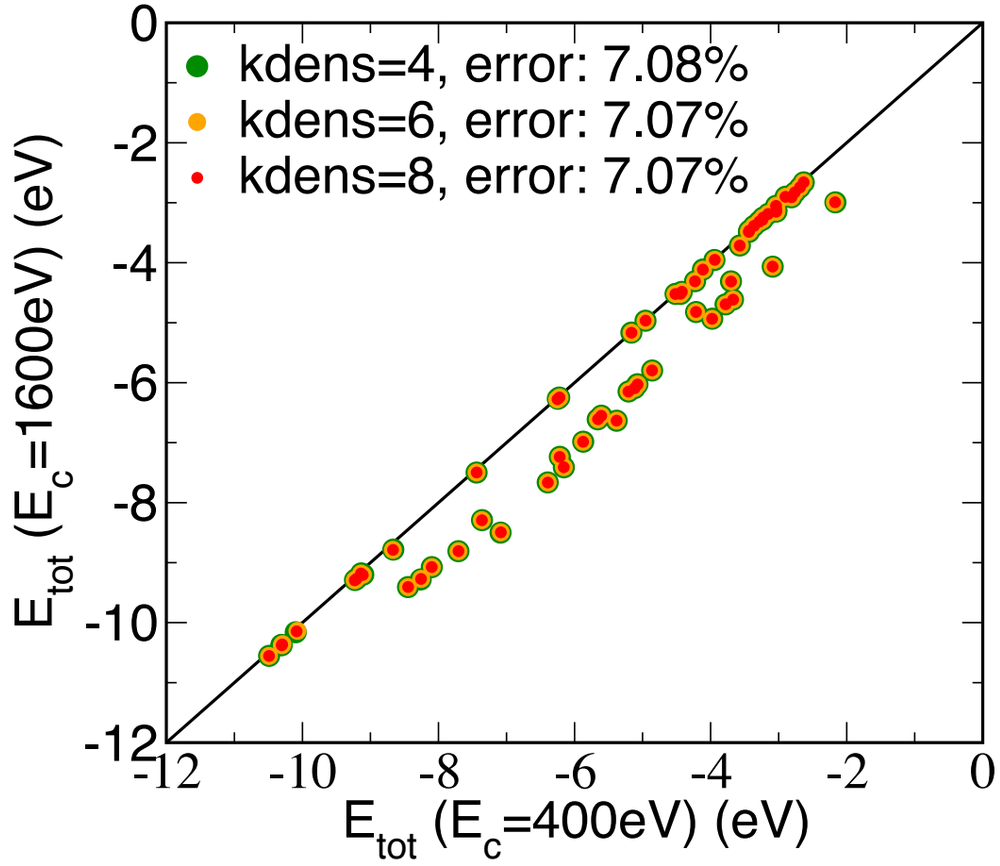
Error bars project

Total energies (binaries): light vs really tight basis

AIMS



GPAW

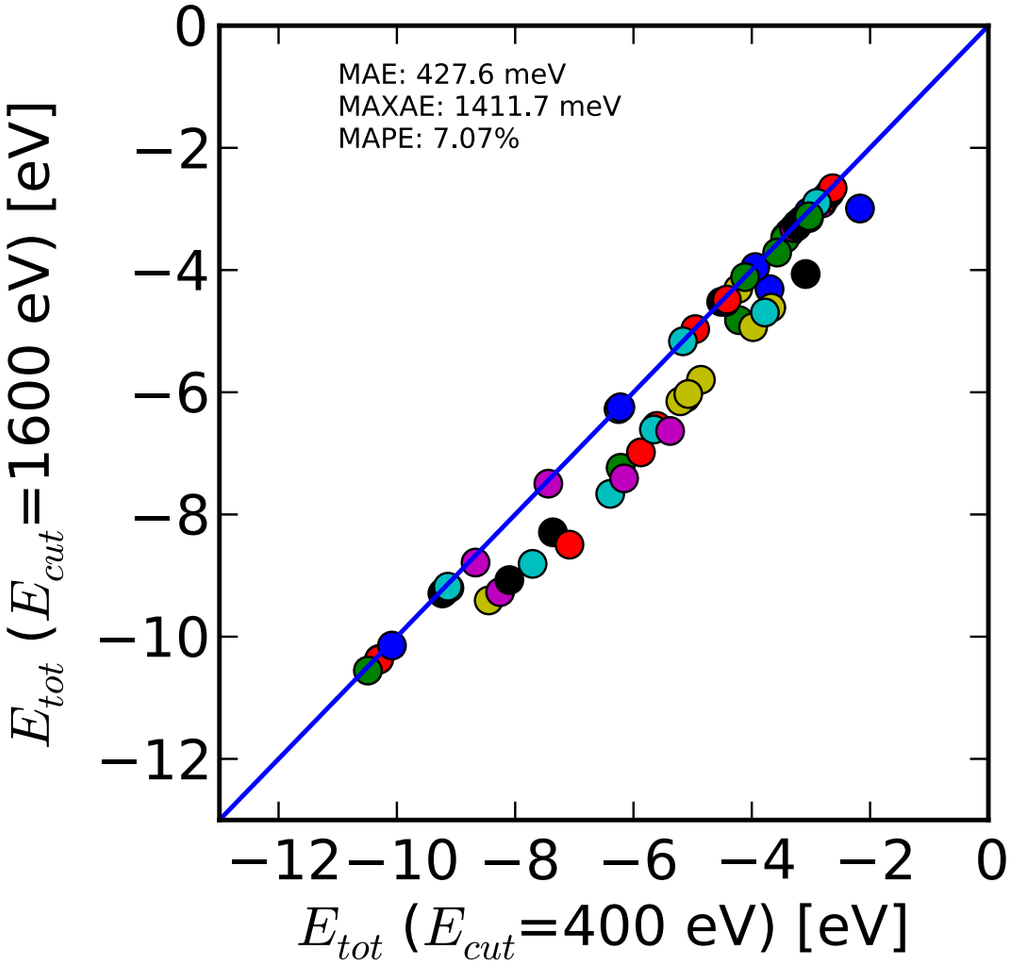


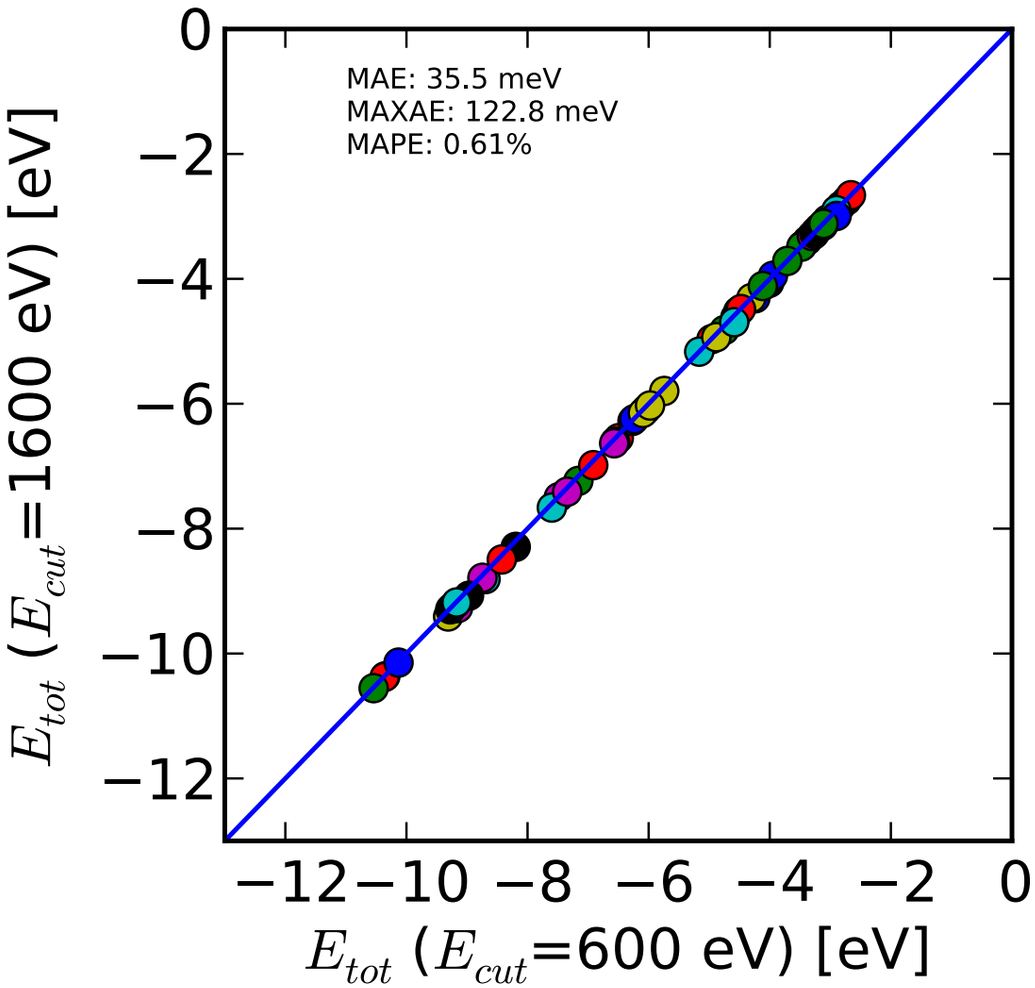
Error from k-point sampling looks “small” compared to basis set

Error bars project

Total energies (binaries)

MAE: Mean absolute error
MAXAE: Max absolute error
MAPE: Mean absolute percentage error



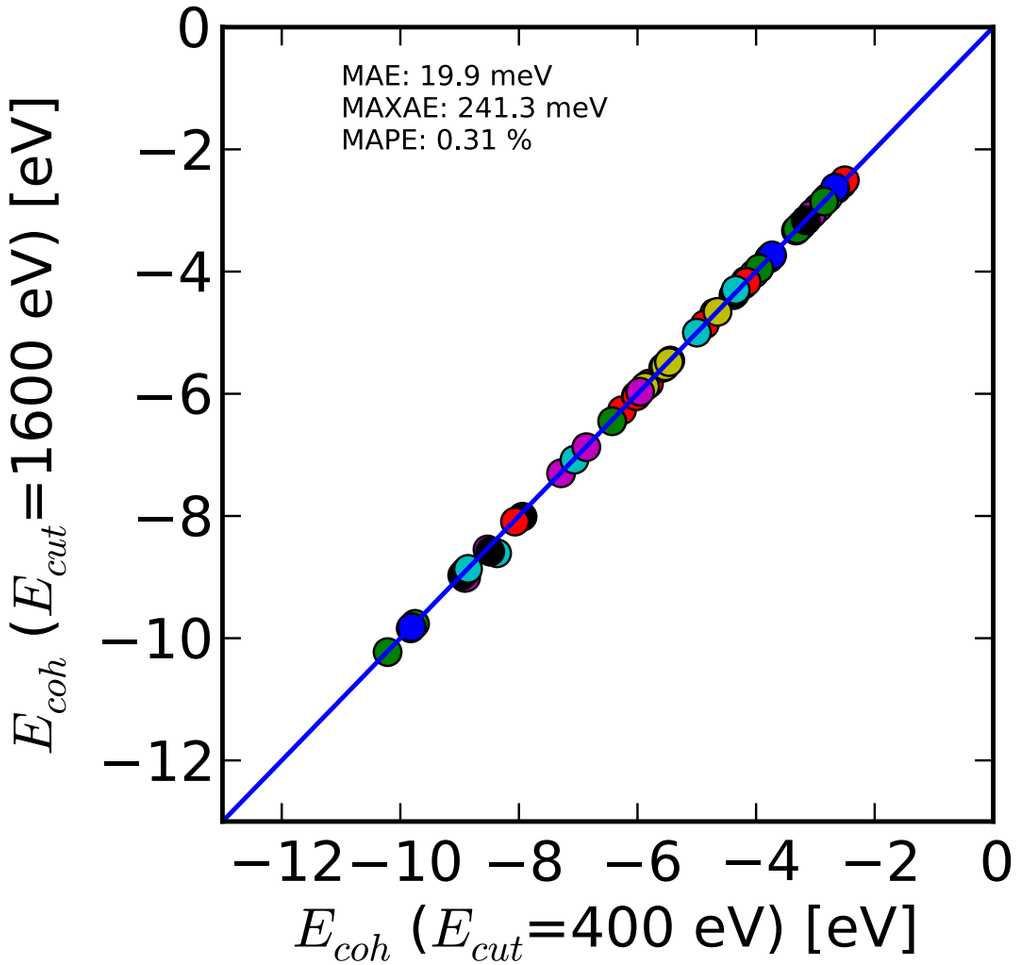


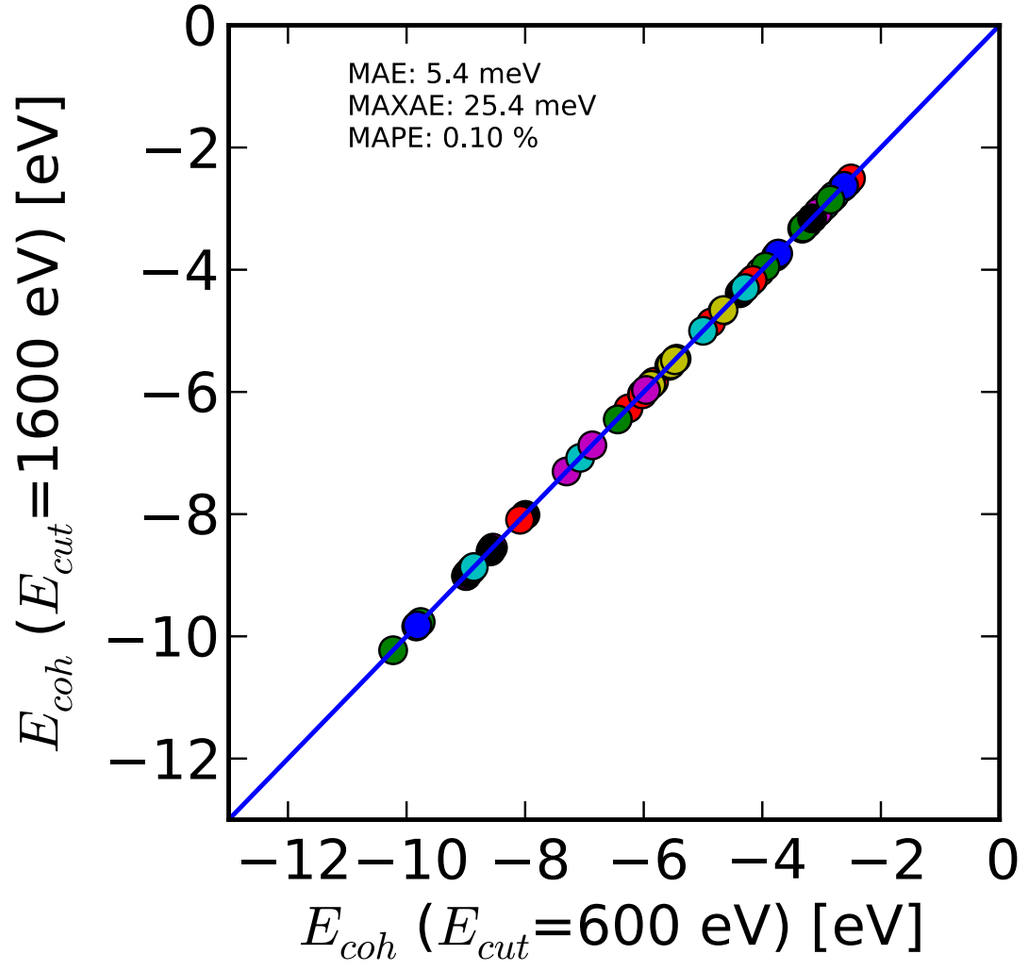
Things really improve at E_{cut} = 600eV!

Error bars project

Cohesive energies (binaries)

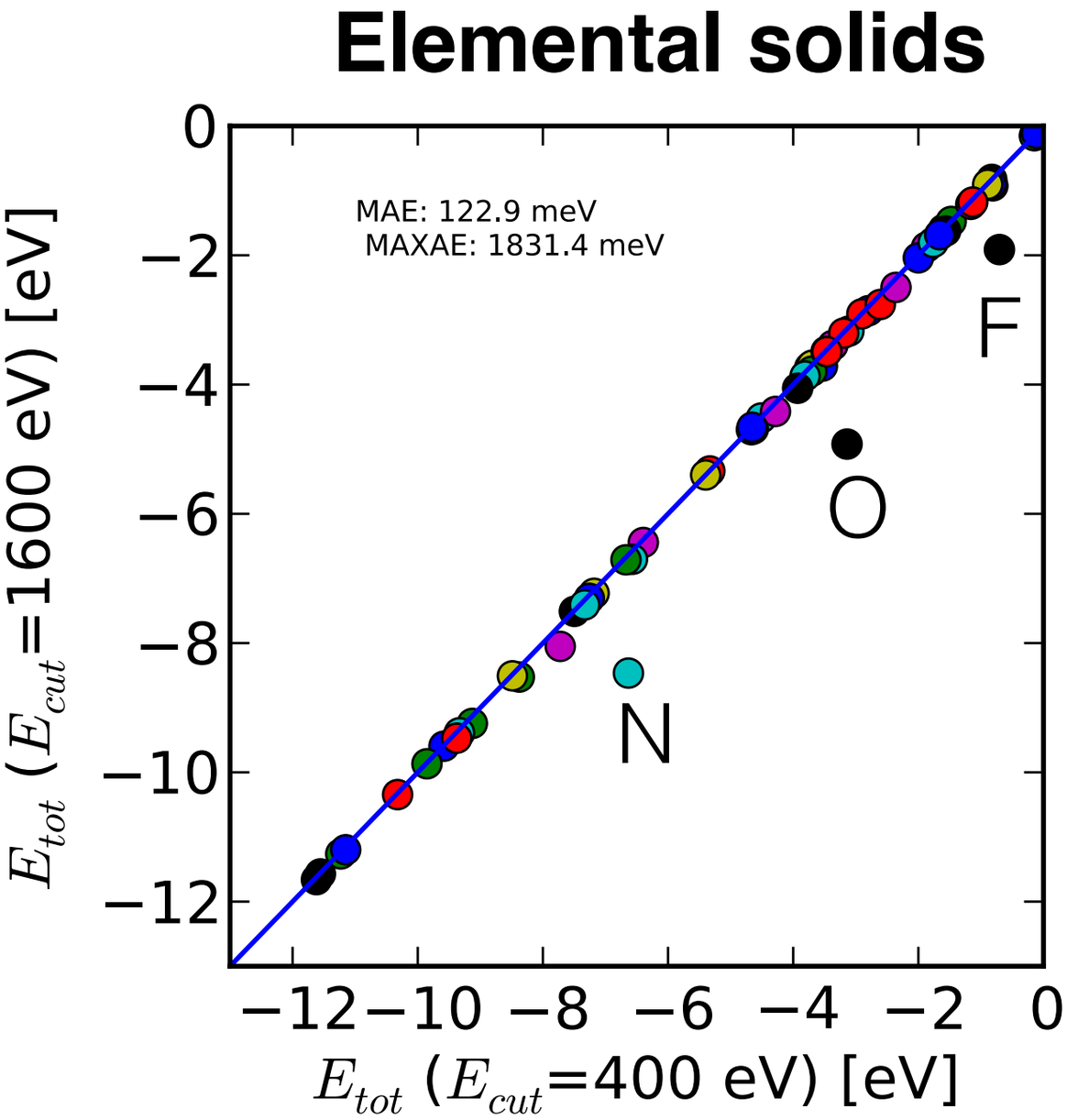
MAE: Mean absolute error
MAXAE: Max absolute error
MAPE: Mean absolute percentage error





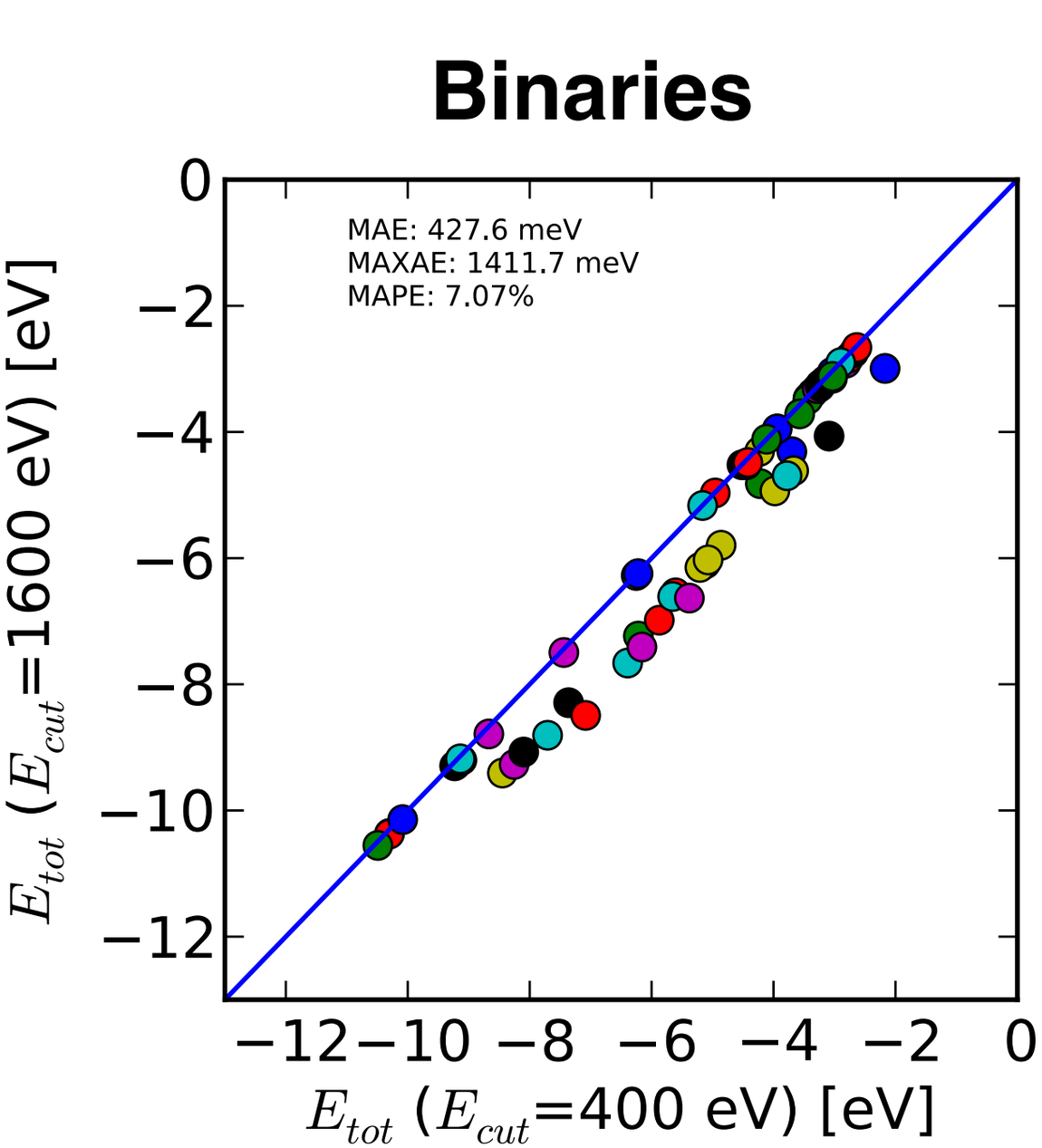
Energy differences benefit
from error cancelation

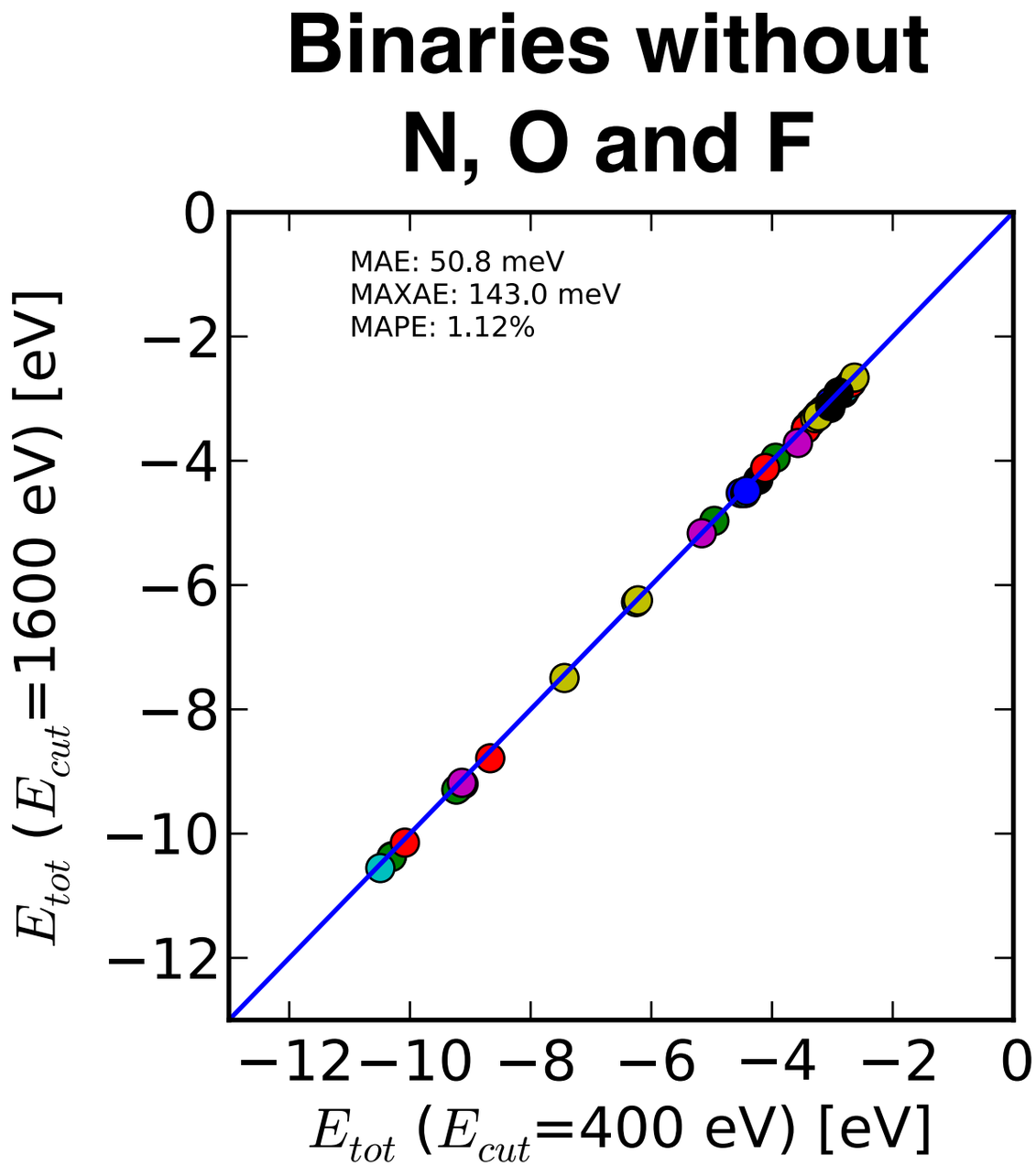
Error bars project



N, O and F are the bad guys!

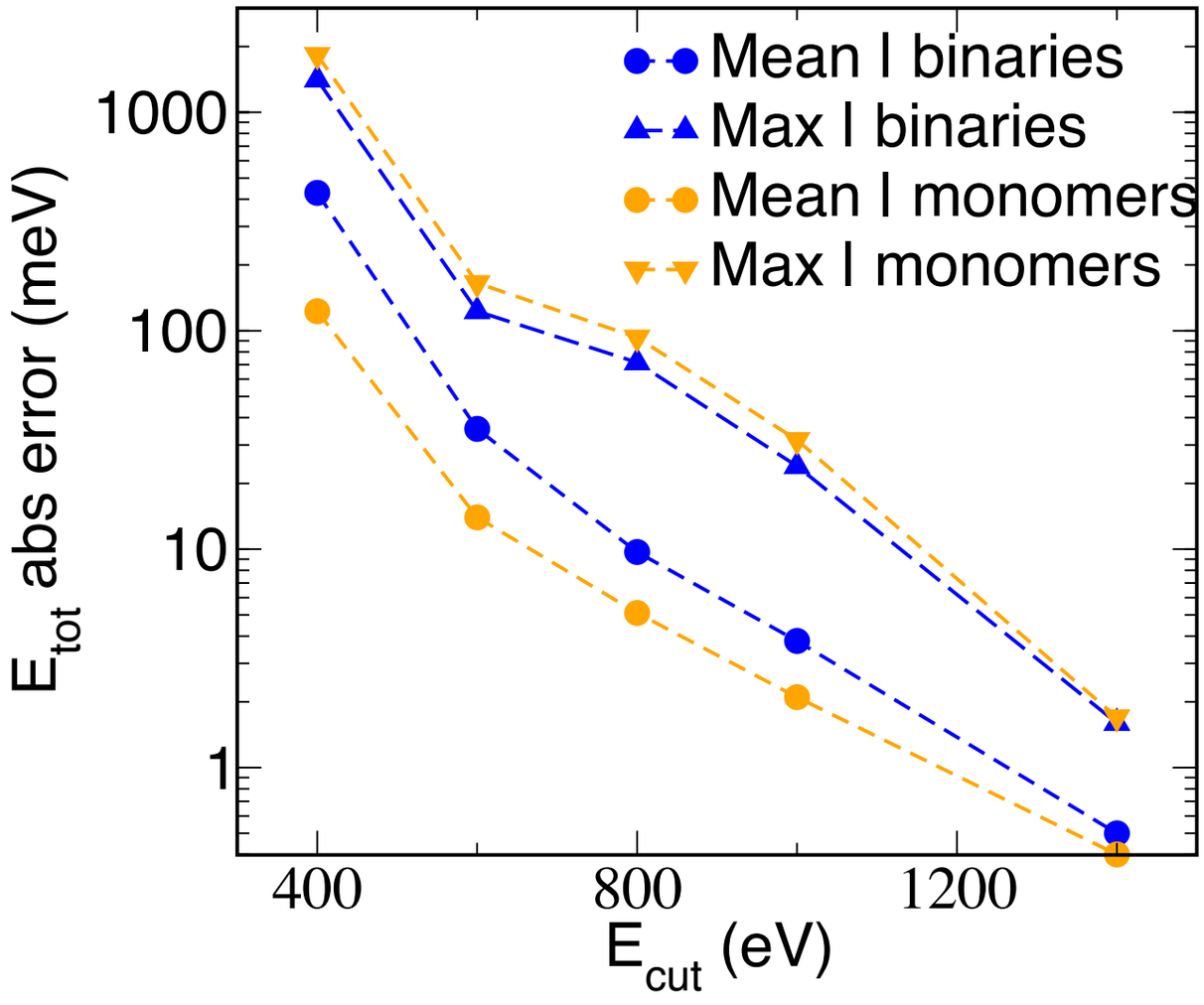
Error bars project





N, O and F are the bad guys!

Error bars project



Max abs error for binaries and elemental solids similar

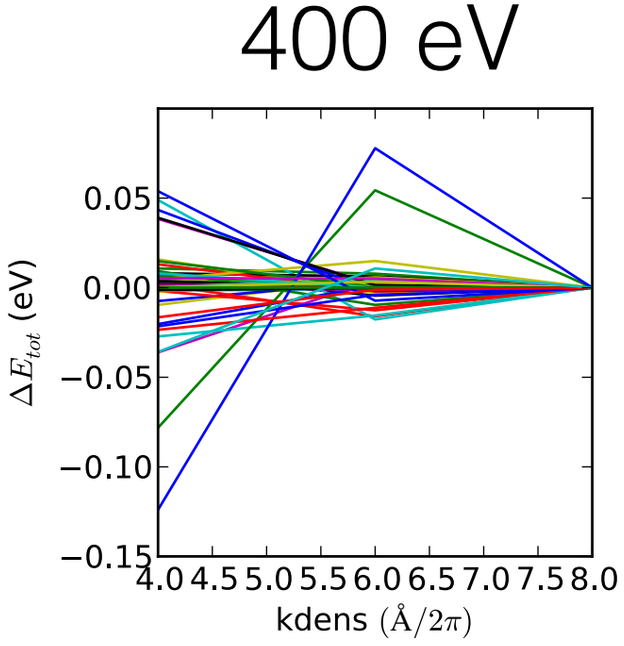
Simple error estimate suggestion: simply use the error for the worst element.

Error bars project

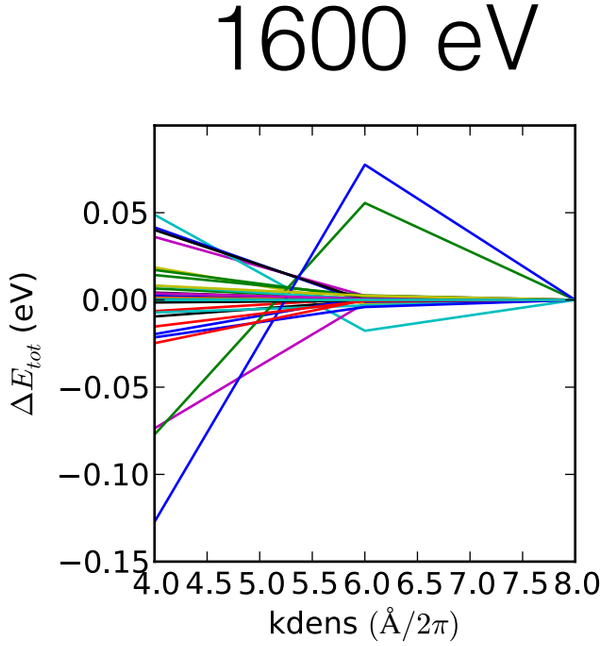
Is convergence with basis set and k-points independent?

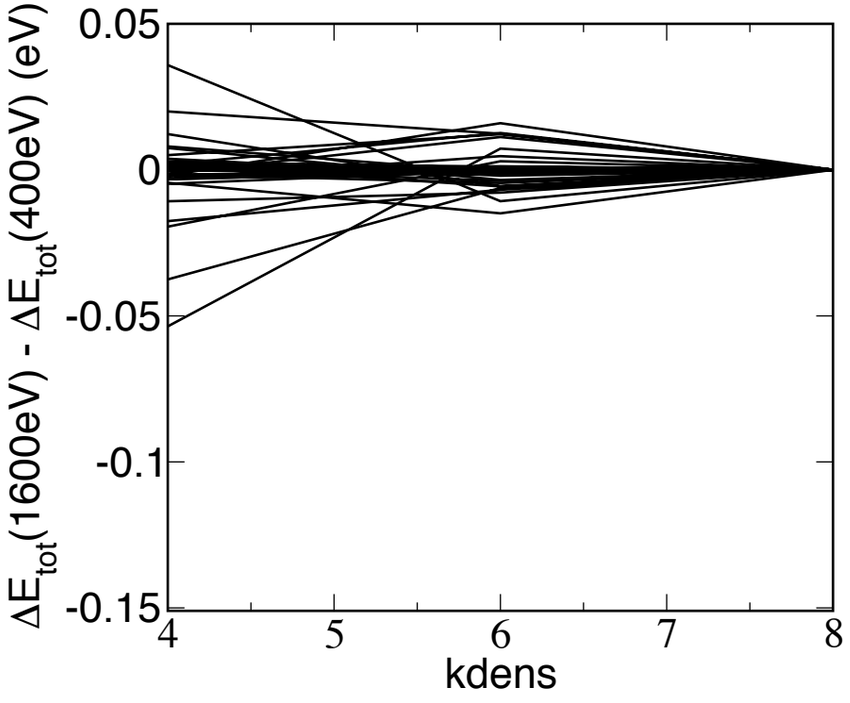
$$E(kpts, basis) = F_1(kpts) + F_2(basis)$$

400 eV



1600 eV





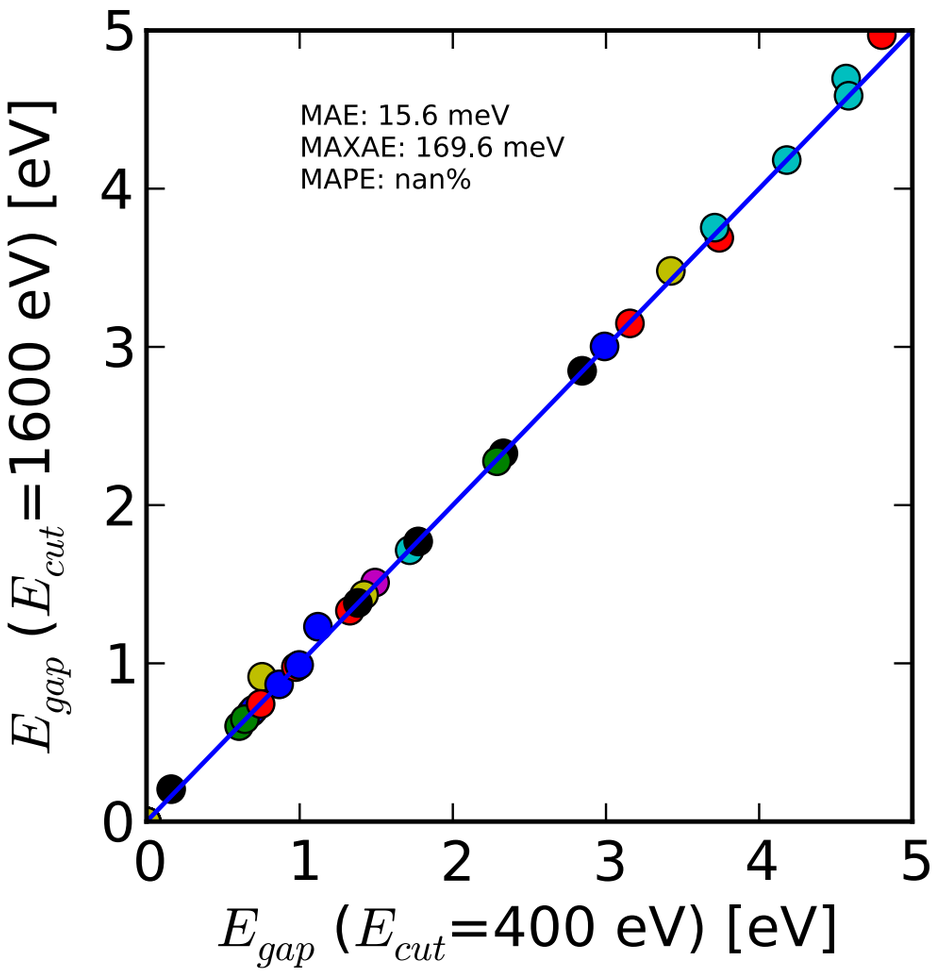
$$\Delta E_{tot}(\rho_k) = E_{tot}(\rho_k = 8) - E_{tot}(\rho_k)$$

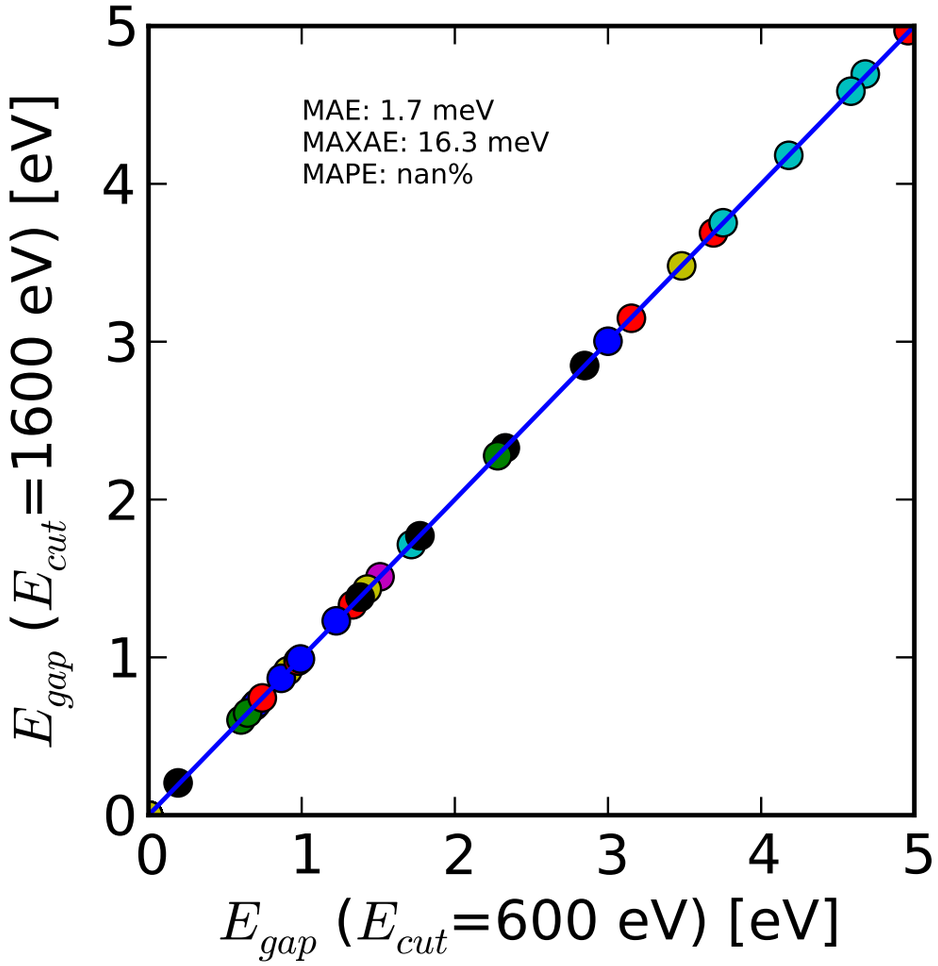
Independent or not?

Error bars project

Also need to look at:

- band gaps
- structures…





Self-consistent hybrid functionals (HSE, PBE0, …)

Currently in GPAW

- Non-SC with PW and k-points
- SC with FD Gamma point only

Challenges:

- Slow (compared to GGA)
- Convergence is supposed to be difficult

VASP tells you to use:
Damped “molecular dynamics”

Self-consistent hybrid functionals (HSE, PBE0, …)

Challenges:

- Convergence is difficult

We are trying with damped molecular dynamics
but also **brute force:**

Hamiltonian in PW basis $\langle g|\hat{h}|g'\rangle$

$$\hat{h}^{HF} = \hat{t} + \hat{v}_H + \hat{v}_F + ...$$

Should be stable, but limited in supercell size

Thank you for the attention!