High-throughput *GW*

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High-throughput *GW*

from a structure

without any human intervention

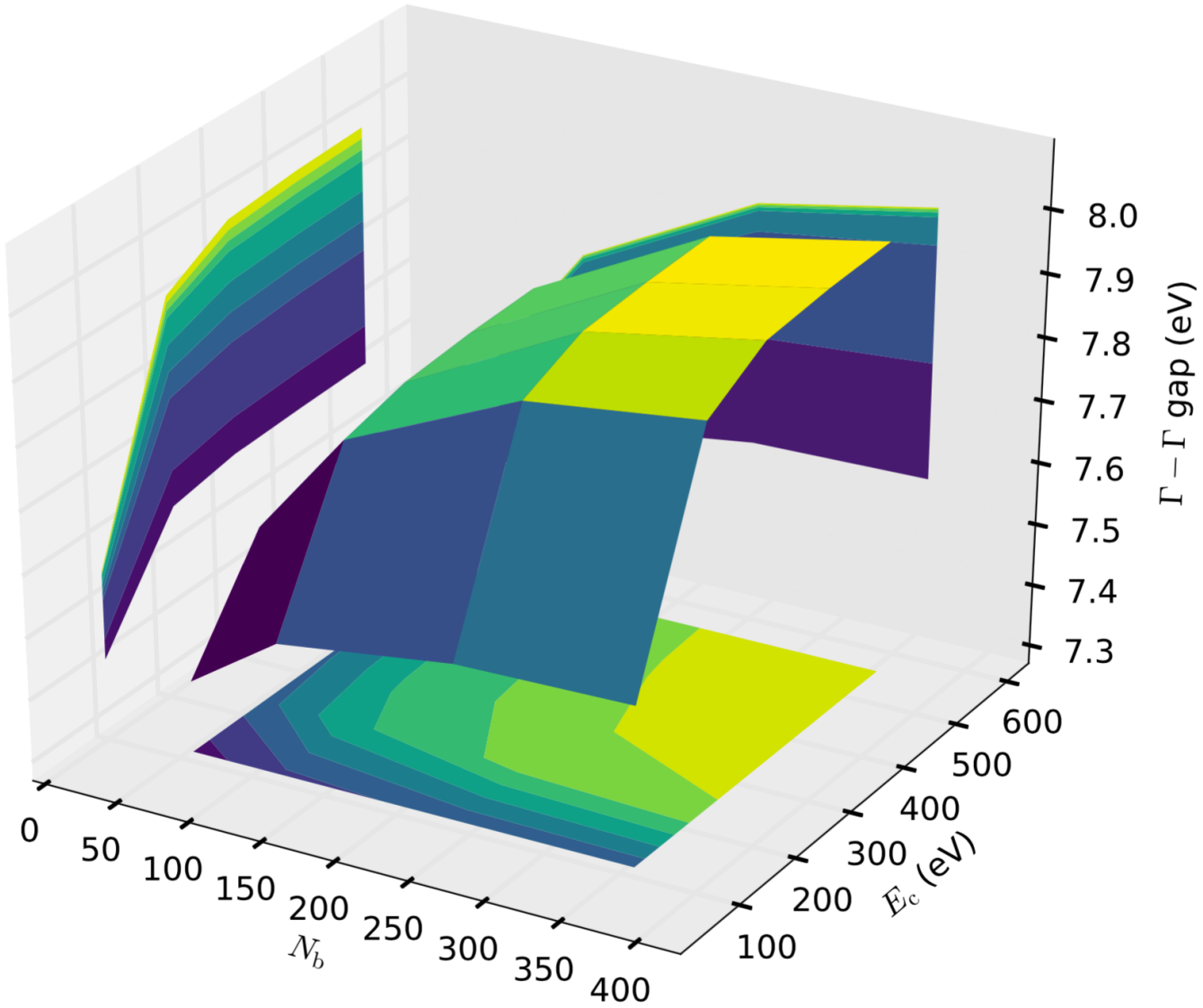
to converged *GW* results

- Automatic calculations
- Screening for new compounds
- Database building
- Uniform results
- No human bias

The Problem

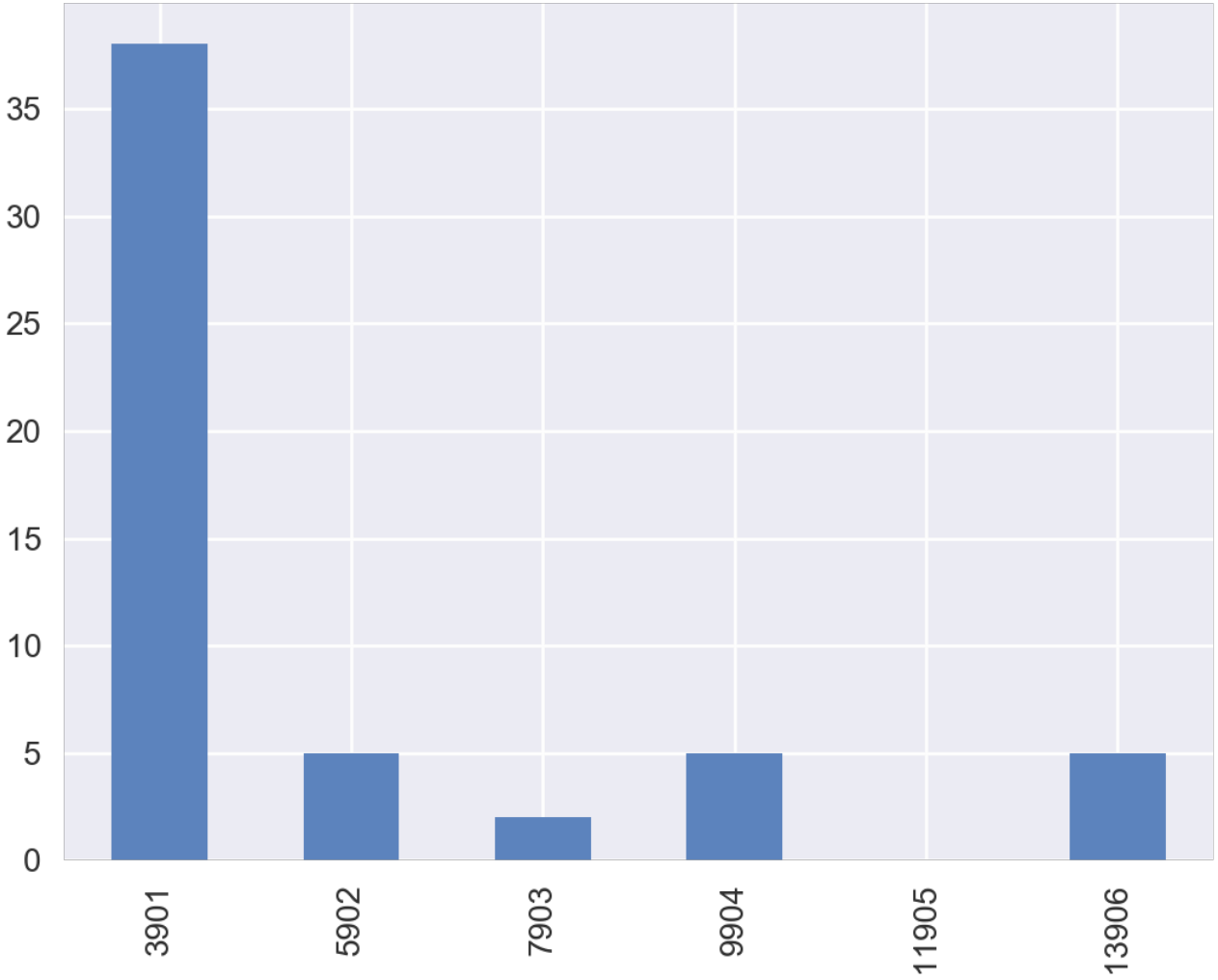
- 'additional' difficulties as compared to DFT
  - Pseudo potentials
  - 4 step calculation
  - N^4 scaling
  - No 'safe' parameter set (converged results for all)
  - No 'safe' computational settings (# cpu's, memory, time, ...)

The convergence problem



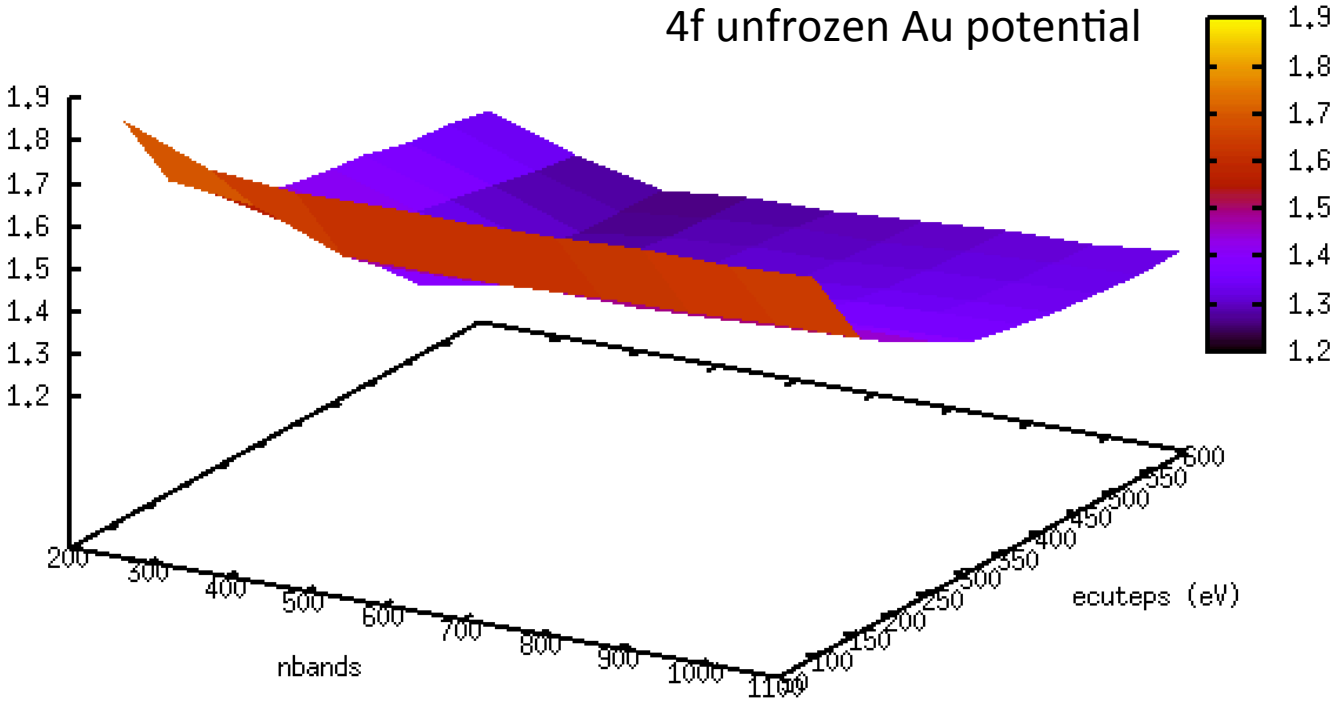
BN

The memory problem

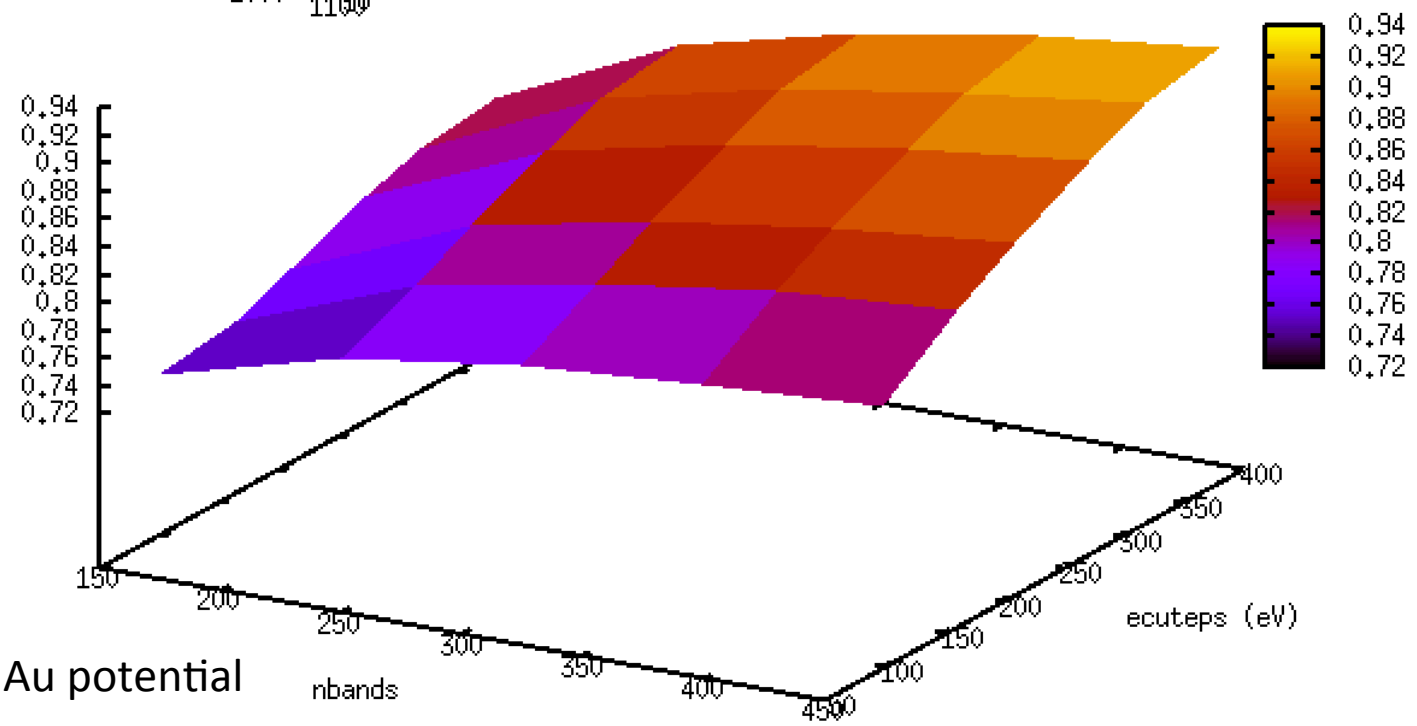


GW tasks that finish at a given memory limit

4f unfrozen Au potential

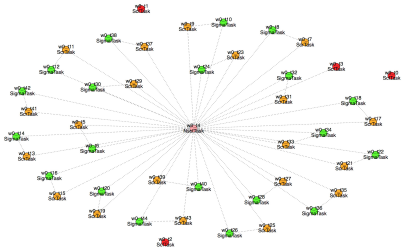


AuCl



Normal 19 electron Au potential

Our solution

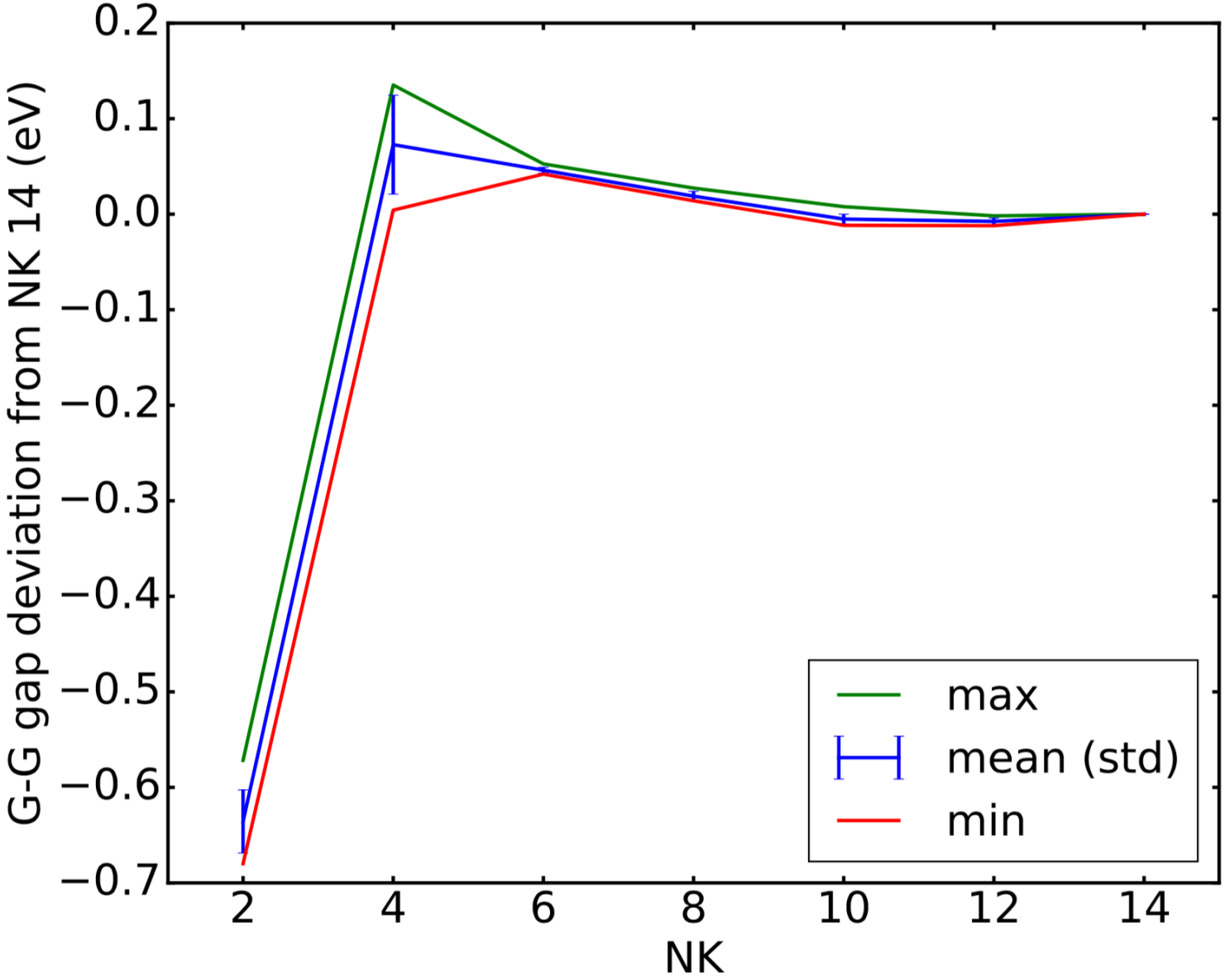


Convergence study

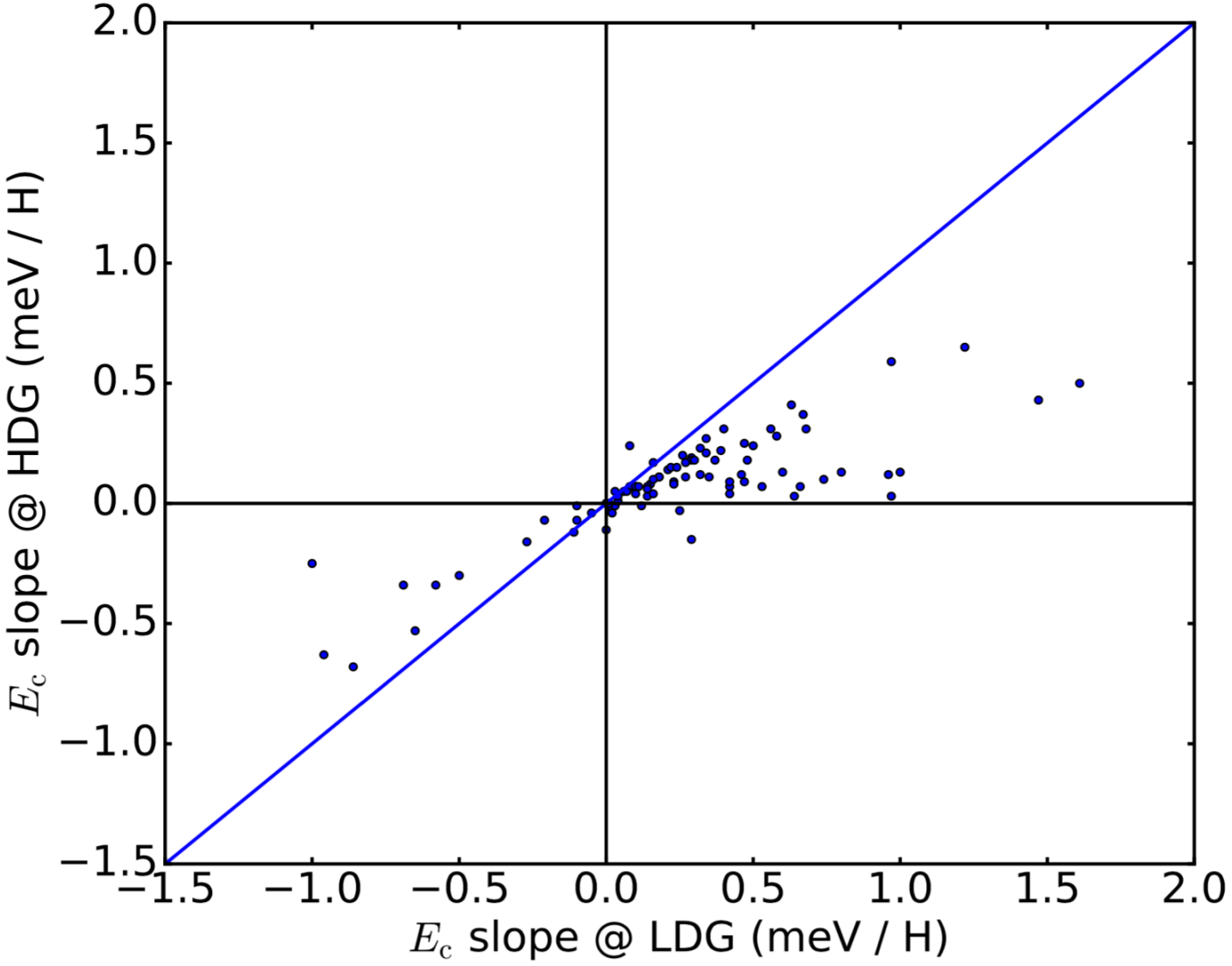
- On a low k-point density (2x2x2): (pw cutoff, …)
  - Set of single parameter ground state convergence studies
  - Grid of nbands X encuteps
  - For each nbands find converged encuteps
  - For the converged encuteps find the converged nbands
  - if not found > extend grid and retest
- On the final high k-point density:
  - Test derivatives.
    (in most cases the high density derivatives turn out smaller)
  - Post process
    (create scissor, apply scissor, plots, statistical analysis…)

abipy

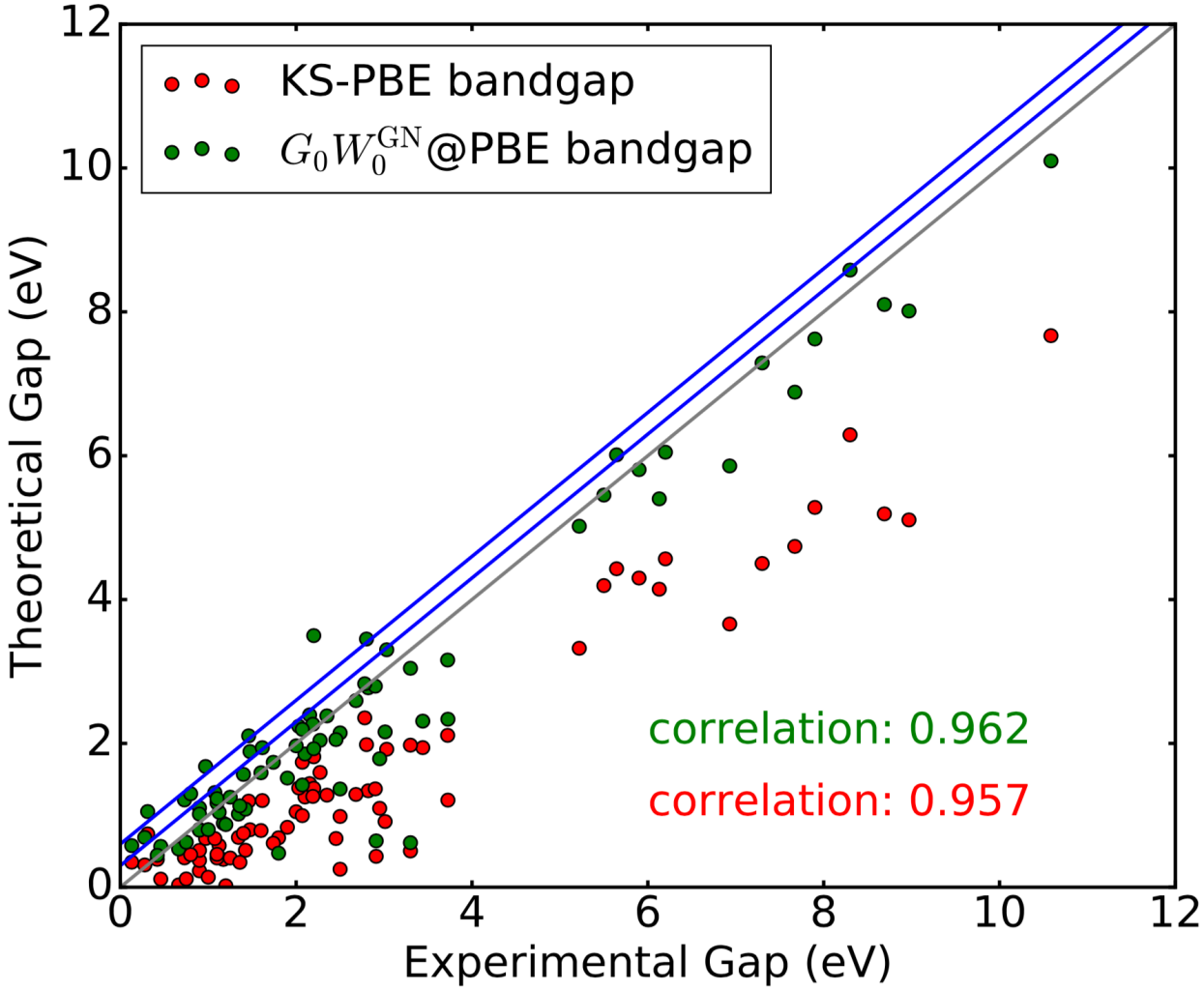
Transferring parameters over k-grids

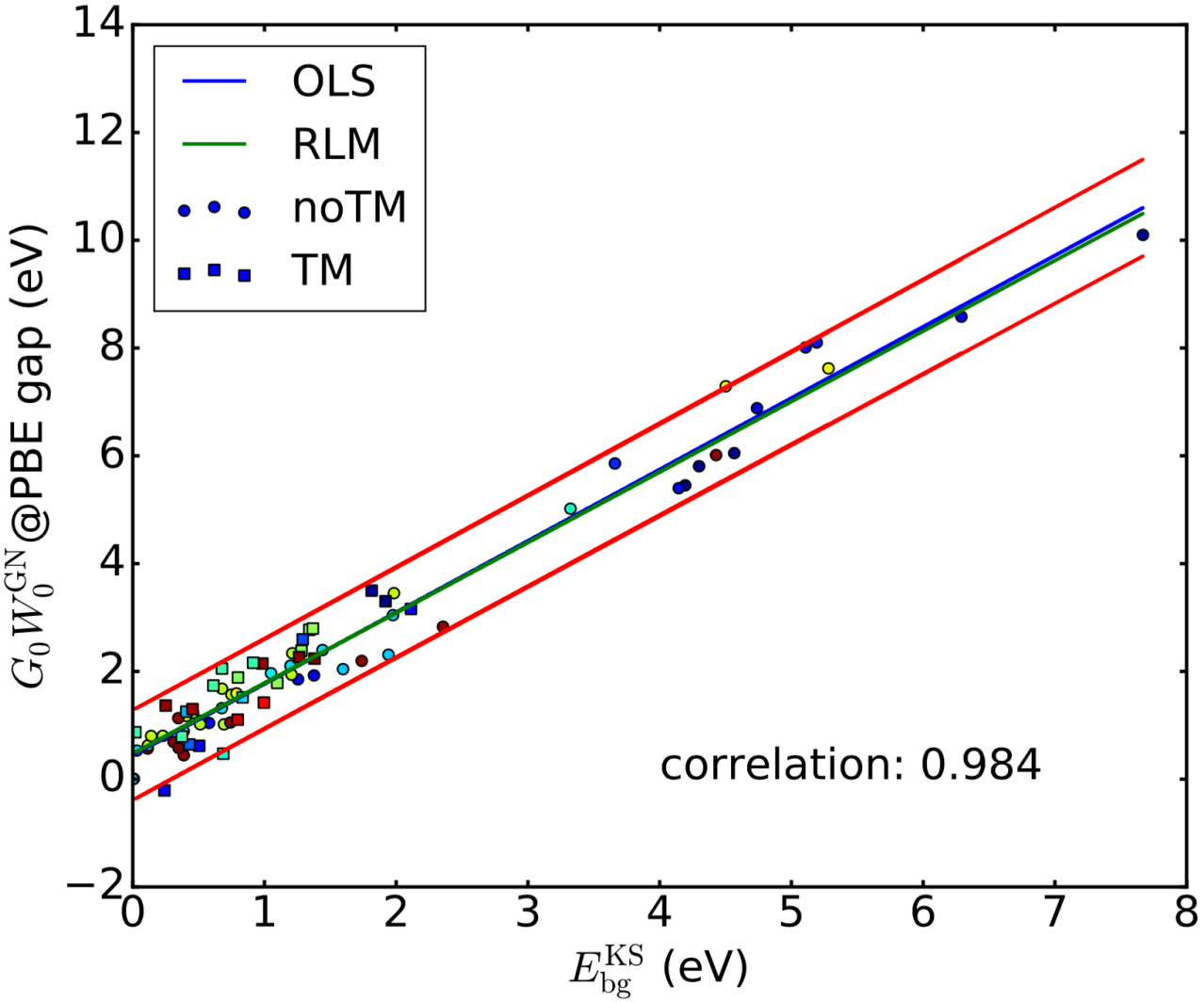


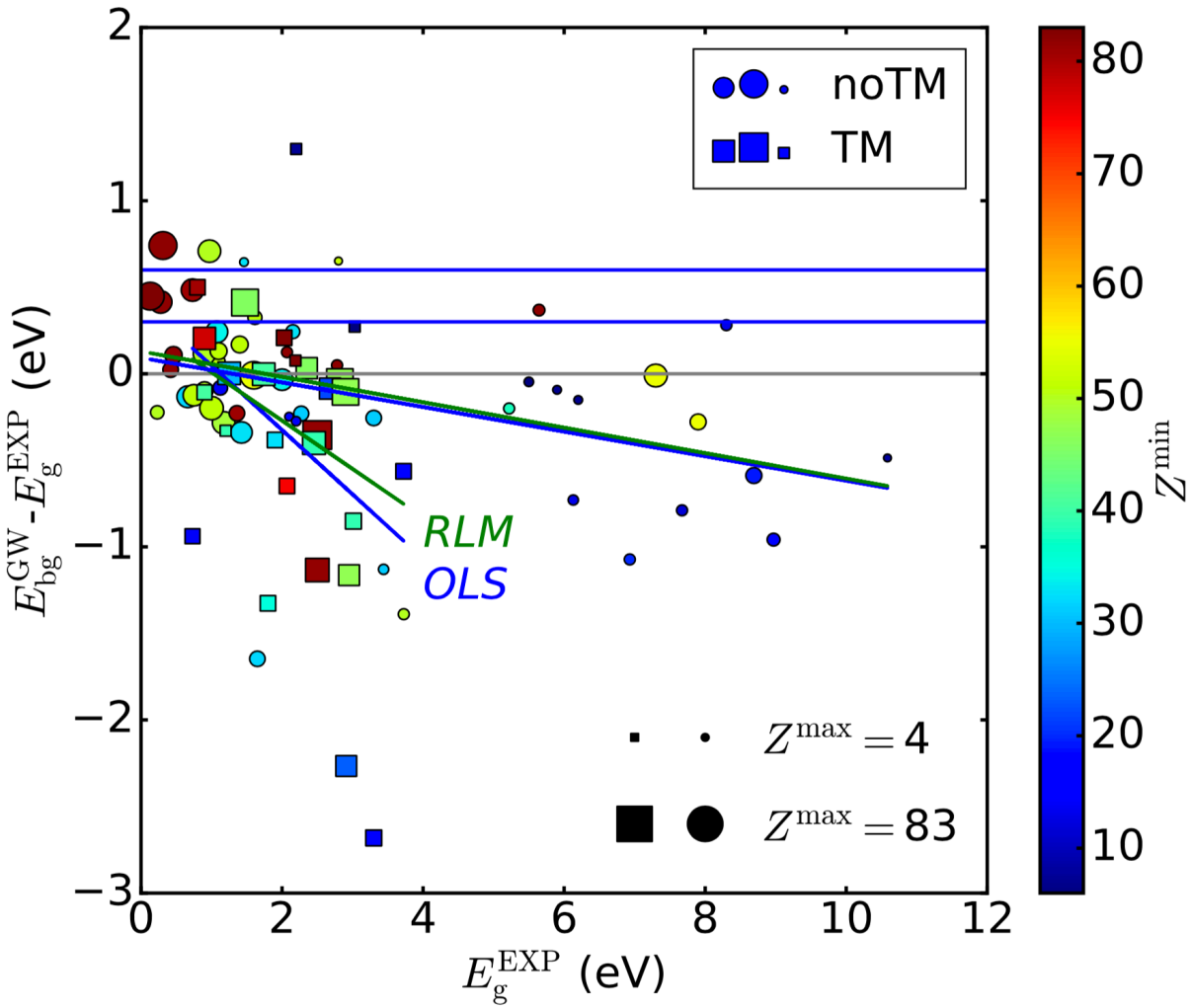
Transferring parameters over k-grids

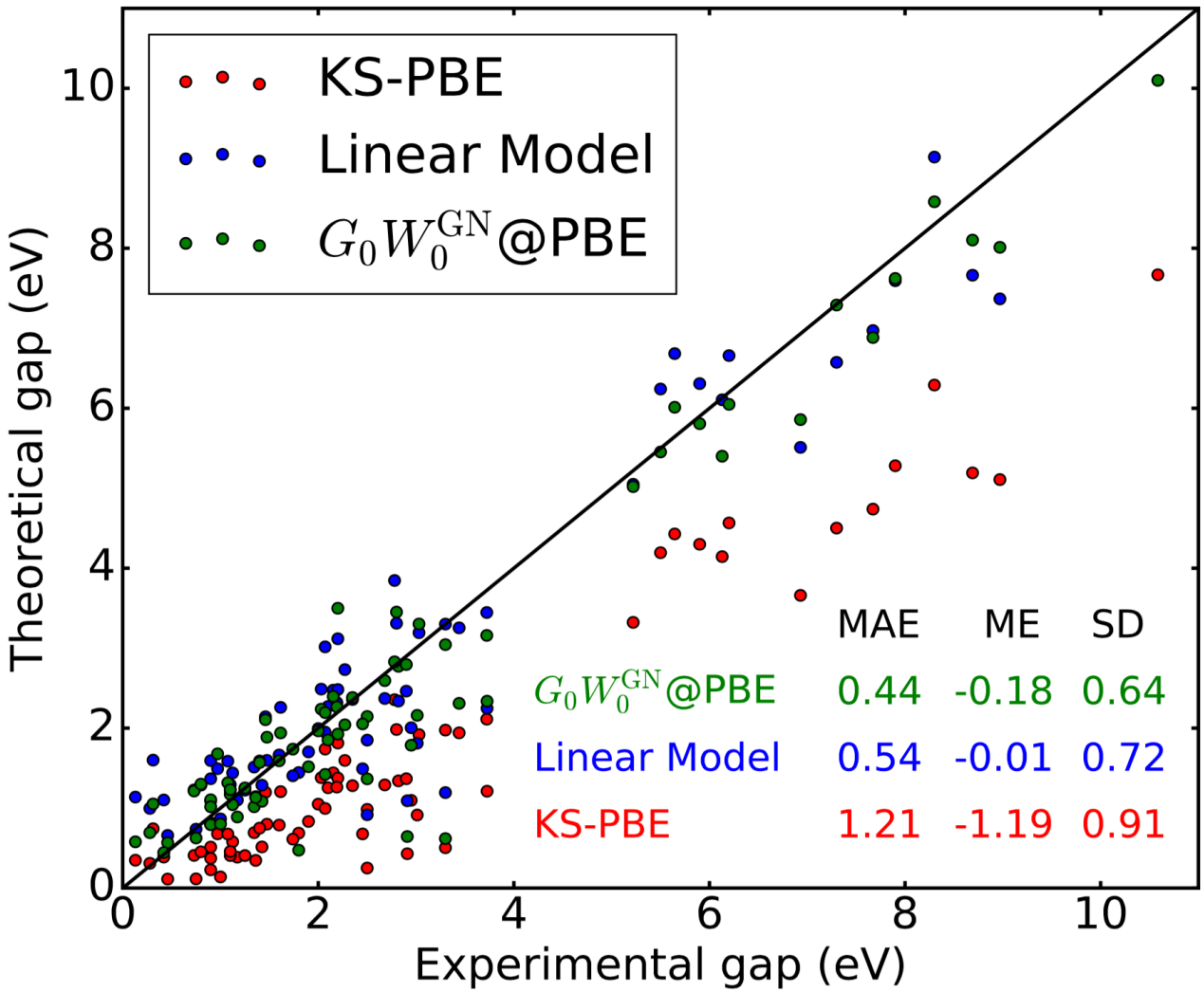


Some results


KS-PBE bandgap
$G_0W_0^{\mathrm{GN}}$@PBE bandgap
correlation: 0.962
correlation: 0.957
Theoretical Gap (eV)
Experimental Gap (eV)
0
2
4
6
8
10
12


OLS
RLM
noTM
TM
correlation: 0.984
$G_0W_0^{\mathrm{GN}}$@PBE gap (eV)
$E_{\mathrm{bg}}^{\mathrm{KS}}$ (eV)
14
12
10
8
6
4
2
0
−2
0
1
2
3
4
5
6
7
8


noTM
TM
RLM
OLS
$Z^{\max} = 4$
$Z^{\max} = 83$
$E_{\mathrm{bg}}^{\mathrm{GW}}$-$E_{\mathrm{g}}^{\mathrm{EXP}}$ (eV)
$E_{\mathrm{g}}^{\mathrm{EXP}}$ (eV)
$Z^{\min}$
2
1
0
−1
−2
−3
0
2
4
6
8
10
12
80
70
60
50
40
30
20
10


KS-PBE
Linear Model
$G_0W_0^{\mathrm{GN}}$@PBE
Theoretical gap (eV)
Experimental gap (eV)
0
2
4
6
8
10
MAE ME SD
$G_0W_0^{\mathrm{GN}}$@PBE 0.44 -0.18 0.64
Linear Model 0.54 -0.01 0.72
KS-PBE 1.21 -1.19 0.91

Collaborators

- Matteo Giantomassi
- Geoffroy Hautier
- Gian-Marco Rignanese
- Don Hamann
- Xavier Gonze

pymatgen