An obvious truth:
Any two independently written DFT codes that solve the Kohn-Sham equations in a numerically exact way, should produce identical predictions for any solid (provided the same XC-functional is used and full numerical accuracy is reached).

Goal of this work
Verify this statement, by comparing predictions by different codes/methods for a standardized benchmark set of elemental solids.

Benchmark set
- Elemental materials in their ground state crystal structure (except for Mn and S).
- 7 data points in a range of ±6% around the equilibrium geometry predicted by VASP.
- Frozen geometry: only volume change, no cell shape or internal positions.

Gauge: Δ

APW+lo as implemented in WIEN2k
PBE functional
\( \text{Rmt} = 2.30 \text{ a.u. or touching}
\)

basis set: very large (see bottom left table)

k-grid : corresponding to 31x31x31 for Au

\( I_{\text{max}} = 14 \)

\( G_{\text{max}} = 3 \text{ G_{min}} \)

FFT-mesh: factor 4

Birch-Murnaghan fits for volume per atom \((\text{Å}^3)\), bulk modulus (GPa) and its pressure derivative

Conclusions and Outlook
- Convenient test set for code accuracy verification
- Convenient test set for pseudopotential and PAW projector generation
- Disagreement between codes/methods is one order of magnitude smaller than disagreement between DFT and experiment (good !)
- General call: run this test for your favourite code (all input and scripts available)
- Interesting question: would other APW-lo implementations yield \( \Delta \)-values well below 1.6 meV/atom?

References
[2] By M. Dutko
[4] By T. Oulek

Input files to run your own tests as well as scripts for analysis are available at http://molmod.ugent.be/DeltaCodesDFT