

GBRV v1.5 + Elemental Testing

Kevin F. Garrity*

*National Institute of Standards and Technology,
Gaithersburg, MD 20899*

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Abstract

These notes contain a very brief discussion of version 1.5 the GBRV potentials for Quantum Espresso and Abinit and testing based on updated all-electron results for elemental ground states.

Recently, there has been a significant effort to produce extremely accurate all-electron and pseudopotential/PAW calculations for elemental ground states. This work was started in Ref. [1] and an expanded version will be described in an upcoming paper co-authored by many experts in DFT numerics (see also molmod.ugent.be/deltacodesdft). Details of the structures tested are in Ref. [1]; they are all elemental ground states. Based up this updated reference data, I am updating the QE version of Cr/Fe/Mn/P and the Abinit version of P, which displayed sub-optimal results for these accurate tests. My previous tests were limited in their testing of spin-polarized structures and failed to identify the under-performance of Fe/Cr/Mn for QE in elemental structures. In addition, my previous tests of P did not include P-P covalent bonding. I also reran my previous tests and there was very little change.

These calculations are all done with the standard low GBRV plane-wave and charge density cutoffs (40 Ryd and 200 Ryd). Results with much higher cutoffs will be presented in the upcoming paper, but are very similar. The reference data is an average of very well converged all-electron calculations from the WIEN2k and exciting codes. The average Δ is 0.8 meV/atom for both codes, and the mean absolute effective lattice constant ($V^{1/3}$) error is 0.10%.

See figures 1 and 2 for element-by-element results. Overall performance is good, especially considering the low convergence parameters. One exception is H/N/O/F, which is due to the fact that it is very difficult to describe short covalent bonds for these atoms with a low cutoff. As emphasized previously, I recommend potentials designed for a higher cutoff when studying organic molecules. However, as shown in my previous testing[2], the performance in typical solids (*e.g.* oxides, nitrides) is very good.

* Electronic address: kgarrity@physics.rutgers.edu

- [1] K. Lejaeghere, V. V. Speybroeck, G. V. Oost, and S. Cottenier, *Crit. Rev. Solid State Mater. Sci* **39**, 1 (2014).
- [2] K. F. Garrity, J. W. Bennett, K. M. Rabe, and D. Vanderbilt, *Comput. Mater. Sci* **81**, 446 (2014).

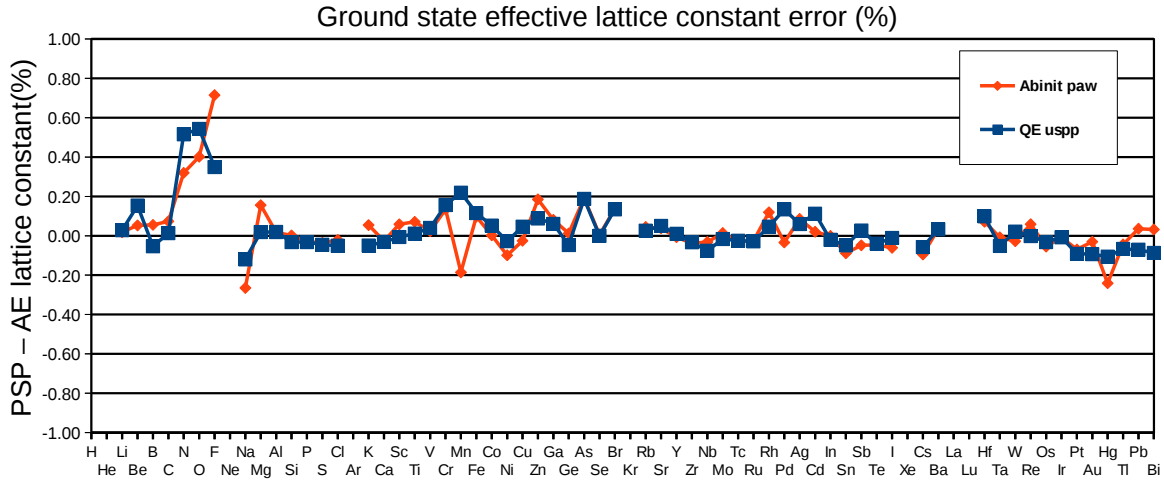


FIG. 1: Percent difference in AE versus pseudopotential calculations for effective lattice constant. GBRV QE USPP results (v1.4) are blue squares, GBRV ABINIT PAW results are red diamonds.

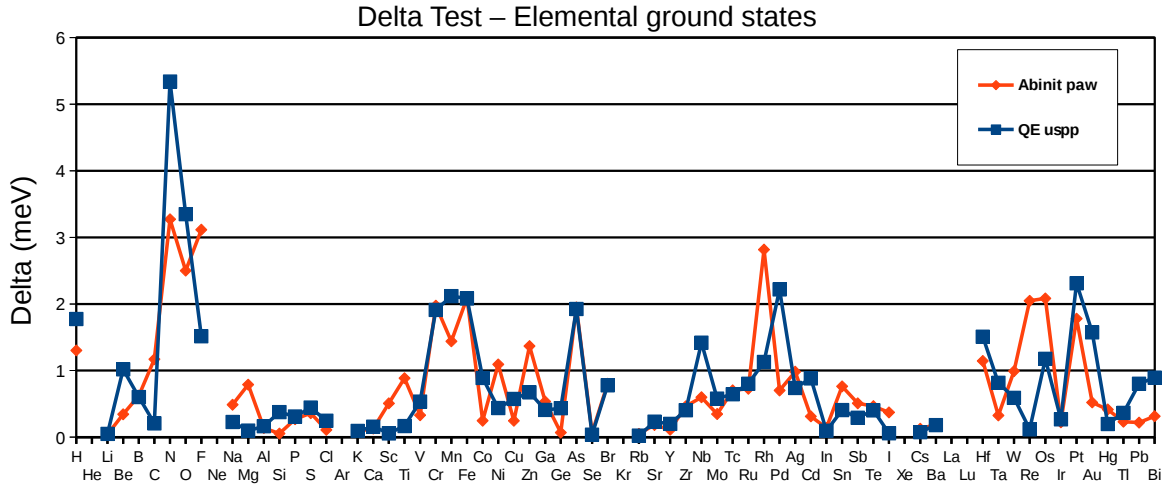


FIG. 2: meV/atom for Δ parameter (see [1]), relative to all-electron results (smaller is better). Calculations with Δ below 1-2 meV/atom are indistinguishable for most purposes.