GBRV update and JTH testing

Kevin F. Garrity*

Department of Physics & Astronomy,

Rutgers University, Piscataway,

New Jersey 08854-8019, USA

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Abstract

These notes contain a discussion of a minor update of the GBRV potentials as well as new testing data on both the GBRV potentials and the recently released JTH PAW set. This testing includes a new zinc blende test set, which has been examined with the Δ-factor test[1]. The updated testing data are consistent with earlier tests which show very good performance for the GBRV potential set. The tests on the JTH set indicate that while the majority of the PAWs are sufficiently accurate, the JTH PAW table requires revisions before it is sufficiently robust for general use in high-throughput computations.

These notes will briefly discuss some updates of the GBRV potential set[2–4], as well as new tests of the GBRV potentials and other potential sets.

First, several GBRV potentials have been updated with the goal of improving their convergence versus both energy cutoff and the double grid or charge density cutoff. Modified potentials include Be-F, V-Cu, Ga, Ru-Pd, W-Ir, and Tl, although in some cases only one of the USPP or PAW versions was modified. The modifications largely were to details of the pseudization, especially of the inner/augmentation regions, and were typically minor adjustments. For most purposes the updated potentials will give the same results as previous versions, which can be seen by comparing the updated tests in these notes with our original papers[2, 3].

Nearly all of these potentials have the same or slightly improved properties on our tests, but with improvement of the numerical performance of the potentials. The improvement was tested by calculating the *fcc-bcc* energy difference. According to this test, all of the potentials should have a convergence error for energy differences of 1 meV/atom or less at 40 Ry plane-wave cutoff, with most of the potentials having even better convergence. The hardest potentials are C-N, Mn-Cu, Ru-Ag, W-Ir. It may be possible to run other elements at lower cutoffs, although as always care should be taken to test that the property you are interested in is converged. By the same test, the charge density is converged at 160 Ry using Quantum Espresso and the double grid at 100 Ry using Abinit in all cases.

In addition to the update of the GBRV potentials, I wanted test the performance of the PAW atomic data library recently published by F. Jollet, M. Torrent and N. Holzwarth (JTH) (available online[5]). JTH test their PAWs as well as version 1.0 of the GBRV PAWs using Abinit on a variety of elemental crystals[6] using the Δ-factor test[1]. The Δ-factor summarizes in one number the RMS difference of the energy versus volume curve as compared to all-electron results, rather than just the lattice constant or bulk modulus, by fitting both to a Birch-Murnaghan equation of state. JTH find good results overall for the GBRV potentials, especially after switching to version 1.01 of the GBRV potentials (see footnotes in [6]); however, they find significantly better results for their own potentials. I decided to study this issue by applying the tests used in the GBRV paper to their potentials.

In addition, I am including a new zinc blende testing set (with the same procedure as in [2]), which includes a calculation of the Δ-factor[1] for these compounds. This new test set is designed to address the possibility that the GBRV potentials are either overfit to the

tests which were used to help design them or that the performance of the GBRV set is worse using the Δ-factor methodology, which are possibilities raised by the JTH study.

My testing results on the previous testing data (Tables I-II and Figures 1-5), indicate that the JTH library performs worse than either the GBRV potentials or VASP when using the GBRV testing data[2, 7]. The tests are done with the same scripts/input parameters that I used to test the GBRV ABINIT potentials[3]. Most of the JTH outliers are in ionic/covalent materials; the *fcc* and *bcc* results are in better agreement with the other potential sets. A few JTH potentials perform very poorly (e.g. Os bonded to O), which may be due to PAW overlap; however, more typical results for the JTH potentials are also generally worse, especially for ionic materials. Tl(+3) and In(+3) are particularly poor.

The tests on the new zinc blende test set, presented in Figs. 6-7, are consistent with previous test sets, especially the comparable NaCl test set. Both lattice constant errors and the Δ-factor indicate very good and very similar performance for the GBRV and VASP potentials, while the JTH set has several outliers. These results seem to indicate that previous testing of the GBRV potential set is a reliable indicator of its performance in comparable new structures, and that its performance in Δ-factor tests is consistent with other testing methods.

This work shows that the JTH PAW set requires further testing before it is appropriate for general purpose high-throughput calculations, especially in ionic materials. It remains somewhat unclear why the JTH set gives excellent results for the JTH tests, but underperforms here, to some extent even on the *fcc* and *bcc* structures.

Notes:

–The JTH set currently lacks a La (GBRV lacks Lu and the noble gases, which are not tested here). La-containing materials are not included in the reported summary data, so the reported summary data are for the same materials.

–Some of the JTH magnetic moments are sensitive to pawecutdg, which I set to 200 Ry for magnetic testing and 100 or 200 Ry for structural testing.

–I used the default for bxctmindg and other PAW variables related to angular momentum sums, etc.

–Thanks to E. Bousquet for discussions.

TABLE I: Summary of pseudopotential testing results. Lattice constant and magnetic moment testing data is presented as either RMS errors relative to AE calculations or percent of lattice constants outside ±0.2%, Δ-factor is a simple average (smaller is better). La is removed from summary results. zb no TlP indicates the zinc blende testing set with TlP removed, which is an obvious outlier for the JTH set.

Test	GBRV QE	GBRV ABINIT	JTH	VASP
fcc latt. const. (%)	0.13	0.13	0.17	0.11
bcc latt. const. (%)	0.15	0.14	0.18	0.12
rock salt latt. const. (%)	0.12	0.13	0.48	0.15
rock salt mag. mom. (μ_B)	0.08	0.09	0.55	0.22
perovskite latt. const. (%)	0.08	0.09	0.29	0.13
half-Heusler latt. const. (%)	0.11	0.12	0.25	0.14
zinc blende latt. const. (%)	0.12	0.12	0.46	0.11
zb no TlP (%)	0.12	0.12	0.24	0.11
fcc latt. const. $>\pm0.2\%$ (%)	8.3	8.3	21.7	8.3
bcc latt. const. $>\pm0.2\%$ (%)	10.0	8.3	26.7	6.7
rock salt latt. const. $>\pm0.2\%$ (%)	9.7	8.1	27.4	12.9
perovskite latt. const. $>\pm0.2\%$ (%)	1.9	1.9	24.5	15.1
half-Heusler latt. const. $>\pm0.2\%$ (%)	2.4	6.3	29.1	15.7
zinc blende latt. const. $>\pm0.2\%$ (%)	5.4	7.1	23.2	7.1
zinc blende Δ (meV)	1.2	1.2	2.8	1.0
zb no TlP, Δ (meV)	1.2	1.3	2.0	1.0

* 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).

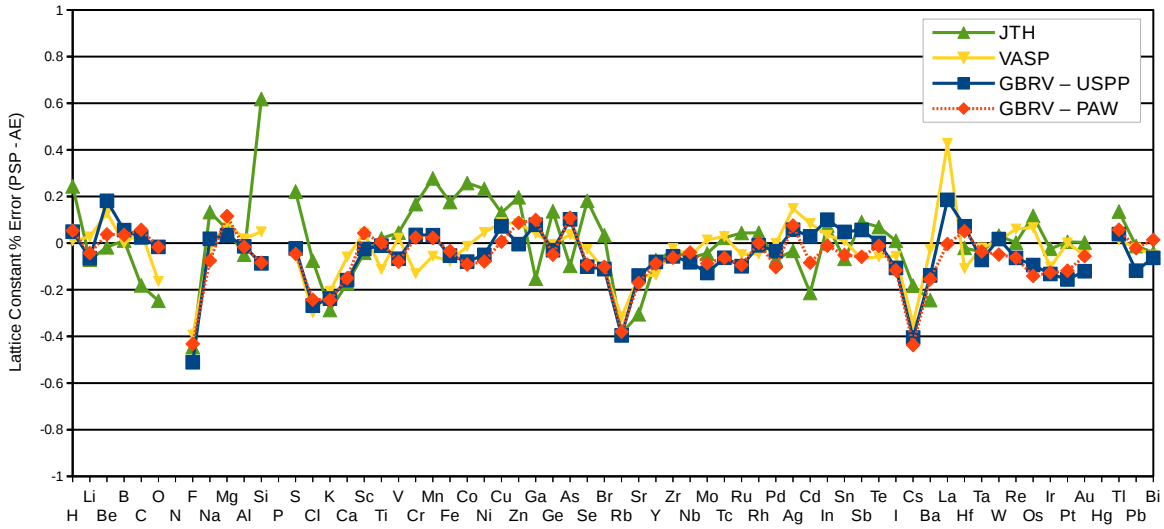

FIG. 1: Percent difference in AE versus pseudopotential calculations for *fcc* lattice constant. GBRV QE USPP results are blue squares, GBRV ABINIT PAW results are red diamonds, VASP results are yellow downward triangles, and JTH results are upward green triangles.

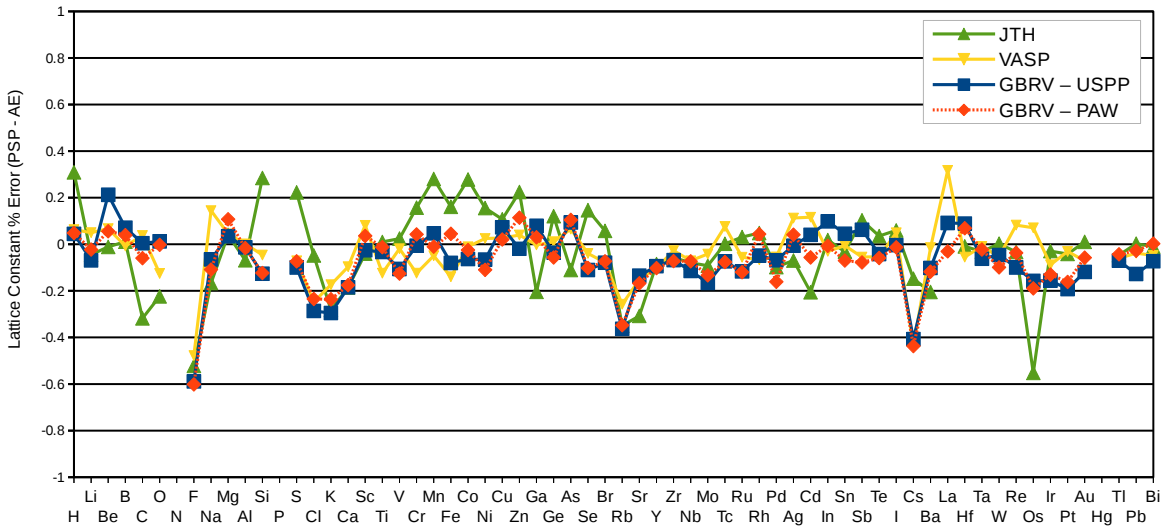

FIG. 2: Percent difference in AE versus pseudopotential calculations for *bcc* lattice constants. Colors as in Fig. 1.

[3] K. F. Garrity, *Notes on abinit gbrv paws* (2013), URL `http://www.physics.rutgers.edu/gbrv/notes_on_abinit3.pdf`.

[4] K. F. Garrity, J. W. Bennett, K. M. Rabe, and D. Vanderbilt, URL `http://physics.rutgers.edu/gbrv`.

[5] M. T. F. Jollet and N. Holzwarth (2013), URL `http://www.abinit.org/downloads/PAW2/`

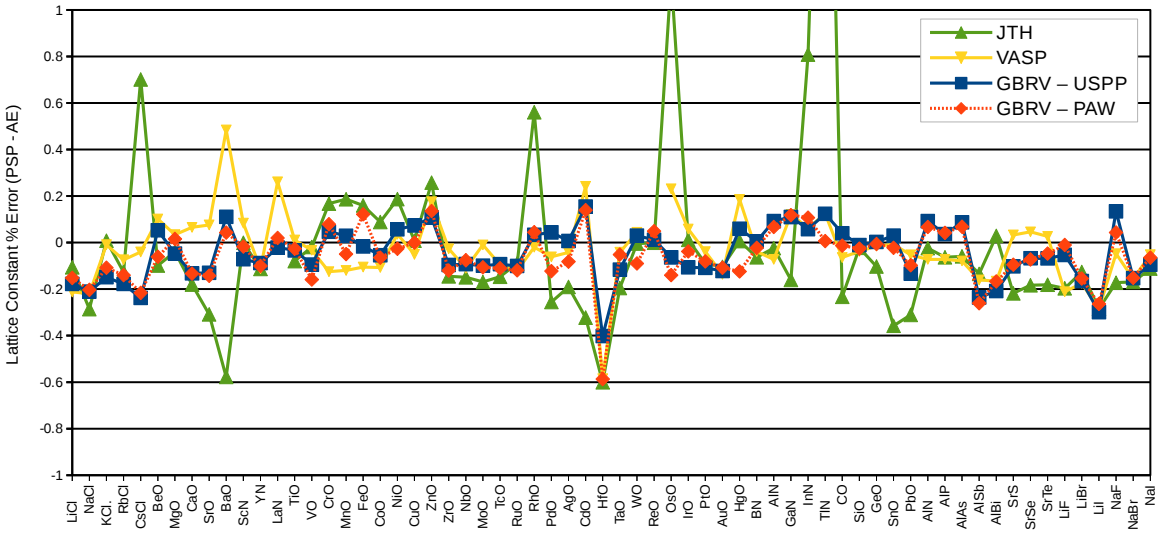

FIG. 3: Percent difference in AE versus pseudopotential calculations for rocksalt lattice constants. Colors as in Fig. 1.

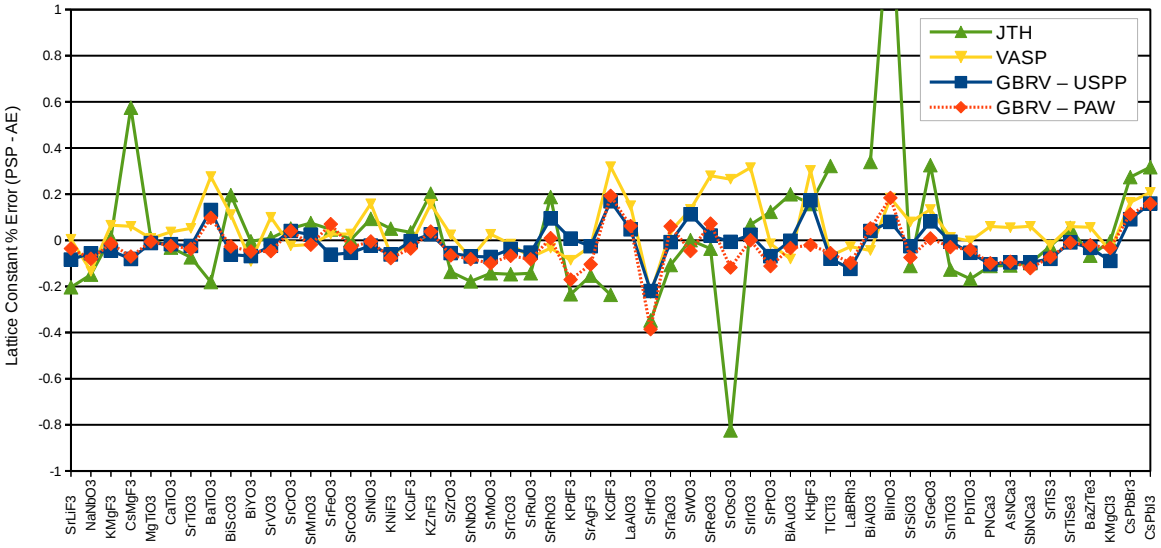

FIG. 4: Percent difference in AE versus pseudopotential calculations for perovskite lattice constants. Colors as in Fig. 1.

`JTH-TABLE/index.html`.

[6] M. T. F. Jollet and N. Holzwarth, arXiv:1309.7274 (2013).

[7] K. F. Garrity, J. W. Bennett, K. M. Rabe, and D. Vanderbilt (2013), URL `http://www.physics.rutgers.edu/gbrv/psp_supp.pdf`.

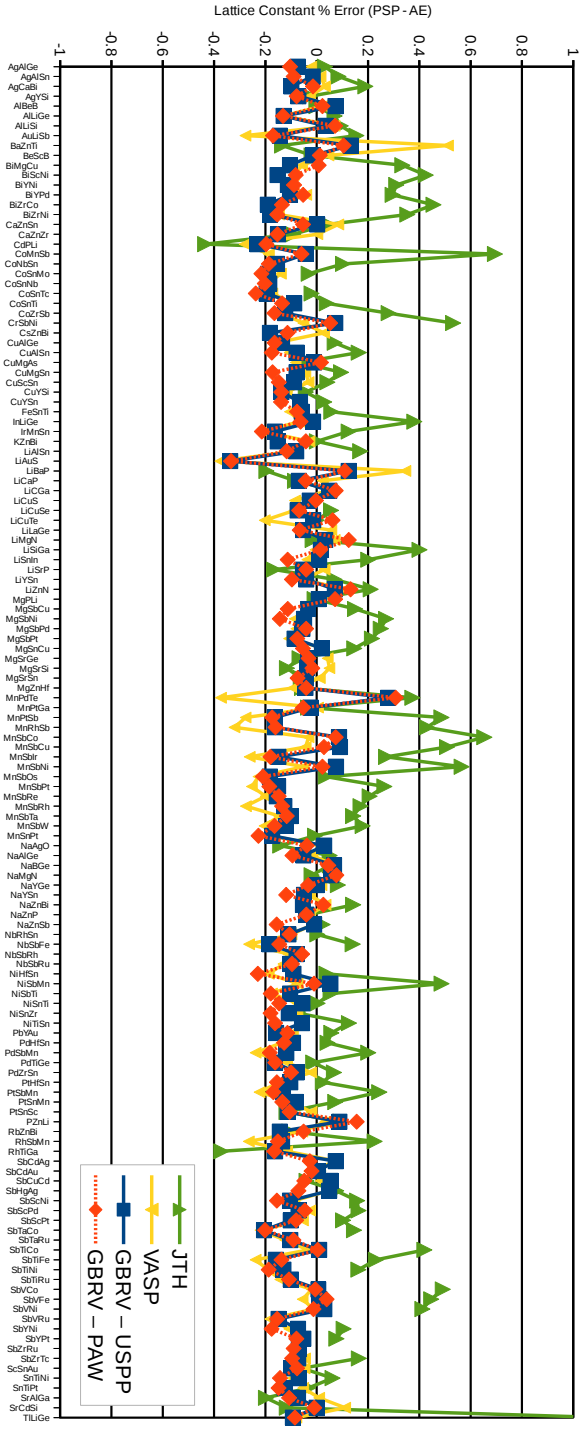

FIG. 5: Percent difference in AE versus pseudopotential calculations for half-Heusler lattice constants.

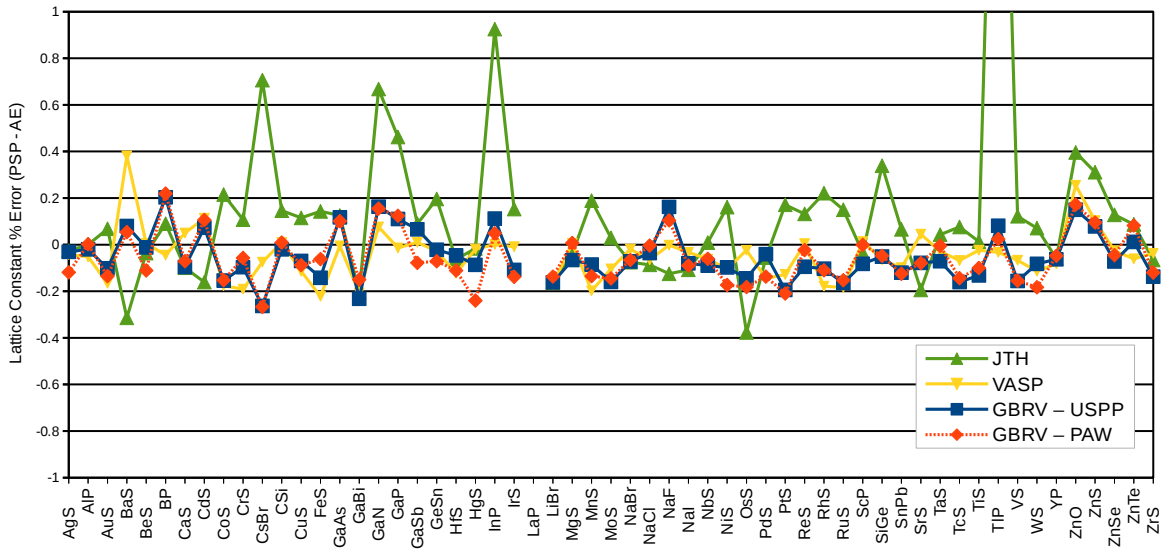

FIG. 6: Percent difference in AE versus pseudopotential calculations for zinc blende lattice constants. Colors as in Fig. 1.

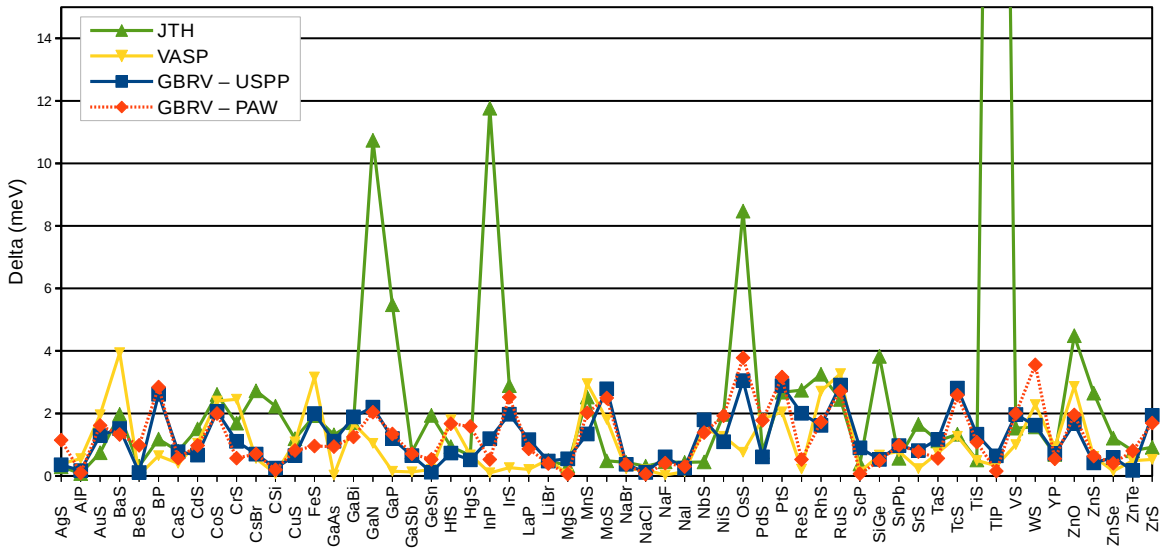

FIG. 7: Delta-factor (meV) in AE versus pseudopotential calculations for zinc blende structure. Colors as in Fig. 1.

TABLE II: Testing data for magnetic moments of transition metal oxides with non-zero magnetic moments at the AE non-spin polarized lattice constant. All magnetic moments in μ_B per primitive cell. Notable discrepancies with AE in bold.

Compound	μ_{AE}	μ_{GBRVQE}	$\mu_{GBRVABINIT}$	μ_{JTH}	μ_{VASP}
TiO	0.08	0.09	0.06	0.04	0.04
VO	1.55	1.54	1.45	1.41	1.44
CrO	2.91	3.01	3.02	3.04	2.97
MnO	3.83	3.90	3.83	3.85	3.84
FeO	3.83	3.85	3.83	3.83	3.83
CoO	2.59	2.81	2.74	2.77	2.69
NiO	1.82	1.63	1.58	**0.74**	**1.01**
MoO	0.42	0.42	0.41	0.40	0.42
TcO	2.02	2.01	2.00	**0.97**	2.01
RuO	1.44	1.42	1.44	1.58	1.45
RhO	0.36	0.37	0.37	0.38	0.37
ReO	0.11	0.11	0.11	0.08	0.09
OsO	1.79	1.79	1.79	**0.44**	1.79
IrO	0.79	0.80	0.79	0.79	0.79