Notes on ABINIT GBRV PAW's

Kevin F. Garrity*

Department of Physics & Astronomy,

Rutgers University, Piscataway,

New Jersey 08854-8019, USA

(Dated: August 16, 2013)

Abstract

Notes on and testing results for the ABINIT PAW versions of the GBRV pseudopotential library.

The major design and testing of the GBRV pseudopotential library was done with QUANTUM ESPRESSO (QE), using ultrasoft pseudopotentials (USPP)[1] generated with the Vanderbilt ultrasoft code[2]. Later, I generated PAW's[3] compatible with ABINIT using the uspp2abinit[4] add-on to the Vanderbilt code. As shown in table I, after optimization of the PAW's (see below), the two potential sets, tested with QE and ABINIT, generate results which are of equivalent accuracy. In figures 1-6 and table II, we present all of our testing data for both potential sets. The tests are compared to all-electron calculations for equivalent convergence parameters; see paper for details of testing procedure and results for other potential sets in the literature. We note that the differences in the RMS error for the rocksalt and perovskite tests are largely due to differences in the PAW and USPP Hf potential; however, we provide an alternative Hf(4+) potential which eliminates those differences, resulting in equivalent accuracy for the two potential sets (see figures 4–5).

While closely related, the formalism of PAW's and USPP's is not identical[5], and the meaning of the various parameters in the input file for the Vanderbilt generator for USPP's is not exactly the same as the meaning for PAW's. Many of the PAW's were generated using exactly the same input file as for USPP's; however, a significant fraction required adjustments. The most common and easiest adjustment was to potentials with projectors for unoccupied states (e.g. a d projector for Br), which I often set to have a relatively large r_c. These large r_c's cause problems for the PAW's, such as PAW overlap, but the problematic r_c's can usually be reduced without difficulty as long as doing so does not to introduce ghost states.

Another set of difficult cases are elements which have many complicated semicore states and problems with ghost states, and sometimes the choices I made to avoid ghosts, like increasing the local core radius, did not work as well for the PAW's. These cases included La, Hf, Cu to Ga, Pd to I, and Hg to Tl. Also note, in some cases, installing the uspp2abinit patch and using different linear algebra libraries resulted in slightly different performance for the USPP's as well, even for identical input files. To try to fix the PAW's, I eliminated any ghost states or convergence issues by moving various cutoff radii around. I note that Ir and Pt, which do not include the $5s$ state in the valence, require large r_c's to avoid introducing ghost states into the s channel, which seems to degrade the performance of these potentials slightly relative to the USPP's.

The other set of potentials which were difficult to convert to ABINIT are potentials like

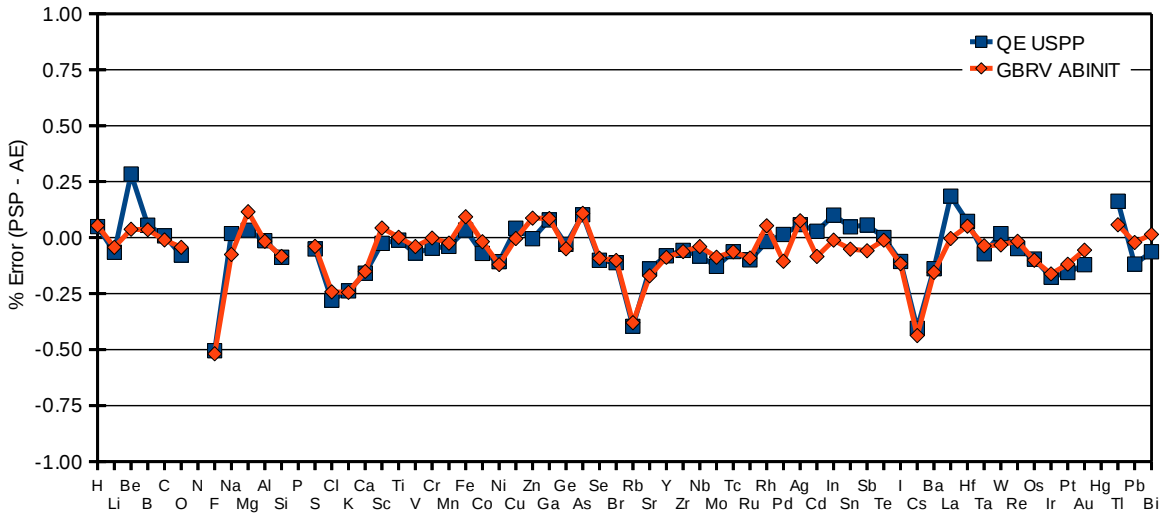

FIG. 1: Percent difference in AE versus pseudopotential calculations for *fcc* lattice constant. USPP QE GBRV results in blue squares, PAW ABINIT GBRV results in red diamonds.

Li, Be, and Ni, which required careful adjustment of the trade-off between accuracy and hardness. Some of these choices had to be adjusted when switching to PAW's.

For cases where I had to change the input files to generate good PAW's, I've included an ABINIT version of the input file. In most but not all cases, this input file will generate an USPP of similar quality to the GBRV USPP set. I did not attempt to do any real-space optimization of the PAW's. Some technical notes:

–As mentioned in the ABINIT documentation, the "Double Counting" energy converges significantly better than the normal energy for PAW's.

–Some of the PAW's produce warnings regarding possible numerical instability, but I have not observed any difficulties with convergence yet.

---

* Electronic address: `kgarrity@physics.rutgers.edu`

[1] D. Vanderbilt, Phys. Rev. B **41**, 7892 (1990).

[2] http://www.physics.rutgers.edu/ dhv/uspp/.

[3] P. E. Blöchl, Phys. Rev. B **50**, 17953 (1994).

[4] M. Torrent and F. Jollet, URL `http://www.abinit.org/downloads/PAW2/USpp2Abinit-Manual-html/USppPAW2.htm`.

[5] G. Kresse and D. Joubert, Phys. Rev. B **59**, 1758 (1999).

TABLE I: Summary of pseudopotential testing results. All testing data is presented as either RMS errors relative to AE calculations or percent of lattice constants outside ±0.2% .

Test	QE USPP	ABINIT PAW
fcc latt. const. (%)	0.14	0.13
bcc latt. const. (%)	0.15	0.14
fcc bulk modulus (%)	3.6	4.0
bcc bulk modulus (%)	5.3	5.0
fcc-*bcc* Energy (meV)	3.7	3.4
rock salt latt. const. (%)	0.13	0.13
rock salt bulk modulus (%)	5.0	4.7
rock salt mag. mom. (μ_B)	0.08	0.09
perovskite latt. const. (%)	0.08	0.09
perovskite bulk modulus (%)	5.5	6.1
half-Heusler latt. const. (%)	0.11	0.13
half-Heusler bulk modulus (%)	5.4	5.6
fcc latt. const. $> \pm 0.2\%$ (%)	9.8	8.2
bcc latt. const. $> \pm 0.2\%$ (%)	9.8	8.2
rock salt latt. const. $> \pm 0.2\%$ (%)	7.8	9.38
perovskite latt. const. $> \pm 0.2\%$ (%)	0.0	3.6
half-Heusler latt. const. $> \pm 0.2\%$ (%)	3.6	5.9

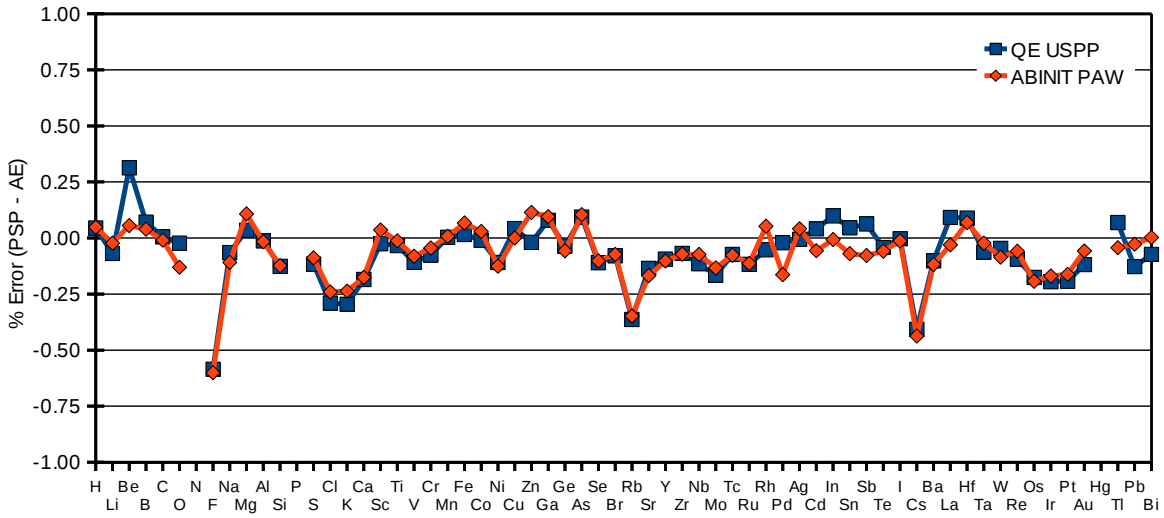

FIG. 2: Percent difference in AE versus pseudopotential calculations for *bcc* lattice constant. USPP QE GBRV results in blue squares, PAW ABINIT GBRV results in red diamonds.

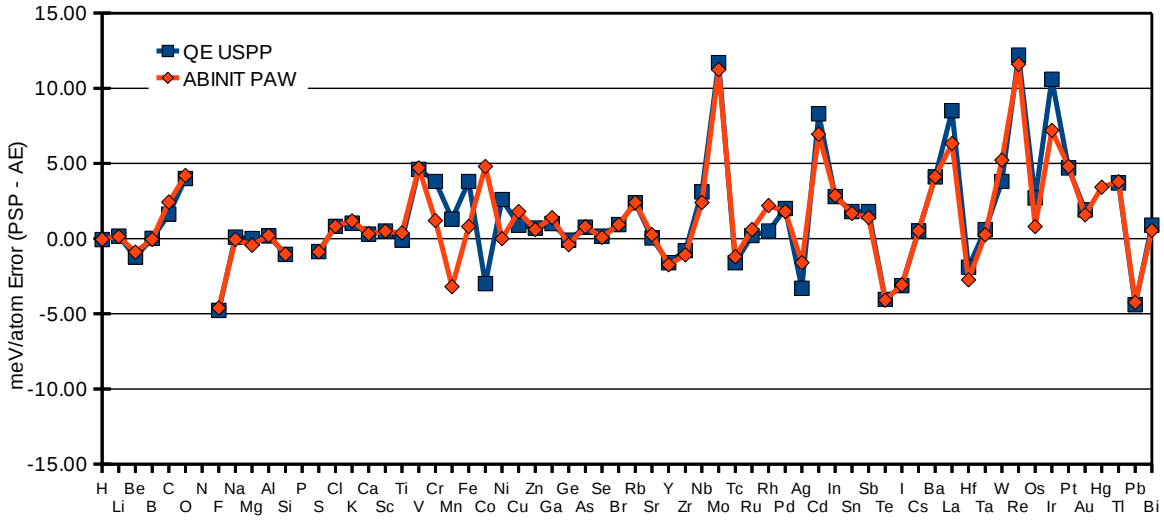

FIG. 3: Energy difference error (meV) for *fcc*−*bcc* structures, AE versus pseudopotential calculations. USPP QE GBRV results in blue squares, PAW ABINIT GBRV results in red diamonds.

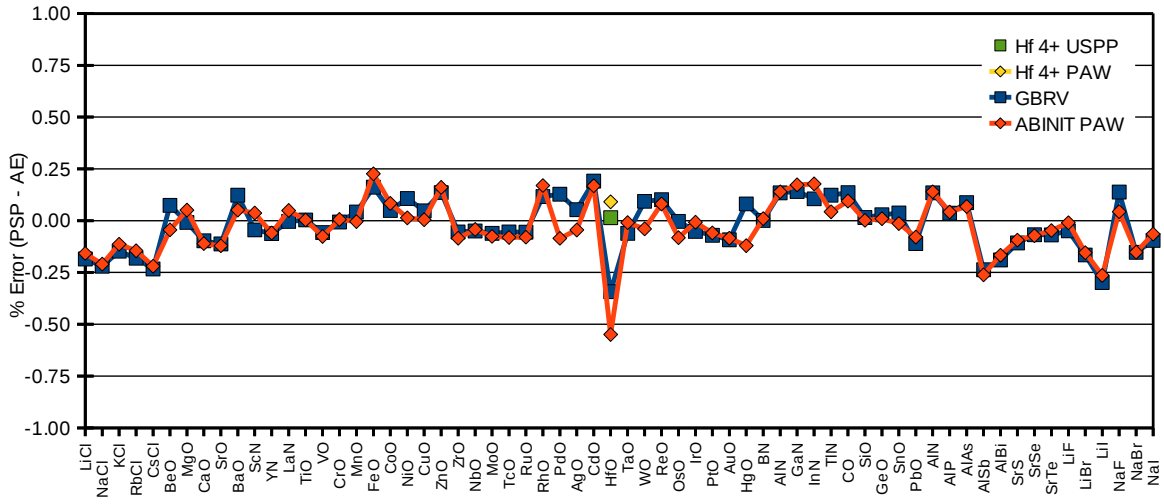

FIG. 4: Percent difference in AE versus pseudopotential calculations for rocksalt lattice constant. USPP QE GBRV results in blue squares, PAW ABINIT GBRV results in red diamonds, Hf (4+) USPP in green square, Hf (4+) PAW in yellow diamond.

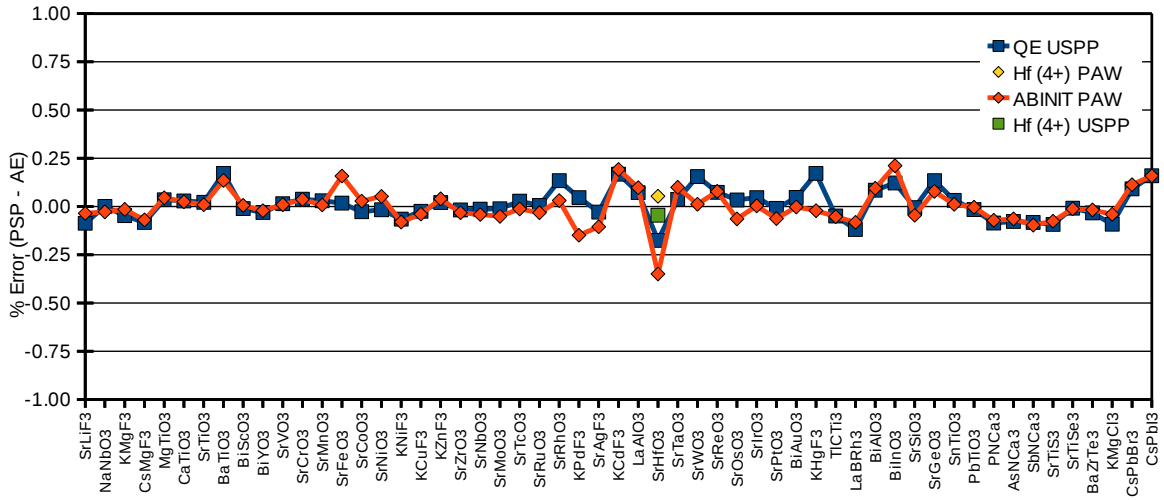

FIG. 5: Percent difference in AE versus pseudopotential calculations for perovskite lattice constant. USPP QE GBRV results in blue squares, PAW ABINIT GBRV results in red diamonds, Hf (4+) USPP in green square, Hf (4+) PAW in yellow diamond.

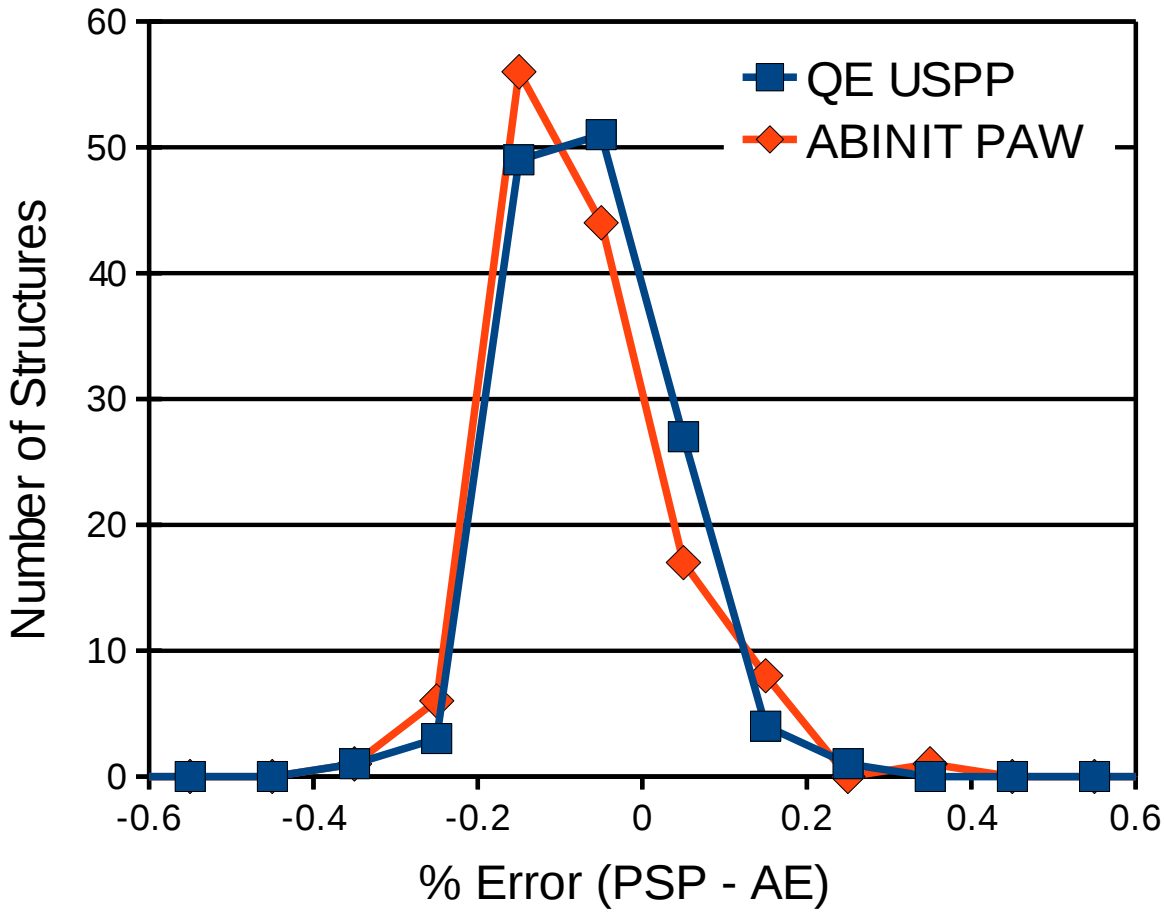

FIG. 6: Histogram of % difference in AE versus pseudopotential calculations for half-Heusler lattice constants. USPP QE GBRV results in blue squares, PAW ABINIT GBRV results in red diamonds.

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.

Compound	μ_{AE}	μ_{USPP}	μ_{PAW}
TiO	0.08	0.08	0.04
VO	1.55	1.54	1.44
CrO	2.91	2.98	3.03
MnO	3.83	3.90	3.83
FeO	3.83	3.85	3.83
CoO	2.59	2.78	2.72
NiO	1.82	1.75	1.56
MoO	0.42	0.43	0.41
TcO	2.02	2.01	2.01
RuO	1.44	1.43	1.44
RhO	0.36	0.36	0.37
ReO	0.11	0.11	0.11
OsO	1.79	1.79	1.79
IrO	0.79	0.80	0.79