SSSPacc/QE

SSSP accuracy mixed PAW-USPP-NCPP dataset / QUANTUM ESPRESSO 5.1

`name and version of the code:` QUANTUM ESPRESSO 5.1
`type of basis set:` plane waves
`method:` mixed projector-augmented wave, ultrasoft pseudopotentials and norm-conserving pseudopotentials (SSSP accuracy)

GENERAL INFORMATION

`exchange-correlation functional`	PBE
`relativistic scheme`	core and valence scalar relativistic (Koelling-Harmon)
`assignment of core / valence states`	see table I
`basis set size`	see table I (wave function cutoff e_{cut}^{wfc})
`k-mesh density`	$20 \times 20 \times 20$
`reciprocal-space integration method`	Marzari-Vanderbilt cold smearing with a fictitious temperature corresponding to 0.002 Ry (0.02 Ry when required to achieve convergence)

METHOD-SPECIFIC INFORMATION

`wave function cutoff`	see table I (e_{cut}^{wfc})
`density cutoff`	see table I (e_{cut}^{rho})

ADDITIONAL COMMENTS

Optimally efficient potentials have been selected for each element. The investigated libraries are: pslibrary.0.3.1 (US and PAW), pslibrary.1.0.0 (US and PAW), GBRV v1.2 and v1.4 (US), and SG15 (NC). The selection criteria for the SSSP accuracy are: smallest Δ, convergence of the phonons mode within 2 %, convergence of the standard heat of formation with respect to the isolated atom (within 3 meV), not too computationally costly. The pseudopotential for N (labeled as THEOS) has been obtained tuning the matching radius starting from the pseudopotential in pslib031 US to improve the Δ.

REFERENCES

`potentials`

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Table I. Calculation settings per element: potential library from which the used potential is taken, wave function cutoff e_{cut}^{wfc}, density cutoff e_{cut}^{rho}, valence.

	library	e_{cut}^{wfc} [Ry]	e_{cut}^{rho} [Ry]	valence
H	pslib031 US	58	276	$1s^1$
He	SG15	100	400	$1s^2$
Li	GBRV-1.4	50	250	$1s^2 2s^{0.55} 2p^0$
Be	SG15	100	400	$1s^2 2s^2$
B	pslib031 PAW	86	340	$2s^2 2p^1$
C	GBRV-1.2	50	250	$2s^2 2p^2$
N	THEOS	100	400	$2s^2 2p^3$
O	pslib031 PAW	94	374	$2s^2 2p^4$
F	GBRV-1.4	50	250	$2s^2 2p^5$
Ne	pslib100 PAW	110	530	$2s^2 2p^6$
Na	GBRV-1.2	50	250	$2s^2 2p^6 3s^1$
Mg	GBRV-1.4	50	250	$2s^2 2p^6 3s^{1.7}$
Al	pslib100 PAW	60	290	$3s^2 3p^1$
Si	pslib100 US	56	219	$3s^2 3p^2$
P	pslib100 US	44	219	$3s^2 3p^3$
S	GBRV-1.2	50	250	$3s^2 3p^4$
Cl	pslib100 US	57	282	$3s^2 3p^5$
Ar	pslib100 US	63	281	$3s^2 3p^6$
K	pslib100 US	56	350	$3s^2 3p^6 4s^1 4p^0$
Ca	GBRV-1.2	50	250	$3s^2 3p^6 4s^2 4p^0$
Sc	GBRV-1.2	50	250	$3s^2 3p^6 3d^1 4s^2 4p^0$
Ti	GBRV-1.4	50	250	$3s^2 3p^6 3d^1 4s^2$
V	GBRV-1.2	50	250	$3s^2 3p^6 3d^3 4s^2$
Cr	pslib100 PAW	125	1150	$3s^2 3p^6 3d^4 4s^2$
Mn	pslib100 PAW	120	1410	$3s^2 3p^6 3d^5 4s^2$
Fe	pslib031 PAW	128	1564	$3s^2 3p^6 3d^6 4s^2 4p^0$
Co	GBRV-1.2	50	250	$3s^2 3p^6 3d^7 4s^1 4p^0$
Ni	GBRV-1.4	50	250	$3s^2 3p^6 3d^8 4s^0 4p^0$
Cu	GBRV-1.2	50	250	$3s^2 3p^6 3d^8 4s^2 4p^0$
Zn	GBRV-1.2	50	250	$3s^2 3p^6 3d^{10} 4s^2 4p^0$
Ga	pslib100 PAW	120	490	$3d^{10} 4s^2 4p^1$
Ge	pslib100 PAW	90	480	$3d^{10} 4s^2 4p^2$
As	pslib031 US	40	206	$4s^2 4p^3$
Se	GBRV-1.2	50	250	$4s^2 4p^4$
Br	GBRV-1.4	50	250	$4s^2 4p^5$
Kr	pslib031 US	56	440	$4s^2 4p^6$
Rb	SG15	100	400	$4s^2 4p^6 5s^1 5p^0$
Sr	pslib100 US	50	331	$4s^2 4p^6 5s^2 5p^0$
Y	GBRV-1.2	50	250	$4s^2 4p^6 4d^1 5s^2 5p^0$
Zr	GBRV-1.2	50	250	$4s^2 4p^6 4d^2 5s^2 5p^0$
Nb	pslib031 PAW	84	728	$4s^2 4p^6 4d^4 5s^1$
Mo	SG15	100	400	$4s^2 4p^6 4d^4 5s^2$
Tc	SG15	100	400	$4s^2 4p^6 4d^5 5s^2$
Ru	SG15	100	400	$4s^2 4p^6 4d^6 5s^2$
Rh	pslib100 PAW	110	730	$4s^2 4p^6 4d^7 5s^2$
Pd	pslib100 PAW	120	1080	$4s^2 4p^6 4d^8 5s^2$
Ag	GBRV-1.4	50	250	$4s^2 4p^6 4d^{10} 5s^{0.5}$
Cd	pslib031 US	74	358	$4d^{9.5} 5s^2 5p^{0.5}$
In	pslib031 US	96	380	$4d^{10} 5s^2 5p^1$

Sn	GBRV-1.2	50	250	$4d^{10}5s^{2}5p^{1}$
Sb	GBRV-1.4	50	250	$4d^{10}5s^{2}5p^{2}$
Te	GBRV-1.2	50	250	$5s^{2}5p^{4}$
I	GBRV-1.2	50	250	$5s^{2}5p^{5}$
Xe	pslib100 US	56	269	$4d^{10}5s^{2}5p^{6}$
Cs	GBRV-1.2	50	250	$5s^{2}5p^{6}5d^{0}6s^{1}6p^{0}$
Ba	SG15	100	400	$5s^{2}5p^{6}5d^{1}6s^{1}$
Lu	*N/A*	*N/A*	*N/A*	*N/A*
Hf	pslib100 PAW	100	640	$4d^{10}4f^{14}5s^{2}5p^{6}5d^{2}6s^{2}$
Ta	pslib100 US	69	663	$4f^{14}5s^{2}5p^{6}5d^{3}6s^{2}$
W	GBRV-1.2	50	250	$5s^{2}5p^{6}5d^{3.9}6s^{2}6p^{0}$
Re	GBRV-1.2	50	250	$5s^{2}5p^{6}5d^{4.5}6s^{2}6p^{0}$
Os	pslib100 US	88	563	$4f^{14}5s^{2}5p^{6}5d^{6}6s^{2}6p^{0}$
Ir	GBRV-1.2	50	250	$5p^{6}5d^{8.5}6s^{0}6p^{0}$
Pt	pslib100 US	100	500	$4f^{14}5s^{2}5p^{6}5d^{8}6s^{2}$
Au	SG15	100	400	$5s^{0}5p^{6}5d^{9}6s^{2}$
Hg	GBRV-1.2	50	250	$5d^{10}6s^{2}6p^{0}$
Tl	pslib100 US	57	263	$5d^{10}6s^{2}6p^{1}$
Pb	pslib031 PAW	94	378	$5d^{10}6s^{2}6p^{2}$
Bi	pslib031 PAW	86	344	$5d^{10}6s^{2}6p^{3}$
Po	pslib100 US	63	569	$5d^{10}6s^{2}6p^{4}$
Rn	pslib100 US	63	269	$5d^{10}6s^{2}6p^{6}$

Table II. Calculation results per element: equilibrium volume per atom V_0, bulk modulus B_0, pressure derivative of the bulk modulus B_1.

	V_0 [Å^3/atom]	B_0 [GPa]	B_1 [–]
H	17.411	10.296	2.720
He	17.709	0.881	6.427
Li	20.231	13.846	3.338
Be	7.934	123.635	3.292
B	7.245	235.870	3.158
C	11.633	207.935	3.551
N	28.943	53.955	3.826
O	19.227	52.194	3.986
F	19.236	34.327	4.085
Ne	24.253	1.431	13.082
Na	37.083	7.697	3.895
Mg	22.938	36.123	4.021
Al	16.476	77.977	4.664
Si	20.452	88.698	4.318
P	21.474	68.262	4.351
S	17.200	82.677	3.692
Cl	38.872	19.085	4.286
Ar	52.437	0.760	3.250
K	73.726	3.594	3.795
Ca	42.226	17.369	3.032
Sc	24.607	54.521	3.398
Ti	17.380	112.192	3.573
V	13.443	182.712	4.061
Cr	11.837	182.041	6.560
Mn	11.443	115.696	2.712
Fe	11.355	204.968	4.680
Co	10.852	216.635	4.919
Ni	10.893	198.736	4.873
Cu	11.982	140.397	5.031
Zn	15.219	74.684	5.409
Ga	20.299	49.119	5.293
Ge	23.905	59.055	4.823
As	22.628	68.628	4.293
Se	29.737	47.281	4.516
Br	39.389	23.016	4.889
Kr	65.885	0.649	7.490
Rb	90.990	2.795	3.776
Sr	54.501	11.400	4.544
Y	32.856	41.199	3.007
Zr	23.381	94.498	3.430
Nb	18.149	170.207	3.713
Mo	15.788	260.913	4.172
Tc	14.438	298.975	4.474
Ru	13.770	312.211	4.855
Rh	14.051	257.621	5.205
Pd	15.307	169.707	5.540
Ag	17.867	91.228	5.918
Cd	22.834	44.725	6.919
In	27.502	35.824	4.850

Sn	36.849	35.709	4.957
Sb	31.765	50.368	4.537
Te	34.931	45.243	4.735
I	50.215	18.707	5.020
Xe	86.674	0.551	6.869
Cs	116.846	1.965	3.423
Ba	63.188	8.727	2.913
Lu	*N/A*	*N/A*	*N/A*
Hf	22.521	107.118	4.290
Ta	18.291	195.230	3.715
W	16.142	305.193	4.334
Re	14.951	364.312	4.428
Os	14.270	397.156	4.805
Ir	14.499	347.354	5.121
Pt	15.638	248.621	5.494
Au	17.982	139.246	5.994
Hg	29.922	7.435	2.338
Tl	31.386	26.834	5.610
Pb	31.993	39.669	4.767
Bi	36.885	42.820	4.643
Po	37.590	45.667	4.856
Rn	92.763	0.541	8.111