SSSPeff/QE

SSSP efficiency 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 efficiency)

GENERAL INFORMATION

exchange-correlation functional	PBE
relativistic scheme	core and valence scalar relativistic (Koelling-Harmon)
assignment of core / valence states	see table
basis set size	see table (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

METHOD-SPECIFIC INFORMATION

wave function cutoff	see table (e_{cut}^{wfc})
density cutoff	see table (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 efficiency are: small Δ (< 1 meV if possible), convergence of the phonons mode within 2 %, convergence of the standard heat of formation with respect to the isolated atom (within 3 meV), low computational cost. 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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code

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Table I. Calculation settings and results per element: potential library from which the used potential is taken, wave function cutoff e_{cut}^{wfc}, density cutoff e_{cut}^{rho}, valence, equilibrium volume per atom V_0, bulk modulus B_0, pressure derivative of the bulk modulus B_1.

	library	e_{cut}^{wfc} [Ry]	e_{cut}^{rho} [Ry]	valence	V_0 [Å^3/atom]	B_0 [GPa]	B_1 [–]
H	pslib031 US	58	276	$1s^1$	17.411	10.296	2.720
He	SG15	100	400	$1s^2$	17.709	0.881	6.427
Li	GBRV-1.4	50	250	$1s^2 2s^{0.55} 2p^0$	20.231	13.846	3.338
Be	GBRV-1.4	50	250	$1s^2 2s^2$	7.944	123.316	3.316
B	pslib031 PAW	86	340	$2s^2 2p^1$	7.245	235.870	3.158
C	GBRV-1.2	50	250	$2s^2 2p^2$	11.633	207.935	3.551
N	THEOS	100	400	$2s^2 2p^3$	28.943	53.955	3.826
O	GBRV-1.2	50	250	$2s^2 2p^4$	19.364	51.605	4.061
F	GBRV-1.4	50	250	$2s^2 2p^5$	19.236	34.327	4.085
Ne	pslib100 PAW	110	530	$2s^2 2p^6$	24.253	1.431	13.082
Na	GBRV-1.2	50	250	$2s^2 2p^6 3s^1$	37.083	7.697	3.895
Mg	GBRV-1.4	50	250	$2s^2 2p^6 3s^{1.7}$	22.938	36.123	4.021
Al	pslib100 PAW	60	290	$3s^2 3p^1$	16.476	77.977	4.664
Si	pslib100 US	56	219	$3s^2 3p^2$	20.452	88.698	4.318
P	pslib100 US	44	219	$3s^2 3p^3$	21.474	68.262	4.351
S	GBRV-1.2	50	250	$3s^2 3p^4$	17.200	82.677	3.692
Cl	GBRV-1.4	50	250	$3s^2 3p^5$	38.435	19.508	4.477
Ar	pslib100 US	63	281	$3s^2 3p^6$	52.437	0.760	3.250
K	pslib100 US	56	350	$3s^2 3p^6 4s^1 4p^0$	73.726	3.594	3.795
Ca	GBRV-1.2	50	250	$3s^2 3p^6 4s^2 4p^0$	42.226	17.369	3.032
Sc	GBRV-1.2	50	250	$3s^2 3p^6 3d^1 4s^2 4p^0$	24.607	54.521	3.398
Ti	GBRV-1.4	50	250	$3s^2 3p^6 3d^1 4s^2$	17.380	112.192	3.573
V	GBRV-1.2	50	250	$3s^2 3p^6 3d^3 4s^2$	13.443	182.712	4.061
Cr	GBRV-1.2	50	250	$3s^2 3p^6 3d^3 4s^2$	11.869	174.060	6.711
Mn	pslib031 PAW	92	488	$3s^2 3p^6 3d^5 4s^2$	11.486	115.607	2.903
Fe	pslib031 PAW	128	1564	$3s^2 3p^6 3d^6 4s^2 4p^0$	11.355	204.968	4.680
Co	GBRV-1.2	50	250	$3s^2 3p^6 3d^7 4s^1 4p^0$	10.852	216.635	4.919
Ni	GBRV-1.4	50	250	$3s^2 3p^6 3d^8 4s^0 4p^0$	10.893	198.736	4.873
Cu	GBRV-1.2	50	250	$3s^2 3p^6 3d^8 4s^2 4p^0$	11.982	140.397	5.031
Zn	GBRV-1.2	50	250	$3s^2 3p^6 3d^{10} 4s^2 4p^0$	15.219	74.684	5.409
Ga	pslib031 US	66	360	$3d^{10} 4s^2 4p^1$	20.356	49.001	5.500
Ge	pslib100 PAW	90	480	$3d^{10} 4s^2 4p^2$	23.905	59.055	4.823
As	pslib031 US	40	206	$4s^2 4p^3$	22.628	68.628	4.293
Se	GBRV-1.2	50	250	$4s^2 4p^4$	29.737	47.281	4.516
Br	GBRV-1.4	50	250	$4s^2 4p^5$	39.389	23.016	4.889
Kr	pslib031 US	56	440	$4s^2 4p^6$	65.885	0.649	7.490
Rb	SG15	100	400	$4s^2 4p^6 5s^1 5p^0$	90.990	2.795	3.776
Sr	pslib100 US	50	331	$4s^2 4p^6 5s^2 5p^0$	54.501	11.400	4.544
Y	GBRV-1.2	50	250	$4s^2 4p^6 4d^1 5s^2 5p^0$	32.856	41.199	3.007
Zr	GBRV-1.2	50	250	$4s^2 4p^6 4d^2 5s^2 5p^0$	23.381	94.498	3.430
Nb	pslib031 PAW	84	728	$4s^2 4p^6 4d^4 5s^1$	18.149	170.207	3.713
Mo	SG15	100	400	$4s^2 4p^6 4d^4 5s^2$	15.788	260.913	4.172
Tc	SG15	100	400	$4s^2 4p^6 4d^5 5s^2$	14.438	298.975	4.474
Ru	SG15	100	400	$4s^2 4p^6 4d^6 5s^2$	13.770	312.211	4.855
Rh	pslib100 PAW	110	730	$4s^2 4p^6 4d^7 5s^2$	14.051	257.621	5.205
Pd	pslib100 PAW	120	1080	$4s^2 4p^6 4d^8 5s^2$	15.307	169.707	5.540
Ag	GBRV-1.4	50	250	$4s^2 4p^6 4d^{10} 5s^{0.5}$	17.867	91.228	5.918
Cd	pslib031 US	74	358	$4d^{9.5} 5s^2 5p^{0.5}$	22.834	44.725	6.919

In	pslib031 US	96	380	$4d^{10}5s^25p^1$	27.502	35.824	4.850
Sn	GBRV-1.2	50	250	$4d^{10}5s^25p^1$	36.849	35.709	4.957
Sb	GBRV-1.4	50	250	$4d^{10}5s^25p^2$	31.765	50.368	4.537
Te	GBRV-1.2	50	250	$5s^25p^4$	34.931	45.243	4.735
I	GBRV-1.2	50	250	$5s^25p^5$	50.215	18.707	5.020
Xe	pslib100 US	56	269	$4d^{10}5s^25p^6$	86.674	0.551	6.869
Cs	GBRV-1.2	50	250	$5s^25p^65d^06s^16p^0$	116.846	1.965	3.423
Ba	SG15	100	400	$5s^25p^65d^16s^1$	63.188	8.727	2.913
Hf	pslib031 US	86	622	$5s^25p^65d^26s^26p^0$	22.471	107.626	3.281
Ta	GBRV-1.2	50	250	$5s^25p^65d^36s^26p^0$	18.275	195.901	3.723
W	GBRV-1.2	50	250	$5s^25p^65d^{3.9}6s^26p^0$	16.142	305.193	4.334
Re	GBRV-1.2	50	250	$5s^25p^65d^{4.5}6s^26p^0$	14.951	364.312	4.428
Os	GBRV-1.2	50	250	$5s^25p^65d^{5.5}6s^26p^0$	14.263	398.882	4.820
Ir	GBRV-1.2	50	250	$5p^65d^{8.5}6s^06p^0$	14.499	347.354	5.121
Pt	GBRV-1.4	50	250	$5p^65d^{9.5}6s^06p^0$	15.604	250.116	5.497
Au	SG15	100	400	$5s^05p^65d^96s^2$	17.982	139.246	5.994
Hg	GBRV-1.2	50	250	$5d^{10}6s^26p^0$	29.922	7.435	2.338
Tl	pslib031 US	70	300	$5d^{10}6s^26p^1$	31.358	26.895	5.689
Pb	pslib031 PAW	94	378	$5d^{10}6s^26p^2$	31.993	39.669	4.767
Bi	pslib031 PAW	86	344	$5d^{10}6s^26p^3$	36.885	42.820	4.643
Po	pslib100 US	63	569	$5d^{10}6s^26p^4$	37.590	45.667	4.856
Rn	pslib100 US	63	269	$5d^{10}6s^26p^6$	92.763	0.541	8.111