

14 outliers of SSSP-precision v1.1.2 found from the previous run of ACWF-QE-SSSP. The newly released v1.2-precision has the pseudopotentials updated with selecting from other libraries. The outlier pseudos are (Te, Na, Cu, Cs, Cd, Ba, As, Hg, I, Ne, Ar, Kr, Xe, Rn).

Latest ACWF runs by Marnik with new pseudos I provide. (Note: psl for PSLibrary)

element	SSSP-precision-v1.1.2	SSSP-precision-v1.2
Te	z_6 Ultrasoft GBRV uspp v1	z_6 Ultrasoft psl ld1 v1.0.0-low
Na	z_9 NC dojo oncvpsp3 v4-std	z_9 PAW psl ld1 v1.0.0-low
Cu	z_19 NC dojo oncvpsp3 v4-std	z_11 PAW psl ld1 v1.0.0-low
Cs	z_9 Ultrasoft GBRV uspp v1	z_9 NC dojo oncvpsp3 v4-str
Cd	z_12 Ultrasoft psl ld1 v0.3.1	z_20 PAW psl ld1 v1.0.0-high
Ba	z_10 PAW psl ld1 v1.0.0-high	z_10 NC dojo oncvpsp4 v4-sp
As	z_5 Ultrasoft psl ld1 v0.2	z_15 NC dojo oncvpsp3 v4-std
I	z_17 PAW psl ld1 v1.0.0-high	z_17 NC dojo oncvpsp3 v4-std
Hg	z_20 NC SG15 oncvpsp3 v0	z_12 Ultrasoft gbrv uspp v1
Ne	z_8 NC sg15 oncvpsp4 v0	z_8 PAW psl ld1 v1.0.0-high
Ar	z_8 NC sg15 oncvpsp4 v0	z_8 PAW psl ld1 v1.0.0-high
Kr	z_8 NC sg15 oncvpsp4 v0	z_18 PAW psl ld1 v1.0.0-high
Xe	z_18 NC sg15 oncvpsp4 v0	z_18 PAW psl ld1 v1.0.0-high
Rn	z_18 NC sg15 oncvpsp4 v0	z_18 PAW psl ld1 v1.0.0-high

Benchmark: SsspApp gallery display

Tellurium

	Pseudopotential label	X0	X02	X03	X20	X203	X205	BCC	FCC	SC	Diamond	TYPICAL	Z
0	z_16 NC dojo oncvpsp3 v4-std	0.569	1.016	3.194	0.643	0.262	0.225	1.215	1.408	0.776	0.366	0.286	z_16
1	z_16 NC sg15 oncvpsp4 v0	0.618	1.020	2.626	0.670	0.260	0.226	1.322	1.503	0.869	0.441	0.318	z_16
2	z_24 NC dojo oncvpsp3 v4-str	0.497	0.600	1.613	0.640	0.169	0.151	1.620	1.355	1.424	0.875	0.451	z_24
3	z_16 PAW psl ld1 v1.0.0-high	0.882	1.321	3.871	0.958	0.359	0.287	2.008	2.303	1.362	0.699	0.451	z_16
4	z_6 PAW psl ld1 v1.0.0-low	0.235	0.467	3.252	0.283	0.116	0.122	0.458	0.620	0.460	0.144	0.094	z_6
5	z_16 Ultrasoft psl ld1 v1.0.0-high	0.883	1.331	4.106	0.969	0.362	0.289	2.063	2.368	1.417	0.701	0.471	z_16
6	z_6 Ultrasoft psl ld1 v1.0.0-low	0.274	0.435	3.556	0.319	0.114	0.112	0.595	0.781	0.488	0.193	0.207	z_6
7	z_6 Ultrasoft gbrv uspp v1	1.169	2.625	10.003	0.964	0.651	0.524	1.147	1.318	1.859	0.322	0.229	z_6

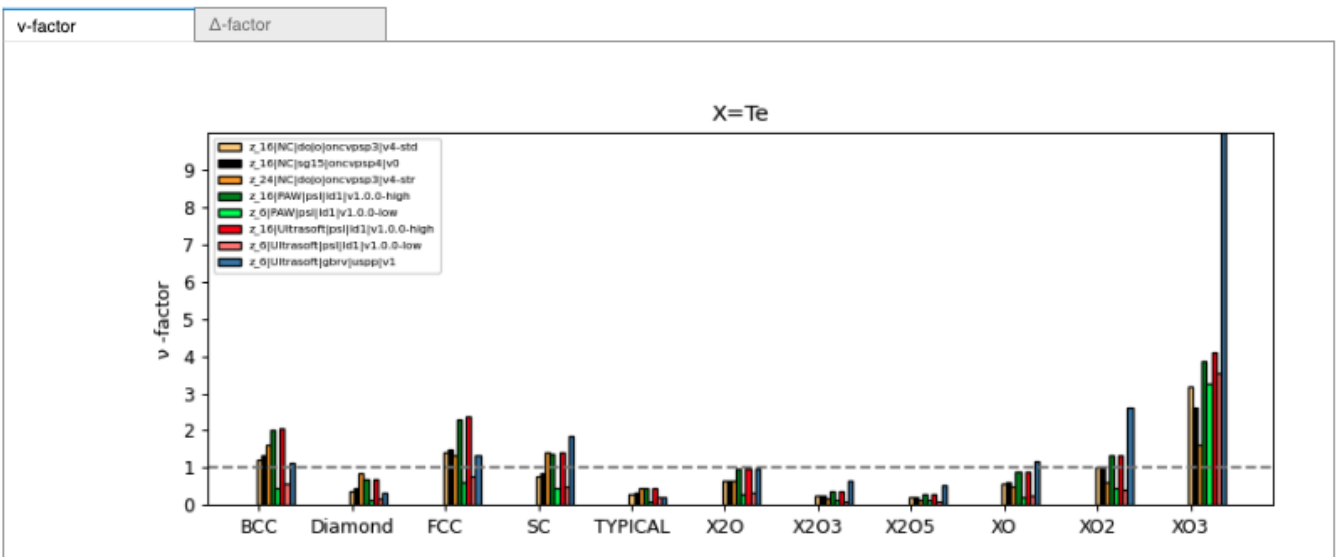
	Pseudopotential label	cohesive energy	phonon frequencies	pressure	delta	bands	Z
0	z_16 NC dojo oncvpsp3 v4-std	60 Ry (3.5)	35 Ry (4.0)	70 Ry (2.5)	65 Ry (3.0)	50 Ry (2.5)	z_16
1	z_16 NC sg15 oncvpsp4 v0	45 Ry (3.5)	45 Ry (3.5)	55 Ry (2.5)	75 Ry (3.5)	35 Ry (2.0)	z_16
2	z_24 NC dojo oncvpsp3 v4-str	80 Ry (3.5)	50 Ry (4.0)	100 Ry (2.5)	90 Ry (3.0)	90 Ry (2.0)	z_24
3	z_16 PAW psl ld1 v1.0.0-high	70 Ry (6.0)	30 Ry (6.0)	75 Ry (6.0)	120 Ry (6.0)	30 Ry (6.0)	z_16
4	z_6 PAW psl ld1 v1.0.0-low	30 Ry (6.0)	30 Ry (6.0)	30 Ry (6.0)	30 Ry (6.0)	30 Ry (8.0)	z_6
5	z_16 Ultrasoft psl ld1 v1.0.0-high	70 Ry (8.0)	30 Ry (6.0)	75 Ry (6.0)	120 Ry (6.0)	35 Ry (6.0)	z_16
6	z_6 Ultrasoft psl ld1 v1.0.0-low	30 Ry (6.0)	30 Ry (6.0)	30 Ry (6.0)	35 Ry (6.0)	30 Ry (6.0)	z_6
7	z_6 Ultrasoft gbrv uspp v1	200 Ry (7.5)	30 Ry (6.0)	30 Ry (6.0)	200 Ry (6.0)	30 Ry (8.0)	z_6

Switch criteria to:

Efficiency
 Precision

Show ρ or dual

Default
 Show ρ cutoff
 Show dual



Na (Sodium)

	Pseudopotential label	X0	XO2	XO3	X20	X2O3	X2O5	BCC	FCC	SC	Diamond	TYPICAL	Z
0	z_9 NC dojo oncvpsp3 v4-std	0.571	0.293	0.626	0.355	0.072	0.025	0.285	0.484	0.596	0.478	1.219	z_9
1	z_9 NC sg15 oncvpsp4 v0	1.197	0.915	1.285	0.945	0.307	0.076	0.504	0.599	0.671	0.421	1.214	z_9
2	z_9 PAW jth atompaw v1.1-std	2.227	1.545	1.807	1.594	0.486	0.166	0.774	0.794	0.886	0.298	1.126	z_9
3	z_9 PAW psl ld1 v0.2	0.264	0.132	0.585	0.042	0.027	0.036	0.047	0.037	0.119	0.080	1.378	z_9
4	z_9 PAW psl ld1 v1.0.0-high	0.762	0.443	0.699	0.518	0.119	0.031	1.060	1.085	1.338	0.542	1.027	z_9
5	z_9 PAW psl ld1 v1.0.0-low	0.299	0.161	0.580	0.149	0.022	0.034	0.083	0.060	0.083	0.095	1.391	z_9
6	z_9 Ultrasoft psl ld1 v0.2	0.929	0.574	0.861	0.706	0.175	0.036	0.606	0.622	0.865	0.098	1.183	z_9
7	z_9 Ultrasoft psl ld1 v1.0.0-high	0.855	0.472	0.711	0.564	0.129	0.034	1.231	1.456	1.641	0.993	0.914	z_9
8	z_9 Ultrasoft psl ld1 v1.0.0-low	0.370	0.178	0.583	0.187	0.028	0.031	0.109	0.301	0.358	0.372	1.279	z_9
9	z_9 Ultrasoft gbrv uspp v1.5	1.875	1.440	1.519	1.153	0.440	0.163	0.441	0.541	0.653	0.330	1.200	z_9

	Pseudopotential label	cohesive energy	phonon frequencies	pressure	delta	bands	Z
0	z_9 NC dojo oncvpsp3 v4-std	70 Ry (3.0)	35 Ry (4.0)	90 Ry (2.5)	90 Ry (3.5)	70 Ry (2.5)	z_9
1	z_9 NC sg15 oncvpsp4 v0	40 Ry (3.0)	30 Ry (3.0)	90 Ry (2.0)	60 Ry (3.5)	40 Ry (4.0)	z_9
2	z_9 PAW jth atompaw v1.1-std	100 Ry (6.5)	30 Ry (6.0)	120 Ry (6.0)	120 Ry (6.0)	30 Ry (6.0)	z_9
3	z_9 PAW psl ld1 v0.2	50 Ry (6.0)	30 Ry (6.0)	55 Ry (6.0)	55 Ry (6.0)	30 Ry (8.0)	z_9
4	z_9 PAW psl ld1 v1.0.0-high	70 Ry (8.0)	30 Ry (6.0)	150 Ry (6.0)	90 Ry (6.0)	45 Ry (6.0)	z_9
5	z_9 PAW psl ld1 v1.0.0-low	70 Ry (8.0)	30 Ry (6.0)	150 Ry (6.0)	75 Ry (7.0)	45 Ry (6.0)	z_9
6	z_9 Ultrasoft psl ld1 v0.2	50 Ry (6.0)	30 Ry (6.0)	55 Ry (6.0)	50 Ry (6.0)	30 Ry (6.0)	z_9
7	z_9 Ultrasoft psl ld1 v1.0.0-high	70 Ry (8.0)	30 Ry (6.0)	150 Ry (6.0)	65 Ry (7.0)	45 Ry (6.0)	z_9
8	z_9 Ultrasoft psl ld1 v1.0.0-low	70 Ry (8.0)	30 Ry (6.0)	150 Ry (6.0)	75 Ry (7.0)	45 Ry (6.0)	z_9
9	z_9 Ultrasoft gbrv uspp v1.5	35 Ry (6.0)	30 Ry (6.0)	40 Ry (6.0)	50 Ry (7.5)	30 Ry (6.0)	z_9

Switch criteria to:

Efficiency

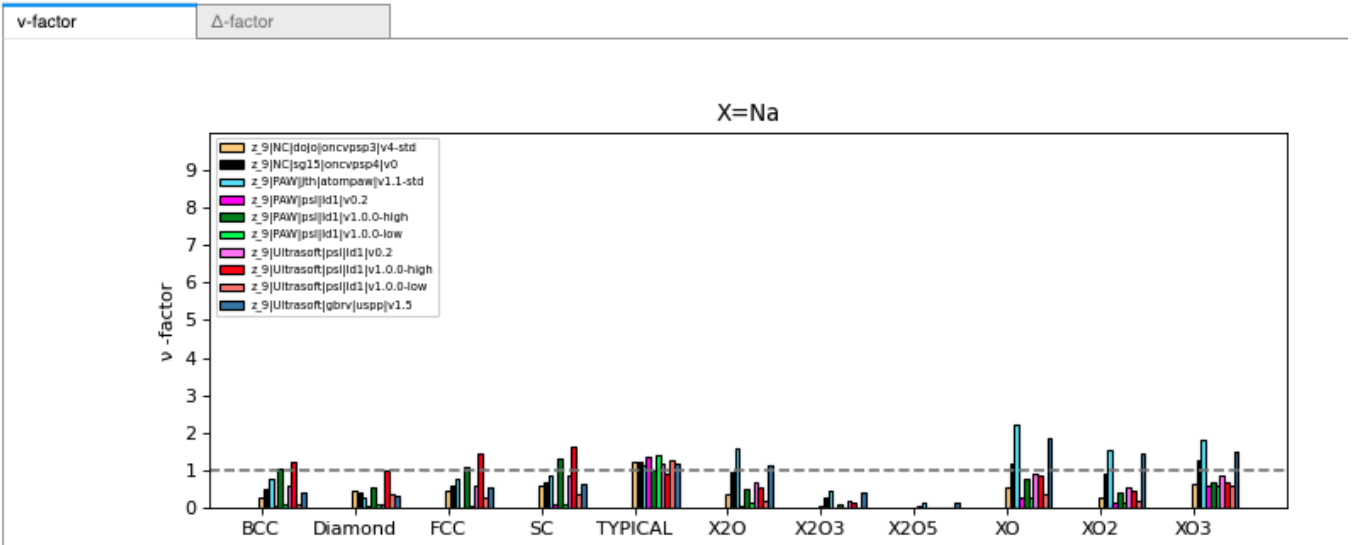
Precision

Show ρ or dual

Default

Show ρ cutoff

Show dual



Cu (Copper)

	Pseudopotential label	XO	XO2	XO3	X2O	X2O3	X2O5	BCC	FCC	SC	Diamond	TYPICAL	Z
0	z_19 NC dojo oncvpsp3 v4-std	1.228	0.899	0.511	3.169	0.533	0.120	15.950	10.187	11.908	3.120	9.642	z_19
1	z_19 NC dojo oncvpsp3 v4-str	1.618	0.810	0.551	3.002	0.533	0.131	16.216	9.530	14.499	2.957	9.046	z_19
2	z_19 NC sg15 oncvpsp4 v0	0.226	0.292	0.553	0.194	0.119	0.057	0.439	1.537	2.093	1.295	1.355	z_19
3	z_11 PAW psl ld1 v0.2	2.506	1.483	1.814	1.435	0.501	0.175	4.834	4.790	4.664	2.739	4.595	z_11
4	z_11 PAW psl ld1 v1.0.0-low	0.229	0.211	0.455	0.106	0.056	0.010	0.310	0.289	0.389	0.346	0.291	z_11
5	z_19 PAW psl ld1 v1.0.0-high	0.463	0.223	0.280	0.262	0.073	0.027	1.330	1.269	1.360	0.711	1.119	z_19
6	z_11 Ultrasoft psl ld1 v0.2	3.618	1.421	1.704	2.242	0.493	0.243	1.950	5.883	12.315	2.903	5.702	z_11
7	z_11 Ultrasoft psl ld1 v1.0.0-low	2.049	0.491	0.818	0.985	0.178	0.112	2.267	2.387	9.578	1.439	2.259	z_11
8	z_19 Ultrasoft psl ld1 v1.0.0-high	39.441	1.591	4.612	6.146	1.057	0.675	36.940	21.564	64.972	9.520	21.260	z_19
9	z_19 Ultrasoft gbrv uspp v1.2	0.861	0.340	0.350	0.494	0.122	0.043	1.359	1.306	1.293	0.626	1.139	z_19

	Pseudopotential label	cohesive energy	phonon frequencies	pressure	delta	bands	Z
0	z_19 NC dojo oncvpsp3 v4-std	80 Ry (3.5)	55 Ry (3.5)	90 Ry (2.5)	90 Ry (3.5)	80 Ry (2.5)	z_19
1	z_19 NC dojo oncvpsp3 v4-str	90 Ry (3.5)	70 Ry (4.0)	100 Ry (3.0)	100 Ry (3.0)	90 Ry (4.0)	z_19
2	z_19 NC sg15 oncvpsp4 v0	70 Ry (3.5)	55 Ry (2.5)	80 Ry (2.5)	75 Ry (2.5)	70 Ry (4.0)	z_19
3	z_11 PAW psl ld1 v0.2	120 Ry (7.5)	30 Ry (6.0)	65 Ry (8.0)	150 Ry (7.5)	30 Ry (6.0)	z_11
4	z_11 PAW psl ld1 v1.0.0-low	70 Ry (8.0)	30 Ry (6.0)	55 Ry (6.0)	50 Ry (6.0)	35 Ry (6.0)	z_11
5	z_19 PAW psl ld1 v1.0.0-high	55 Ry (6.5)	35 Ry (6.0)	120 Ry (6.0)	90 Ry (6.0)	55 Ry (6.0)	z_19
6	z_11 Ultrasoft psl ld1 v0.2	100 Ry (7.5)	30 Ry (6.0)	50 Ry (6.5)	70 Ry (8.0)	30 Ry (6.0)	z_11
7	z_11 Ultrasoft psl ld1 v1.0.0-low	70 Ry (6.5)	30 Ry (6.0)	55 Ry (6.0)	50 Ry (6.0)	35 Ry (6.0)	z_11
8	z_19 Ultrasoft psl ld1 v1.0.0-high	55 Ry (6.5)	35 Ry (6.0)	120 Ry (6.0)	90 Ry (6.0)	55 Ry (8.0)	z_19
9	z_19 Ultrasoft gbrv uspp v1.2	80 Ry (7.5)	30 Ry (6.0)	55 Ry (6.0)	55 Ry (6.0)	35 Ry (6.0)	z_19

Switch criteria to:

Efficiency

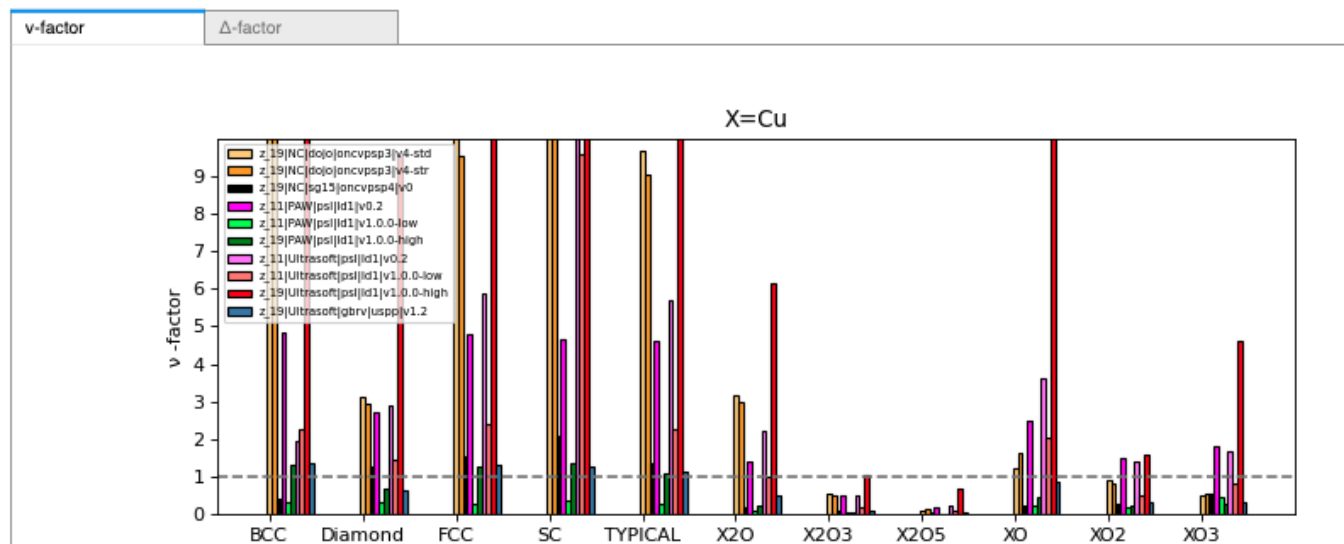
Precision

Show ρ or dual

Default

Show ρ cutoff

Show dual



Cd (Cadmium)

	Pseudopotential label	X0	X02	X03	X20	X203	X205	BCC	FCC	SC	Diamond	TYPICAL	Z
0	z_20 NC dojo oncvpsp3 v4-std	0.569	0.366	0.633	0.468	0.118	0.055	1.871	2.842	1.598	2.136	1.386	z_20
1	z_20 NC dojo oncvpsp3 v4-str	0.313	0.235	0.550	0.227	0.078	0.030	0.539	1.330	0.339	1.079	0.651	z_20
2	z_20 NC sg15 oncvpsp4 v0	0.267	0.419	0.534	0.427	0.100	0.047	1.583	1.919	1.354	0.871	1.107	z_20
3	z_12 PAW psl id1 v0.3.1	0.874	0.607	1.079	0.261	0.184	0.081	1.361	0.569	1.093	0.287	0.366	z_12
4	z_12 PAW psl id1 v1.0.0-low	1.440	1.183	2.031	0.541	0.348	0.165	1.549	0.692	1.060	0.422	0.398	z_12
5	z_20 PAW psl id1 v1.0.0-high	0.209	0.216	0.543	0.051	0.065	0.023	1.080	0.347	1.062	0.319	0.226	z_20
6	z_12 Ultrasoft psl id1 v0.3.1	1.147	0.553	0.982	0.280	0.177	0.081	1.982	1.159	1.672	0.625	0.671	z_12
7	z_12 Ultrasoft psl id1 v1.0.0-low	1.268	1.156	2.026	0.513	0.333	0.157	1.479	0.597	0.972	0.433	0.362	z_12
8	z_12 Ultrasoft gbrv uspp v1	1.442	0.808	1.031	0.518	0.262	0.113	1.560	1.781	1.083	0.534	0.801	z_12
9	z_20 Ultrasoft psl id1 v1.0.0-high	0.236	0.225	0.551	0.081	0.067	0.024	0.817	0.032	0.784	0.088	0.146	z_20

	Pseudopotential label	cohesive energy	phonon frequencies	pressure	delta	bands	Z
0	z_20 NC dojo oncvpsp3 v4-std	90 Ry (3.0)	50 Ry (4.0)	100 Ry (2.0)	90 Ry (2.5)	75 Ry (2.5)	z_20
1	z_20 NC dojo oncvpsp3 v4-str	100 Ry (2.5)	45 Ry (4.0)	120 Ry (2.0)	100 Ry (2.5)	90 Ry (2.5)	z_20
2	z_20 NC sg15 oncvpsp4 v0	35 Ry (2.5)	30 Ry (2.0)	40 Ry (2.0)	35 Ry (2.0)	35 Ry (4.0)	z_20
3	z_12 PAW psl id1 v0.3.1	40 Ry (6.0)	30 Ry (6.0)	60 Ry (6.0)	35 Ry (6.0)	30 Ry (6.0)	z_12
4	z_12 PAW psl id1 v1.0.0-low	80 Ry (8.0)	45 Ry (7.0)	60 Ry (6.0)	55 Ry (8.0)	35 Ry (6.0)	z_12
5	z_20 PAW psl id1 v1.0.0-high	90 Ry (7.5)	70 Ry (7.5)	120 Ry (6.0)	70 Ry (8.0)	55 Ry (6.0)	z_20
6	z_12 Ultrasoft psl id1 v0.3.1	40 Ry (6.0)	30 Ry (6.0)	60 Ry (6.0)	35 Ry (6.0)	30 Ry (6.0)	z_12
7	z_12 Ultrasoft psl id1 v1.0.0-low	80 Ry (8.0)	45 Ry (7.0)	60 Ry (6.0)	55 Ry (8.0)	30 Ry (6.0)	z_12
8	z_12 Ultrasoft gbrv uspp v1	40 Ry (8.0)	30 Ry (6.0)	120 Ry (6.0)	55 Ry (6.0)	30 Ry (6.0)	z_12
9	z_20 Ultrasoft psl id1 v1.0.0-high	90 Ry (7.5)	70 Ry (7.5)	120 Ry (6.0)	65 Ry (7.0)	55 Ry (6.0)	z_20

Switch criteria to:

Efficiency

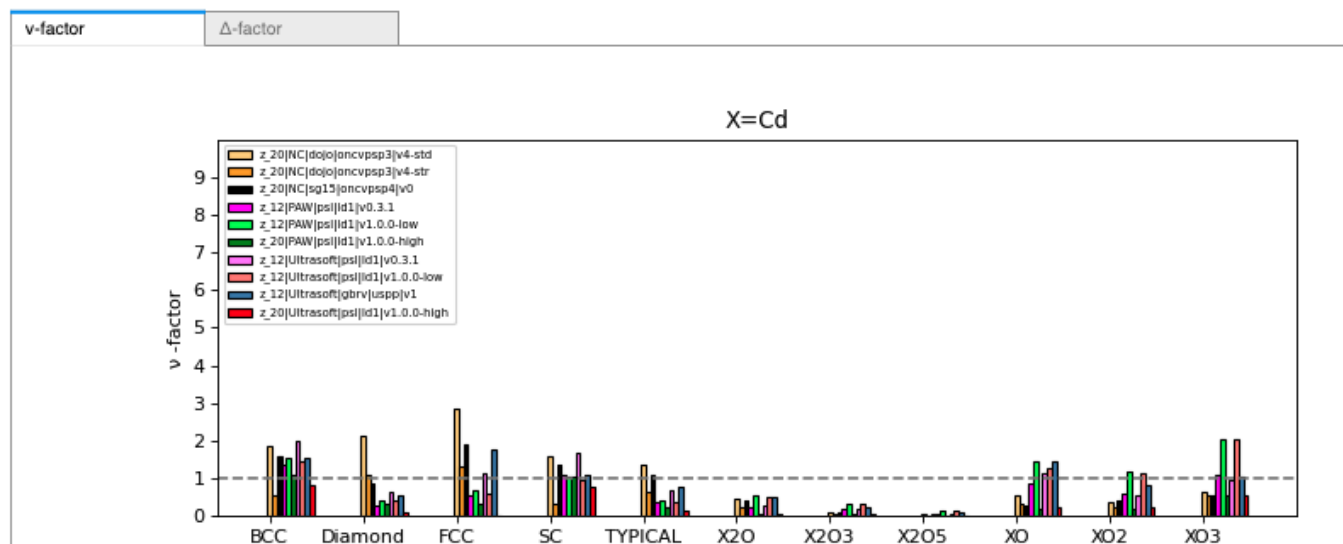
Precision

Show ρ or dual

Default

Show ρ cutoff

Show dual



Ne (Neon)

	Pseudopotential label	X0	X02	X03	X20	X203	X205	BCC	FCC	SC	Diamond	TYPICAL
0	z_8 NC dojo oncvpsp3 v4-std	1.061	0.214	0.715	1.722	0.023	0.042	8.518	8.313	5.973	2.406	6.636
1	z_8 NC sg15 oncvpsp4 v0	5.430	5.817	9.383	1.491	1.957	0.748	3.949	4.406	2.857	2.546	5.375
2	z_8 PAW ps ld1 v1.0.0-high	0.181	0.165	0.701	0.779	0.034	0.053	1.148	2.123	0.273	0.667	6.663
3	z_8 Ultrasoft ps ld1 v1.0.0-high	39.235	9.131	13.909	42.454	4.269	1.510	169.678	105.279	125.960	55.065	106.766

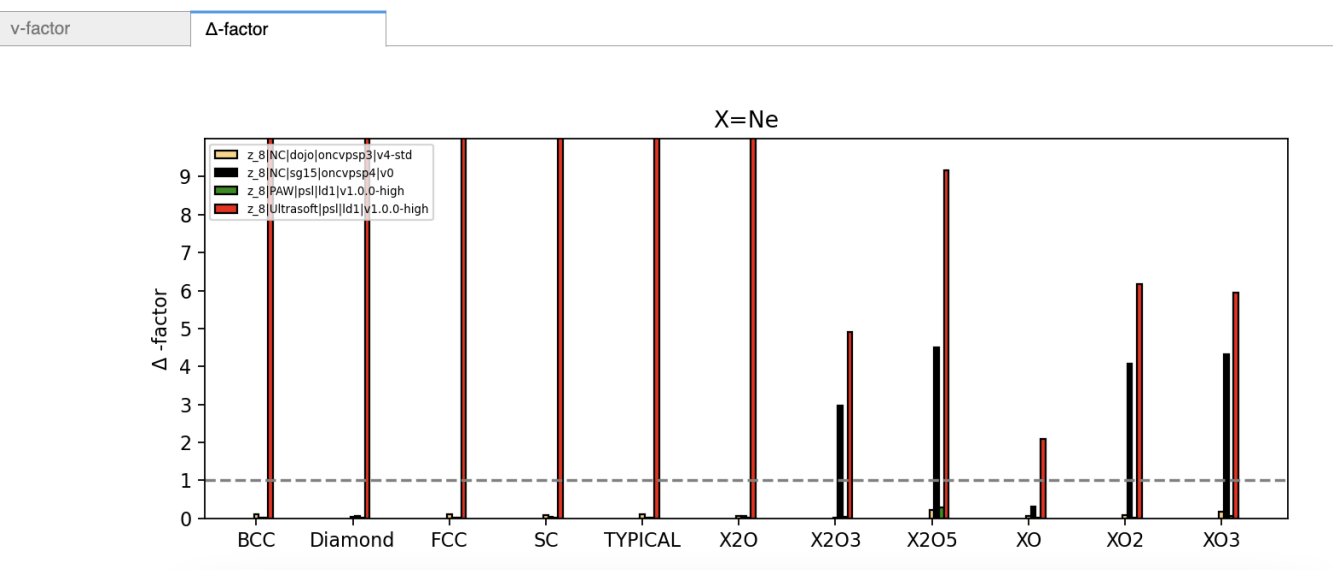
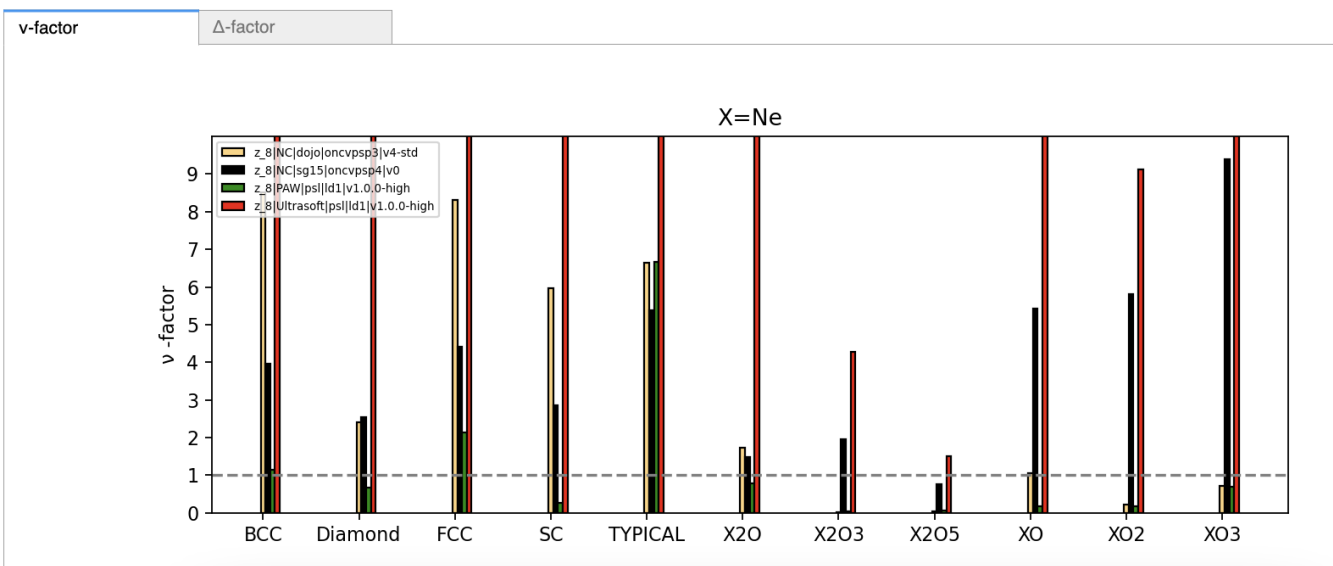
	Pseudopotential label	cohesive energy	phonon frequencies	pressure	delta	bands
0	z_8 NC dojo oncvpsp3 v4-std	55 Ry (165 Ry)	120 Ry (480 Ry)	120 Ry (360 Ry)	55 Ry (165 Ry)	55 Ry (110 Ry)
1	z_8 NC sg15 oncvpsp4 v0	35 Ry (105 Ry)	30 Ry (90 Ry)	45 Ry (112 Ry)	35 Ry (105 Ry)	35 Ry (70 Ry)
2	z_8 PAW ps ld1 v1.0.0-high	40 Ry (280 Ry)	55 Ry (357 Ry)	200 Ry (1200 Ry)	45 Ry (360 Ry)	35 Ry (210 Ry)
3	z_8 Ultrasoft ps ld1 v1.0.0-high	40 Ry (240 Ry)	nan	70 Ry (420 Ry)	65 Ry (390 Ry)	35 Ry (210 Ry)

Switch criteria to:

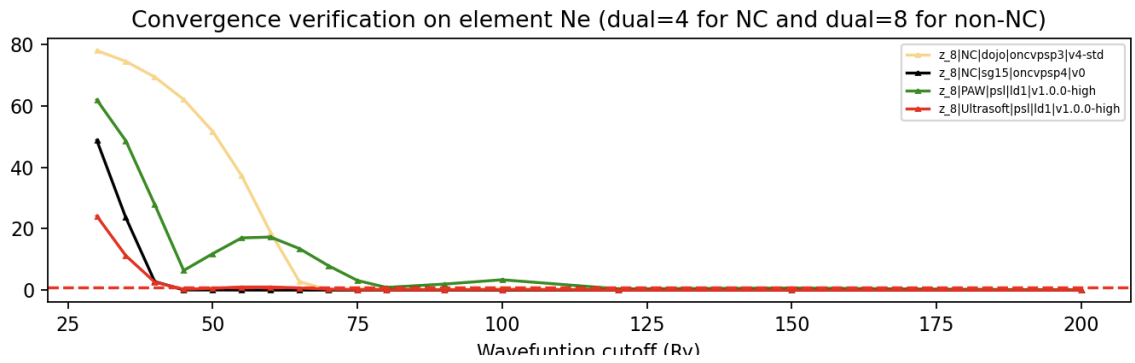
Efficiency
 Precision

Show ρ or dual

Default
 Show ρ cutoff
 Show dual



- Pressure (Relative Error, %)
- Bands distance (Avg. error meV)
- Bands distance (Max. error meV)
- Delta (Relative Error, %)
- Delta (Raw value, meV/cell)



Kr (Krypton)

	Pseudopotential label	XO	XO2	XO3	X2O	X2O3	X2O5	BCC	FCC	SC	Diamond	TYPICAL
0	z_8 NC dojo oncvpsp3 v4-std	0.484	0.237	0.276	0.703	0.067	0.049	6.021	6.134	4.931	3.280	2.069
1	z_8 NC sg15 oncvpsp4 v0	0.763	1.246	2.987	0.482	0.314	0.083	5.518	5.638	4.485	3.082	1.986
2	z_18 PAW psl ld1 v1.0.0-high	0.437	0.432	0.716	0.337	0.106	0.023	2.611	2.991	2.431	2.237	3.267
3	z_18 Ultrasoft psl ld1 v1.0.0-high	0.499	0.589	0.899	0.286	0.149	0.006	4.906	4.380	3.207	2.548	2.302

	Pseudopotential label	cohesive energy	phonon frequencies	pressure	delta	bands
0	z_8 NC dojo oncvpsp3 v4-std	30 Ry (75 Ry)	30 Ry (75 Ry)	70 Ry (140 Ry)	40 Ry (80 Ry)	35 Ry (87 Ry)
1	z_8 NC sg15 oncvpsp4 v0	30 Ry (60 Ry)	30 Ry (60 Ry)	30 Ry (60 Ry)	30 Ry (60 Ry)	30 Ry (90 Ry)
2	z_18 PAW psl ld1 v1.0.0-high	55 Ry (330 Ry)	50 Ry (300 Ry)	200 Ry (1200 Ry)	55 Ry (330 Ry)	45 Ry (270 Ry)
3	z_18 Ultrasoft psl ld1 v1.0.0-high	50 Ry (300 Ry)	65 Ry (487 Ry)	200 Ry (1200 Ry)	50 Ry (300 Ry)	40 Ry (240 Ry)

Switch criteria to:

Efficiency

Precision

Show ρ or dual

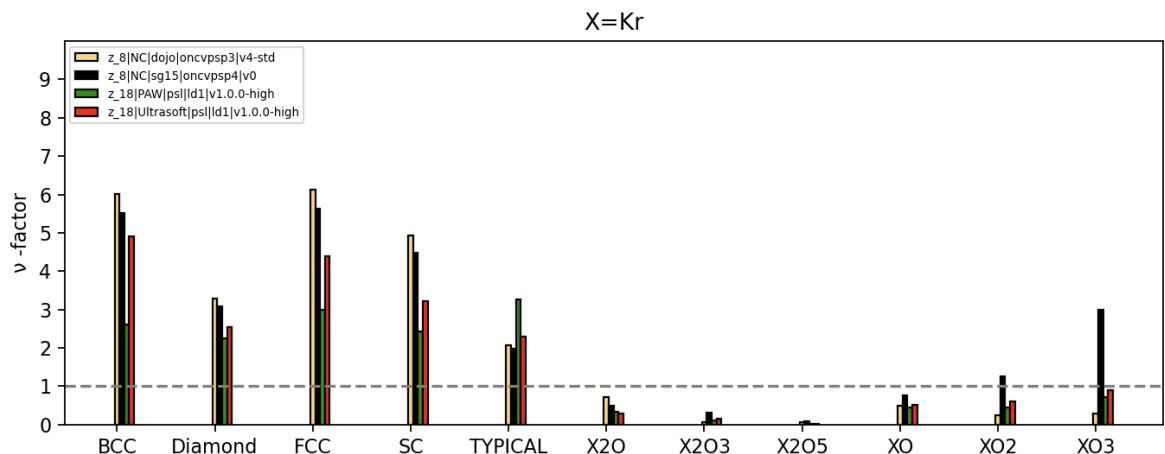
Default

Show ρ cutoff

Show dual

v-factor

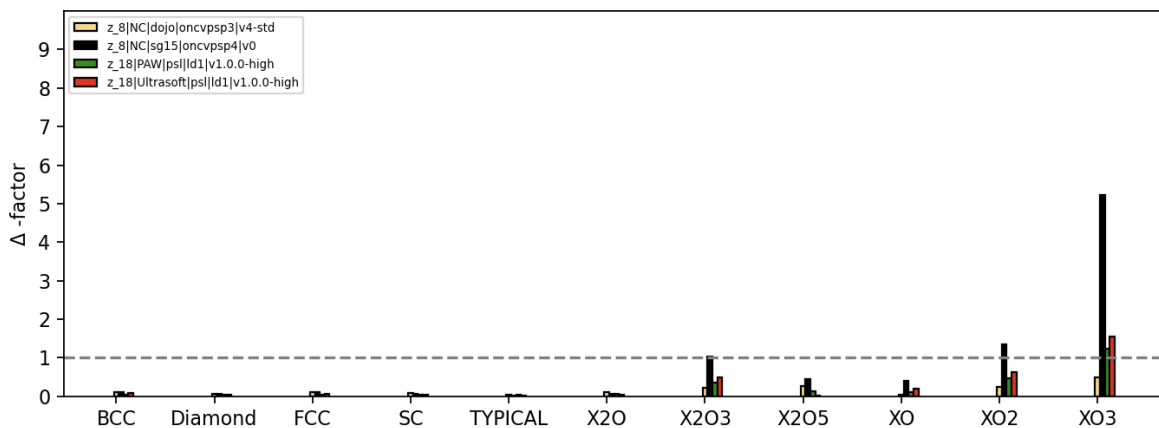
Δ -factor



v-factor

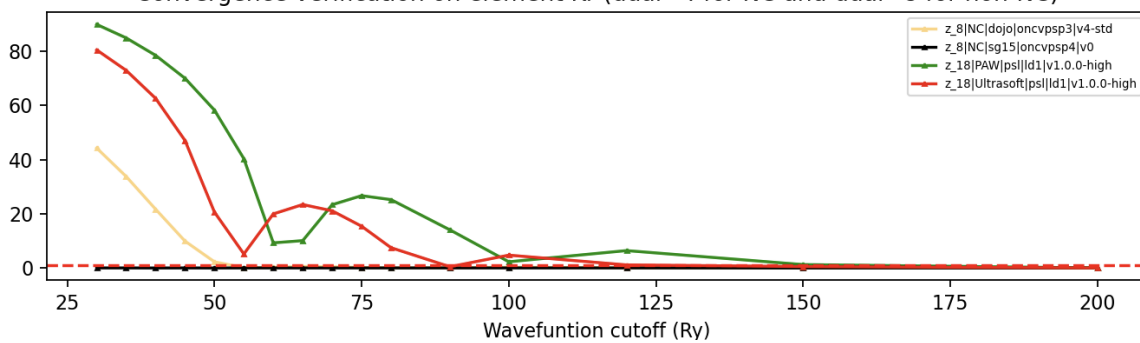
Δ-factor

X=Kr



- Pressure (Relative Error, %)
- Bands distance (Avg. error meV)
- Bands distance (Max. error meV)
- Delta (Relative Error, %)
- Delta (Raw value, meV/cell)

Convergence verification on element Kr (dual=4 for NC and dual=8 for non-NC)



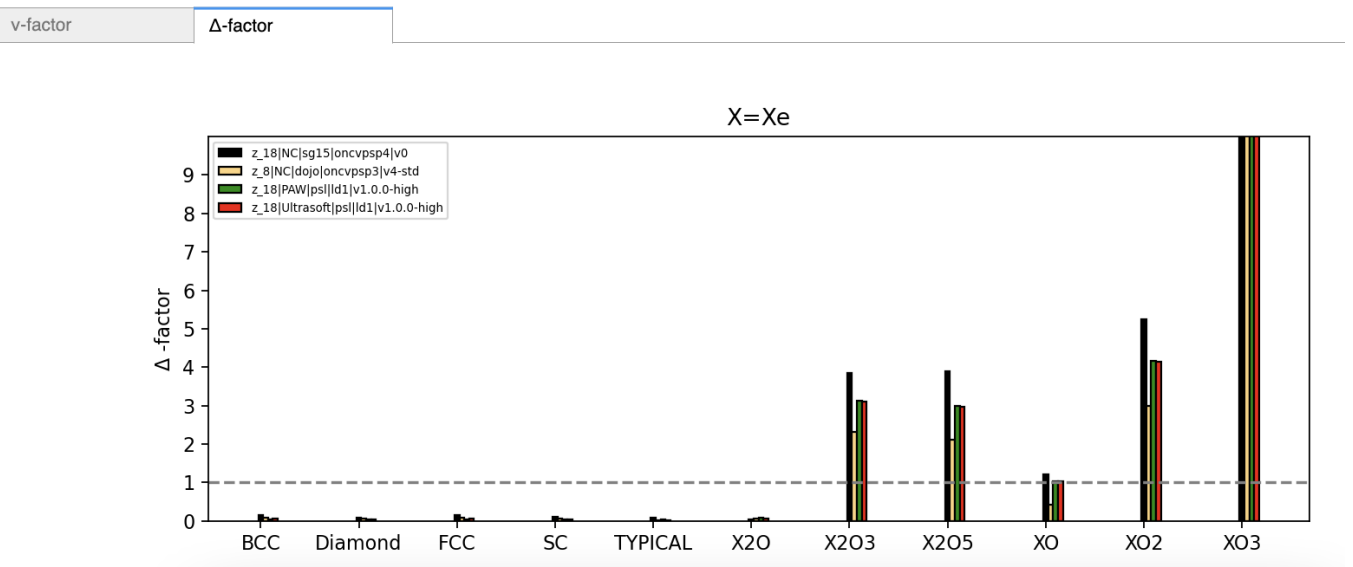
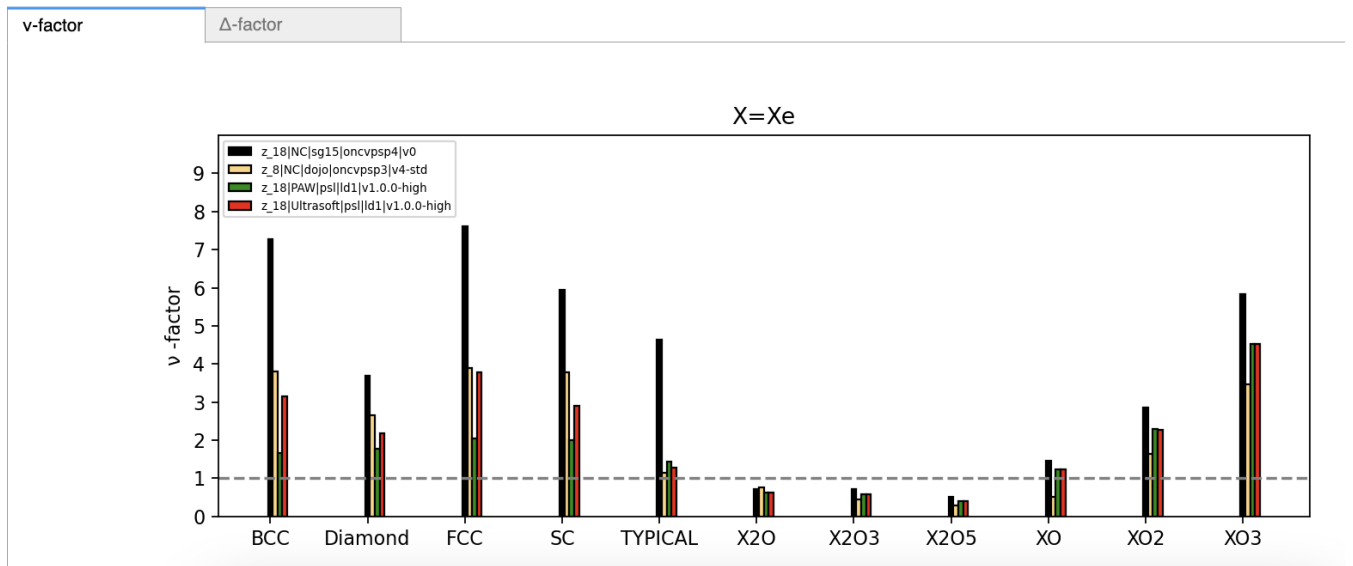
Xe (Xenon)

	Pseudopotential label	X0	XO2	XO3	X20	X2O3	X2O5	BCC	FCC	SC	Diamond	TYPICAL
0	z_18 NC sg15 oncvpsp4 v0	1.450	2.864	5.821	0.714	0.718	0.505	7.270	7.622	5.955	3.695	4.645
1	z_8 NC dojo oncvpsp3 v4-std	0.516	1.646	3.474	0.756	0.434	0.275	3.802	3.895	3.783	2.653	1.131
2	z_18 PAW ps ld1 v1.0.0-high	1.238	2.281	4.524	0.626	0.585	0.389	1.658	2.038	2.007	1.779	1.440
3	z_18 Ultrasoft ps ld1 v1.0.0-high	1.225	2.275	4.524	0.619	0.580	0.387	3.158	3.782	2.897	2.186	1.271

	Pseudopotential label	cohesive energy	phonon frequencies	pressure	delta	bands
0	z_18 NC sg15 oncvpsp4 v0	45 Ry (180 Ry)	70 Ry (280 Ry)	50 Ry (150 Ry)	50 Ry (150 Ry)	35 Ry (70 Ry)
1	z_8 NC dojo oncvpsp3 v4-std	30 Ry (75 Ry)	30 Ry (60 Ry)	150 Ry (300 Ry)	30 Ry (60 Ry)	30 Ry (120 Ry)
2	z_18 PAW ps ld1 v1.0.0-high	40 Ry (240 Ry)	60 Ry (450 Ry)	150 Ry (900 Ry)	45 Ry (270 Ry)	35 Ry (210 Ry)
3	z_18 Ultrasoft ps ld1 v1.0.0-high	40 Ry (240 Ry)	75 Ry (562 Ry)	150 Ry (900 Ry)	45 Ry (270 Ry)	35 Ry (210 Ry)

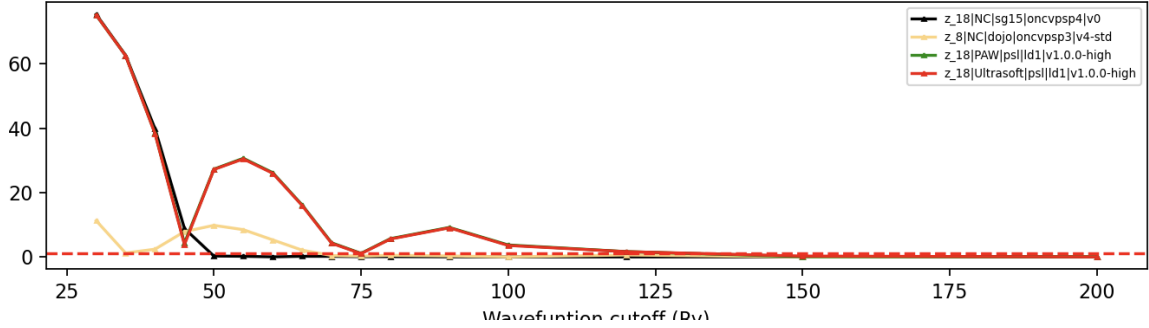
Switch criteria to:

Show p or dual



- Pressure (Relative Error, %)
- Bands distance (Avg. error meV)
- Bands distance (Max. error meV)
- Delta (Relative Error, %)
- Delta (Raw value, meV/cell)

Convergence verification on element Xe (dual=4 for NC and dual=8 for non-NC)



Rn (Radon)

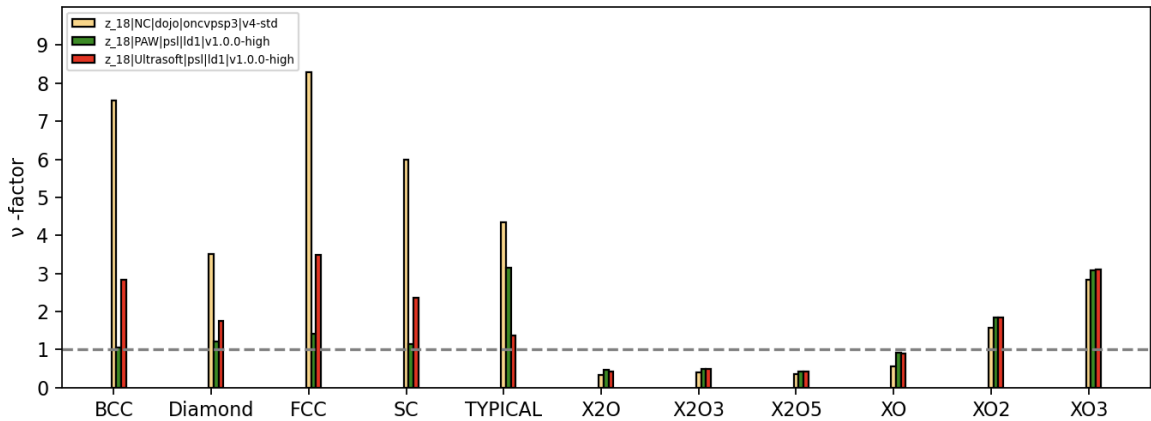
	Pseudopotential label	XO	XO2	XO3	X2O	X2O3	X2O5	BCC	FCC	SC	Diamond	TYPICAL
0	z_18 NC doj oncvpsp3 v4-std	0.562	1.574	2.832	0.327	0.401	0.364	7.555	8.296	5.978	3.512	4.349
1	z_18 PAW psl d1 v1.0.0-high	0.922	1.840	3.072	0.469	0.486	0.424	1.058	1.408	1.147	1.214	3.152
2	z_18 Ultrasoft psl d1 v1.0.0-high	0.894	1.832	3.096	0.431	0.483	0.430	2.835	3.487	2.369	1.747	1.361

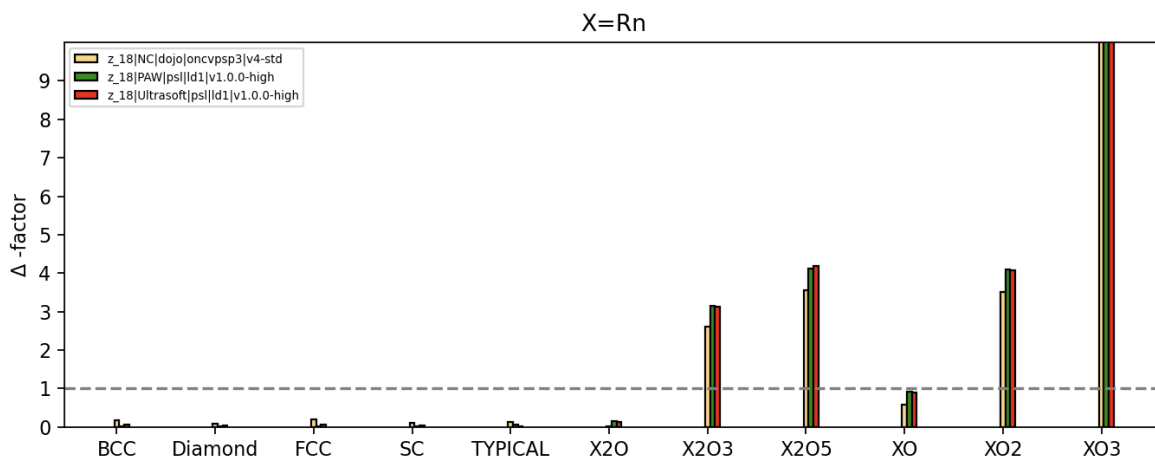
	Pseudopotential label	cohesive energy	phonon frequencies	pressure	delta	bands
0	z_18 NC doj oncvpsp3 v4-std	60 Ry (210 Ry)	100 Ry (400 Ry)	90 Ry (270 Ry)	55 Ry (165 Ry)	45 Ry (90 Ry)
1	z_18 PAW psl d1 v1.0.0-high	45 Ry (270 Ry)	40 Ry (260 Ry)	200 Ry (1200 Ry)	45 Ry (270 Ry)	40 Ry (240 Ry)
2	z_18 Ultrasoft psl d1 v1.0.0-high	45 Ry (270 Ry)	40 Ry (240 Ry)	200 Ry (1500 Ry)	50 Ry (300 Ry)	40 Ry (240 Ry)

Switch criteria to:

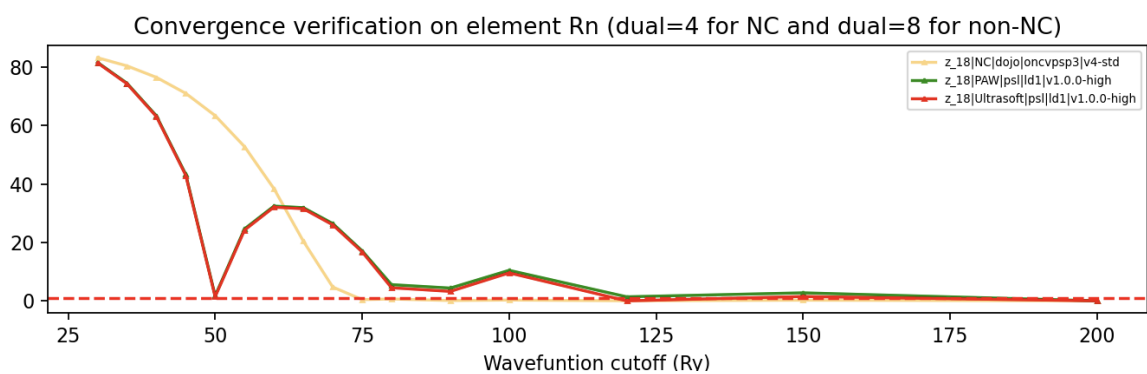
Show ρ or dual

X=Rn





- Pressure (Relative Error, %)
- Bands distance (Avg. error meV)
- Bands distance (Max. error meV)
- Delta (Relative Error, %)
- Delta (Raw value, meV/cell)



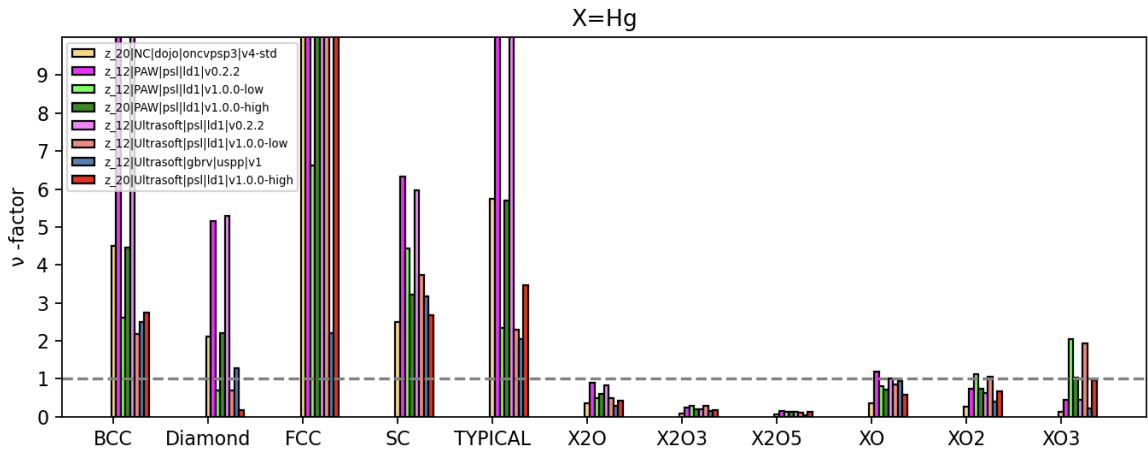
Hg (Mercury)

	Pseudopotential label	X0	X02	X03	X20	X203	X205	BCC	FCC	SC	Diamond	TYPICAL
0	z_20 NC dojo oncvpsp3 v4-std	0.356	0.261	0.134	0.361	0.071	0.062	4.499	27.190	2.504	2.115	5.753
1	z_12 PAW psl ld1 v0.2.2	1.184	0.726	0.448	0.903	0.231	0.154	10.731	47.319	6.329	5.147	12.132
2	z_12 PAW psl ld1 v1.0.0-low	0.805	1.114	2.034	0.496	0.288	0.117	2.610	6.617	4.435	0.683	2.339
3	z_20 PAW psl ld1 v1.0.0-high	0.722	0.727	1.023	0.603	0.184	0.129	4.465	38.706	3.225	2.211	5.689
4	z_12 Ultrasoft psl ld1 v0.2.2	1.016	0.630	0.432	0.818	0.196	0.137	10.452	63.299	5.969	5.301	11.858
5	z_12 Ultrasoft psl ld1 v1.0.0-low	0.845	1.062	1.923	0.488	0.283	0.113	2.181	10.248	3.733	0.689	2.299
6	z_12 Ultrasoft gbrv uspp v1	0.939	0.391	0.207	0.274	0.155	0.033	2.497	2.196	3.177	1.286	2.036
7	z_20 Ultrasoft psl ld1 v1.0.0-high	0.589	0.662	0.971	0.427	0.168	0.117	2.753	14.269	2.679	0.163	3.461

	Pseudopotential label	cohesive energy	phonon frequencies	pressure	delta	bands
0	z_20 NC dojo oncvpsp3 v4-std	45 Ry (157 Ry)	30 Ry (105 Ry)	70 Ry (175 Ry)	55 Ry (137 Ry)	50 Ry (100 Ry)
1	z_12 PAW psl ld1 v0.2.2	30 Ry (180 Ry)	30 Ry (180 Ry)	80 Ry (480 Ry)	35 Ry (210 Ry)	30 Ry (180 Ry)
2	z_12 PAW psl ld1 v1.0.0-low	45 Ry (337 Ry)	30 Ry (180 Ry)	60 Ry (360 Ry)	40 Ry (300 Ry)	30 Ry (180 Ry)
3	z_20 PAW psl ld1 v1.0.0-high	120 Ry (720 Ry)	55 Ry (412 Ry)	200 Ry (1200 Ry)	65 Ry (487 Ry)	50 Ry (300 Ry)
4	z_12 Ultrasoft psl ld1 v0.2.2	30 Ry (180 Ry)	30 Ry (180 Ry)	60 Ry (360 Ry)	35 Ry (210 Ry)	30 Ry (180 Ry)
5	z_12 Ultrasoft psl ld1 v1.0.0-low	45 Ry (337 Ry)	30 Ry (180 Ry)	60 Ry (360 Ry)	45 Ry (337 Ry)	30 Ry (180 Ry)
6	z_12 Ultrasoft gbrv uspp v1	30 Ry (180 Ry)	30 Ry (180 Ry)	90 Ry (540 Ry)	30 Ry (180 Ry)	30 Ry (180 Ry)
7	z_20 Ultrasoft psl ld1 v1.0.0-high	120 Ry (720 Ry)	55 Ry (412 Ry)	200 Ry (1200 Ry)	50 Ry (400 Ry)	50 Ry (300 Ry)

v-factor

Δ -factor



X=Hg

